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Also included in the Onsite Program:

- Program at a Glance Booklet
- Map of Whistler Village

Committees

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Professor, ArcelorMittal Dofasco Chair in Advanced Steel Processing
The University of British Columbia Materials Engineering Department

Gianluigi Botton
Professor, Canada Research Chair in Microscopy of Nanoscale Materials
McMaster University Materials Science and Engineering Department

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Thomas Waltz, Austria
Jer-Ren Yang, Taiwan
Wenzheng Zhang, China
Registration

Your full congress registration includes

- Name Badge
- Onsite Program (including Abstracts)
- Proceedings USB
- Program Sessions
- Welcome Reception on Monday
- Daily Coffee Breaks; Lunch on Monday, Tuesday and Thursday
- Gala Dinner on Thursday

Registration Hours

The registration desk will be located in the Main Foyer of the Hotel

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NETWORKING & SOCIAL EVENTS

Welcome Reception

The Welcome Reception will be held on Monday, June 29 from 18:30–20:30 at the Squamish Lil’wat Cultural Centre Whistler, B.C.

The Welcome Reception is about a 25 min. walk from the Westin. The location and route are highlighted on the enclosed map.

Poster Viewing and Extended Lunch Break

The poster session will be held Tuesday from 13:15–15:00 in the Alpine Foyer and includes lunch. Posters will be on display for the duration of the conference from Monday to Friday.

Congress Dinner

The dinner will be held on Thursday, July 2 from 20:00–22:30 in the Emerald Ballroom.

Internet Access

Complimentary internet access is available for PTM attendees in public areas of the hotel and in the guest rooms.

Technical Sessions

The plenary sessions will be held in the Emerald Ballroom.

The poster presentations will be held in the Alpine Foyer on Level 2. See the Technical Program for room locations.

All other oral presentations will be held in Alpine ABC and Alpine DE, Callaghan Room and the Nordic Room up on Level 2.

POLICIES

Badges

All attendees must wear registration badges at all times during the congress to ensure admission to events included in the paid fee such as technical sessions and receptions.

Photography Notice

By registering for this congress, all attendees acknowledge that they may be photographed by congress personnel while at events and that those photos may be used for promotional purposes.

Audio/Video Recording Policy

Recording of sessions (audio, video, still photography, etc.) intended for personal use, distribution, publication, or copyright without the express written consent of PTM and the individual authors is strictly prohibited.

Cell Phone Use

In consideration of attendees and presenters, we kindly request that you minimize disturbances by setting all cell phones and other devices on “silent” while in meeting rooms.
Exhibition Hours

The exhibition tables will be located in the Emerald Ballroom Foyer

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Toll Free 1.877.991.9988
Email activity@tourismwhistler.com
Location 4230 Gateway Drive
(Adjacent to the Taxi/Bus loop in the centre of Whistler Village)

**Free Parking Options**
Parking in Day Lots 4 and 5 is free for a maximum of 72 hours. Please see map for locations.

**Emergency Services**
The nationwide emergency phone number for the police, ambulance and fire is 911.

**Tipping**
Tipping in Canada is much the same as it is in the U.S. In most cases, a tip in the range of 15%–20% is perfectly acceptable.

**Electricity**
Canada's electrical supply and electrical outlets (sockets, wall plugs) are the same as those found in the United States. The electrical supply is 110 Volts and 60 Hertz (cycles per second).

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Abstracts

10:30
Carbon and Nitrogen Effects on Austenite Decomposition in a Low-Alloyed Steel: Simon D. Cattet1; Julien Texeira1; Jacky Dulvy1; Sabine Denis1; Moukrae Dehmas2; Hugo P. Van Landeghem2; Abdelkrim Redjiam1; Marc Courtaux1; Institut Jean Lamour; PSA Peugeot Citroën

The decomposition of carbon and nitrogen enriched austenites during cooling is studied in a low-alloyed steel, by dilatometry, in-situ synchrotron X-ray diffraction (HEXRD) and TEM. Samples were prepared by using a gas-carbonitriding process to obtain different controlled and homogeneous N and/or C concentrations. The newest results concern the effects of nitrogen and C+N on the isothermal transformation kinetics of the austenite. In the ferrito-austenite domain, an acceleration of the kinetics is observed whereas in the austenitic domain, the kinetics is slowed down. From the in situ HEXRD, it is shown that during the bainitic transformation (400°C) ferrite is formed first and then chromium nitrides (CrN) and cementite precipitate. From the analysis of the austenite lattice parameter evolution and peak profiles, the possible rejection of interstitial elements from the ferrite before the austenite is discussed. Formation of nanometric CrN in the bainitic ferrite is confirmed by TEM.

10:45
Allaying Effects on Microstructure of Fe-1mass%M Binary Alloys Treated by Nitriding and Quenching Process: Hironori Kubo1; Goro Miyamoto1; Tadashi Furuhara1; Nisshin Steel Co.; 2Institute for Materials Research, Tohoku Univ.

In order to reduce long treatment time in nitriding and distortion in carburizing, nitriding and quenching (N-Q) process has been developed recently. In this process, surface hardening is achieved by the formation of high nitrogen austenite during nitriding at high temperature and subsequent martensite transformation by quenching. In this study, in order to clarify the influence of alloying elements, microstructure of Fe-1mass%M (M = Mn, Cr, Si) binary alloys and pure iron after N-Q process were investigated. By the addition of 1%Mn, higher hardness and deeper hardened layer (austenite before quenching) were obtained compared with those for the pure iron. The addition of Si increases the hardness with the reduction of the hardened layer thickness, while both of the hardness and thickness are decreased by the addition of Cr. Those alloying effects will be discussed in terms of precipitation of alloy nitrides, variations in nitrogen contents and austenite/ ferrite phase stability.

11:00
Microstructure Characterization of a Nitrided Fe-3wt.%Cr-0.3wt.%C Model Alloy by Anomalous Small Angle X-ray Scattering: Myriam Dumont1; Sébastien Jegou2; Laurent Barrallier1; 1IM2NP-UMR 7334; 2MSMP

Nitriding is a thermo-chemical surface treatment of steels providing an improved fatigue and wear resistance. This treatment is based on nitrogen diffusion involving the precipitation of nano-scaled nitrides from the solid solution at the near surface of the nitrided piece. Nitriding involves a complex microstructural evolution both in time and depth including diffusion of nitrogen and precipitation of nitrides but also coarsening and dissolution of carbides resulting in diffusion of carbon. However the chemical composition of nano-scaled precipitates remains controversial, in particular regarding the iron content in nano-nitrides that may substitute alloying elements. In this framework, anomalous small-angle X-ray scattering was used to obtain quantitative data on the distribution and composition of the nano-scaled phases in a Fe-3Cr-0.3C steel as a function of depth.

10:00 Invited
Ab Initio Description of Finite Temperature Phase Stabilities and Transformations: Jörg Neugebauer1; Albert Gleinsk1; Blaize Grabowski2; Tilmann Hickel1; Max-Planck-Institut für Eisenforschung

The driving force behind phase transformations is the difference in the chemical potentials of the involved phases. Since for most technologically relevant structural materials the chemical potential differences are strongly temperature dependent an accurate treatment of all free energy contributions (vibrational, electronic, magnetic) is crucial. This turns out to be a major hurdle for empirical potentials as well as for ab initio computations. Over the last years we have therefore developed computationally efficient approaches that allow an accurate and fully ab initio based description of all relevant free energy contributions. The power of these approaches will be shown for examples ranging from the design of new high-strength steels, understanding failure mechanisms such as H embrittlement, or to improve ductility of light-weight alloys.

10:30
Ab Initio Description of the Ti bcc to α Transition at Finite Temperatures: Dominique Kortmacher1; Albert Gleinsk1; Blaize Grabowski2; Tilmann Hickel1; Jörg Neugebauer1; Max-Planck-Institut für Eisenforschung

Ti-based alloys are technologically important materials. A detailed knowledge of their phase diagrams and transitions is crucial for optimizing their properties. However, the occurrence of phases that become stable only at high temperatures makes an ab initio computation of phase diagrams challenging. We have therefore developed and applied an ab initio methodology that allows to accurately compute free energies of unstable phases. The method employs thermodynamic integration starting from a reference of optimized embedded atom potentials that were fitted to reproduce ab initio molecular dynamics data for a narrow temperature range. We apply our technique to the bcc phase of pure Ti and compute its free energy up to the melting point. We predict a second order phase transformation at around 1000 K. A careful investigation of the trajectories allows us to identify the low temperature phase as the technologically important hexagonal α structure.

10:45
First-principles Study of Ni Doping Effect on Mechanical Properties of Dilute Fe-Si Alloy: Ying Chen1; Arkapal Saengdeejing1; Tetsuo Mohri1; Yoshio Uehara2

A drastic change in mechanical properties at Si concentration 5-6wt.% has been intriguing since a long time ago. Our recent DFT calculations reproduced a Si concentration dependence of the elastic properties in dilute Fe-Si alloy, and found a ductile to brittle transition as Si content crosses 4.2wt.%. Further calculations combining CVM (Cluster Variation Method) revealed the origin of the softening transition. In the metastable Si-rich region is the interplay between magnetoelastic effect and structure ordering of D03 in Fe-Si alloy. Electronic structure analysis revealed that the instability at Fermi Energy results in a degradation of ductility at 4.2wt.%. Simulations of Ni-doping into Fe-Si have been performed.
and we found a recovery of elastic properties at critical Si concentration, which is an encouraging experience of tailing band structures intentionally by creating specific atomic configurations which varies bonding states and generates variable, re-distribution of electrons toward enhancing the specific physical property.

11:00 Invited  
Spin Wave Method for the Total Energy of the Paramagnetic State: Practical Applications: Vsevolod Razumovskyi; Andrei Reyes-Huanantico; Andrei Rubani; Materials Center Leiden; KTH Royal Institute of Technology.

The Spin Wave method for the total energy of paramagnetic state represents an alternative to the existing methods for modeling magnetic disorder in Density Functional Theory calculations. One of the main advantages of the method is its applicability to defect calculations in pure metals and alloys. A combination of the SW-method and the supercell approach provides one with a convenient way of ab initio calculations of a number of thermodynamic and kinetic properties using methods based on Hamiltonian formalism like the PAW method as implemented in VASP. The Hamiltonian-based VASP-PAW-SW and Green's function-based EMTO-DLM methods have been used to calculate basic thermodynamic properties of paramagnetic iron and steel (including vacancy formation energy, phonon energy, phonon spectra etc.). The accuracy and efficiency of both methods has been assessed by comparing the obtained results to available experimental and theoretical data.

11:30 Break

### Atomistic Characterization

#### MONDAY AM  ROOM: CALLAGHAN  SESSION CHAIR: FRÉDÉRIC DANOIX, CNRS - UNIVERSITÉ DE ROUEN

10:00 Invited  
Advanced Characterization of Precipitates in Strip Cast Steel Alloys: Nicole Stanford1; Mahendra Ramajayam1; Ross Marceau; Thomas Dorin; Adam Taylor; Deakin University.

During the strip casting of steels, solidification occurs in a matter of milliseconds, and complete cooling to room temperature is complete in under 1 minute. Consequently, the many steel alloys are meta-stable when processed by industry. Much uncertainty remains regarding their short-range ordering, atomic clustering, segregation and growth. We have used aberration-corrected scanning transmission electron microscopy, electron back scattering diffraction, and combined these with multi-component diffusion simulations and FEM simulations to study the microstructural evolution processes that occur during direct metal laser melting of various Ni-based superalloys. Microstructural characterization techniques including scanning and transmission electron microscopy, electron back scattering diffraction, x-ray diffraction, and synchrotron ultra small angle x-ray scattering were used to determine the residual stress distributions, porosity, phase fractions, and the effects of changing cooling conditions of varying processing conditions. These results are compared with multi-component diffusion simulations and FEM simulations that predict the phase fraction, composition, and residual stress as functions of time and temperature that predict the phase fraction, composition, and residual stress as functions of time and temperature.

10:30 Invited  
Atomic-scale Structure and Mechanisms of Phase Transformations of Precipitates in Aluminium Alloys: Laure Bourgeois1; Nikhil Medhekar1; Julian Rosalie2; Tseszhon Khabibulin1; Andrei Reyes-Huamantinco1; Andrei Rubani1; Materials Center Leiden; KTH Royal Institute of Technology; Deakin University; National Institute for Materials Science; Forschungszentrum Jülich.

In precipitate-hardened materials, high strength is achieved through the controlled formation of precipitate phases. These precipitates are often metastable phases which grow into high aspect ratio shapes with nanoscale dimensions. Due to the experimental difficulty in characterising such embedded precipitates, much uncertainty remains regarding their bulk and interface structures, and consequently, the mechanisms of phase transformations for nucleation and growth. We have used aberration-corrected scanning transmission electron microscopy and first-principles calculations to gain a better understanding of the phase-transition pathway, which enables the first design and modelling of the atomic configurations in n-component solid solutions.

10:45 Invited  
Maraging Steel Produced by Laser Additive Manufacturing: Yaniv Idel1; Tzeasan Baturci2; Eric Lass3; Li Ma4; National Institute of Standards and Technology.

Materials produced by Laser Additive Manufacturing (LAM) experience a thermal history that is markedly different from that encountered by conventionally produced materials. In particular, a high cooling rate from the melt is combined with cyclic reheating upon deposition of subsequent layers. Using SEM-EDS, EBSD and atom-probe tomography (APT), we investigated how this nonconventional thermal history influences the phase-transformation behaviour of martensitic steel (Fe-18Cr-1Mo-Cr-Mo, a 21% Cr steel) produced by Laser Additive Manufacturing and electron beam powder melting process, were described using integrated process models.

11:00 Invited  
The Role of Microscopy in Guiding Materials Simulations: Towards Designer Structure-Property Relationships: Simon Ringer; The University of Sydney.

Short-range ordering, atomic clustering, segregation and site-occupancy exert a major influence on the phase transformation pathways, and transformation kinetics in many technologically important solid solutions. Therefore, the questions around how these non-periodic arrangements of solute atoms within a parent crystal lattice can be described, measured precisely and, ultimately, ‘designed’ to understand and create new materials property-performance space, remain of great interest. This is the topic of our recent research. Firstly, I will discuss our recent theory for short-range order, which provides a framework for describing the atomic configurations in n-component solid solutions. The characterisation of such materials for the purposes of measuring the atomic configurations will then be discussed, in detail. The challenging issues associated with scattering based approaches using X-rays, neutrons or electrons, will be mentioned and our approaches to addressing these issues using atom probe microscopy will be featured. We have recently modelled the origins of resolution in the atom probe, computed advanced spatial distribution maps, which are analogous to Patterson functions in scattering experiments, and used these new tools to devise an approach for ‘lattice rectification’. In bringing us closer to atomic resolution tomography, these techniques are revealing a rich and complex hierarchal architecture of atomic structures within solid solutions, and at microstructural interfaces. This opens new opportunities for computational materials science where the input supercells can be derived directly from experiments. Intersecting atomic resolution microscopy and first principles modelling through density functional approaches has great potential impact in advancing our capacity to understand material behaviour, conduct materials discovery and design, new materials. Examples that will be highlighted will include the design of new 3rd generation steels with remarkable balance of high strength and ductility, and materials that exhibit magnetism and superconductivity in the same phase.

11:15 Determination of the Interfacial Atomic Structure of O Phase in In-Cu-Mg-Ag Alloy and Its Role in O Phase Transformation: SungHyun Kung1; Jian-Min Zhao2; Myoung-Ki Lee1; Deakin University; University of Illinois.

Interface plays a critical role in phase transformation of light alloys involving precipitation, but interfacial atomic structures of precipitates are often undetermined, even for common phases in alloys such as Al-Cu. We solved the interface structure of the O phase in Al-Cu-Mg-Ag alloy by using a combination of 3D atomic-resolution imaging obtained by aberration-corrected scanning transmission electron microscopy (STEM) and simulation. The structure is further refined by density functional theory (DFT) calculations. We discovered that the interface of the O phase is substantially stabilized by ordering of Ag atoms in a hexagonal arrangement within a single atomic layer and Mg atoms located in the middle of the hexagonal Ag atoms. In the O phase, the Cu atoms in the interface, which enables Al,Cu, to crystal be form on (111)A. This type of phase transformation seems to occur in several AI alloys providing new insight for light alloy design.

11:30 Break

Additive Manufacturing of Metals

#### MONDAY AM  ROOM: NORDIC  SESSION CHAIR: ADAM FARROW, LOS ALAMOS NATIONAL LABORATORY

10:00 Invited  
Rationalization of Microstructural Heterogeneity in Components Produced by Additive Manufacturing and Welding: Sudarsanan Babu; The University of Tennessee, Knoxville.

Mechanical property of welds and additively manufactured components depend on local microstructural gradients. This paper will focus on fundamental aspects of heat and mass transfer, solidification under large ($10^3$ to $10^4$ K/min) thermal gradients and liquid solid-interface velocities ($10^2$ to $10^3$ m/s), as well as, solid-solid transformation during thousands of thermal gyrations. Need for measurement of these phenomena using in-situ and ex-situ characterization tools, as well as, simulation using integrated process modeling will be highlighted. Two examples will be presented. In the first example, competition between dissolution and growth of M$_2$C$_6$ during normalizing welding and post-weld heat treatment in Cr-Mo steels was described and these changes were correlated to creep fracture. In the second example, the crystallographic heterogeneity, micro-scale segregation features and nano-scale compositional distribution around age-hardening precipitates in Inconel 718 alloys built by laser additively manufacturing and electron beam powder melting process, were described using integrated process models.

10:30 Characterization of Nickel Based Superalloys Technique of Additive Manufacturing: Yaakov Ide1; Yakeov Ide1; Lyle Levine1; Carolyn Campbell1; Eric Lass1; Li Ma4; National Institute of Standards and Technology.

Additive manufacturing of nickel based superalloys will allow direct production of complex shaped components based on 3-D computer aided drawings. The aerospace industry is interested in exploiting this technology to reduce time and cost for production of complex parts; however, the effects resulting from repeated cycles of rapid heating, melting, cooling, and solidification on the microstructure-property relationships are not well understood. We conducted a study investigating the microstructural evolution processes that occur during direct metal laser sintering of various Ni-based superalloys. Microstructural characterization techniques including scanning and transmission electron microscopy, electron back scattering diffraction, x-ray diffraction, and synchrotron ultra small angle x-ray scattering were used to determine the residual stress distributions, porosity, phase fractions, and the effects of changing cooling conditions of varying processing conditions. These results are compared with multi-component diffusion simulations and FEM simulations that predict the phase fraction, composition, and residual stress as functions of time and temperature.

10:45 Maraging Steel Produced by Laser Additive Manufacturing: The influence of Processing Conditions on Precipitation and Austenite Reversion Behaviour: Eric Jaegle1; Zhenghong Sheng1; Puick Jementick2; Vsevolod Razumovskyi1; Andrei Reyes-Huamantinco1; Andrei Rubani1; Max-Planck-Institut für Eisenforschung.

Materials produced by Laser Additive Manufacturing (LAM) experience a thermal history that is markedly different from that encountered by conventionally produced materials. In particular, a high cooling rate from the melt is combined with cyclic reheating upon deposition of subsequent layers. Using SEM-EDS, EBSD and atom-probe tomography (APT), we investigated how this nonconventional thermal history influences the phase-transformation behaviour of maraging steel (Fe-18Ni-3Co-3.4Mo-1.2Ti) produced by LAM. We compared specimen prepared conventionally, by direct Laser Melting produced by Laser Metal Deposition and found differences in the microsegregation, amount of clustering and retained austenite that are not observed in the as-produced state. Up to aging, three different types of precipitates, namely (Fe,Ni,Co), (Ti,Mo), (Fe,Ni,Co), were observed as
well as martensite-to-austenite reverse around regions of the retained austenite. The findings are discussed light the different processing conditions.

11:00 Texture Evolution during Laser Direct Metal Deposition of Ti-6Al-4V: Niyant Shridharan; Anil Chaudhary; Sudarsanam Babu; University of Tennessee Knoxville; Applied Optimization

With the production of near net shapes is achievable in terms of shape, the microstructures obtained via additive manufacturing are not favorable for the full scale production of engineering materials. Titanium alloys are used in a wide variety of high performance applications and hence the processing of the titanium and the resulting microstructures has received significant attention. During additive manufacturing the processing route involves the transition from a liquid to solid state. The addition of successive layers results in a complex microstructure due to size and shape transformations. Since phase transformations in titanium alloys occur with specific orientation relationships the texture in titanium alloys is expected to vary with the addition of every new layer. The aim of this work is to investigate the changes in texture and microstructure as a function of the build height and identify conditions to tailor the texture in the manufactured parts.

11:15 Prediction of Phase Transformation During Electron Beam Additive Manufacturing of Inconel 718: Michael Kerk; Allison Miller; Grant Helmreich; Ryan Dehoyos; Oak Ridge National Laboratory; University of Tennessee; University of Tennessee

Metal powder bed additive manufacturing processes such as electron beam melting (EBM) have emerged as industrial viable tools. Unlike traditional manufacturing processes that are understood and yield predictable microstructures, the EBM processes present new challenges in processing science. Through EBM, components are built layer by layer, during which temperatures are maintained at two-thirds or greater of the material’s melt temperature throughout a component’s build as in the case of Inconel 718, which allows for the precipitation and coarsening of phases as a function of build height. Considered in this work are the influences of EBM build parameters for Inconel 718 that ultimately control the resulting as-built component microstructure. Coupling experimental findings with computational findings obtained from JMatPro, an understanding of the phase transformations that occur during the EBM build process are derived and applied towards the development of optimal process conditions for Inconel 718 EBM components.

11:30 Microstructure and Hardness Evolution During Simulated Coiling of a Direct Strip Cast Low Carbon Low Niobium Steel: Thomas Donn; Adam Taylor; Nicolle Stanford; Peter Hodgson; Deakin University

The novel direct strip casting technology involves extremely rapid cooling. Upon cooling, the steel are maintained at a given temperature for coiling. The temperature and duration of coiling strongly affects the final microstructure and mechanical properties of these metals making it necessary to understand and control it. In this work, we study the microstructure evolution of a low carbon, low-niobium steel for three coiling temperatures, 600°C, 700°C and 850°C. These three temperatures correspond to coiling in the ferrite, during the austenite decomposition and in the austenite. The microstructure exists in different forms: low strain, high strain, SEM and TEM. We show that the coiling temperature strongly affects the final ferrite morphology which ranges from bainite to d 微观组织 and pearlitic ferrite. We show that only coiling in the ferrite provides suitable hardening response. We finally discuss the concurrent strengthening contributions of the microstructure and of the fine Niobium-carbide-nitride precipitates that form during cooling.

11:45 Invited The Effect of Alloy Elements Partition on Kinetics of Deformed Austenite Decomposition in Steels: Zhi-Gang Yang; Chi Zhang; Yuan Xia; Ze nan Yang; T工作者 University.

Due to significant difference between carbon and alloy elements diffusion coefficients, whether the partition of alloy elements during phase transformation happens or not affects the kinetics of austenite decomposition in steel remarkably. Based on the partition local equilibrium (Pele) and negligible partition local equilibrium (NPLe) theory, the formation of pro-eutectoid ferrite from deformed austenite in Fe-C-Mn alloys has been studied in this work. The nucleation rate was calculated with pitbox model on grain boundaries. Under PLE model, the promotion of ferrite nucleation process relates mainly with acceleration of diffusion and increment of grain boundary, whereas under PLE model, the increase of phase transformation driving force dominates. The reason of grain refinement of ferrite from deformed austenite is proposed considering the kinetics of nucleation and growth at different temperatures.

12:15 Modelling the Austenite to Ferrite Phase Transformation in Low Carbon Microalloyed Steels in Terms of Grain Size Distributions: Pedro Manuel García-Rascaza; José María Rodríguez-Iturbe; CITEC and TECNUN

In the present paper, a model to predict the ferrite grain size distribution after transformation at continuous cooling conditions in low carbon microalloyed steels is described. The use of grain size distributions instead of mean grain sizes is very interesting to predict mechanical properties, especially toughness, where the coarsest grains play an important role in fracture. The model has been applied to both, recrystallized and deformed austenite microstructures. The model uses the austenite grain size distribution present before transformation as an input and provides the final ferrite grain size distribution. In the case of deformed austenite, the effect of accumulated strain on ferrite grain size has been implemented. For the validation of the model, thermomechanical simulations were carried out by dilatometry tests. In all cases the prior austenite and the resulting ferrite microstructures were characterized. The critical parameters of the grain size distribution model could be identified.

12:30 Microstructure and Hardness Evolution During Simulated Coiling of a Direct Strip Cast Low Carbon Low Niobium Steel: Thomas Donn; Adam Taylor; Nicolle Stanford; Peter Hodgson; Deakin University

The novel direct strip casting technology involves extremely rapid cooling. Upon cooling, the steel are maintained at a given temperature for coiling. The temperature and duration of coiling strongly affects the final microstructure and mechanical properties of these metals making it necessary to understand and control it. In this work, we study the microstructure evolution of a low carbon, low-niobium steel for three coiling temperatures, 600°C, 700°C and 850°C. These three temperatures correspond to coiling in the ferrite, during the austenite decomposition and in the austenite. The microstructure exists in different forms: low strain, high strain, SEM and TEM. We show that the coiling temperature strongly affects the final ferrite morphology which ranges from bainite to d 微观组织 and pearlitic ferrite. We show that only coiling in the ferrite provides suitable hardening response. We finally discuss the concurrent strengthening contributions of the microstructure and of the fine Niobium-carbide-nitride precipitates that form during cooling.

12:45 Predicting Structure and Energy of Dislocations and Semicoherent Heterophase Interfaces: Aurelien Valette; Michael Denkowicz; CEA, DAM, DIF; MIT

Bicrystals containing semicoherent interfaces exhibit distortions produced by the superposition of coherency strains and the elastic strain fields of interface Volterra dislocations. Using an approach that combines the quan

13:00 Lunch
11:45 Invited
Direct Observation of Step Nucleation and Motion in Faceted Grain Boundaries at Atomic Resolution:
Ulrich Dahmen1; Abhay Gautam2; Colin Ophus3; Frederic Lancer2; LBNL; IIT; CEA
Using aberration-corrected transmission electron microscopy, we make direct atomic resolution observations of structural events such as step and kink motion in solid interfaces. From extended dynamic time sequences recorded at a rapid rate, atomic relaxations in the interface are measured by automated event detection followed by cumulative averaging of images between events. The approach is illustrated for HREM and HAADF images of structural changes that take place in a 90°- tilt grain boundary in Au. By splitting a series of images at sudden events such as step motion or fluctuations between structural states of the interface, image blurring due to overlapping structures can be avoided. This makes it possible to analyze the atomic structure of dynamic defects with sufficient spatial resolution to allow comparison with atomatic simulations. Our results highlight the importance of surfaces and other defects in the nucleation and motion of steps and kinks in flat interfaces.

12:15 Invited
Movie Mode Dynamic Transmission Electron Microscopy: A New Tool for Observing Nanoscale Dynamics in Rapid Phase Transformations:
Thomas LaGrange1; Integrated Dynamic Electron Solutions
Transmission electron microscopy (TEM) is an extraordinarily powerful tool for exploring the dynamics of material phase transitions. However, we are typically confined to observe phase transitions under near equilibrium conditions due to the resolution limitations of conventional analytical techniques and we often miss the rapid salient events associated the phase transitions dynamics. Now, with rapid advances in in situ and time-resolved TEM (including single-shot Dynamic and femtosecond Ultrafast TEM, DTEM and UTEM), it is possible to directly observe the nucleation and growth dynamics of rapid transitions as they unfold, often in the precise physical conditions of real-world applications. This talk will present the most recent technological developments in DTEM(such as the Move-Magnify technique, which allows us to capture multiple images of the same object) and show examples drawn from materials science, chemistry, and nanoscience illustrating how this new instrumentation opens unique windows onto nanoscale phase transformations and structural dynamics associated with real applications.

12:45 TEM Studies of Structure and Magnetism in Thermally-induced Antiphase Boundary:
Yasukazu Murakami1; Koudai Nitsu2; Toshiaki Tanigaki3; Ryosuke Kunimine1; Hiroshi Nakamura1; Hiroo Nakai4; Waseda University; RIKEN; Hitachi Ltd.; D-Ang-D University
Antiphase boundaries (APBs) in ordered alloys/compounds induce material functional properties such as pinning of magnetic domain walls, large critical fields for magnetic saturation, magnetoresistance, etc. These functionalities are due to atomic disordering in the APB region, which deteriorates ferromagnetic spin order. Our transmission electron microscopy demonstrated the unusual relationship between APBs and ferromagnetism in the Fe-30at%Al alloy. The thermally-induced APBs showed a finite strength (approximately 2 nm) in which significant atomic disordering was observed. Electron holography studies revealed an unexpectedly large magnetic flux density in the APB region, amplified by 60 % (at 293 K) compared with the matrix value. The observations provide novel insights for materials engineering using thermally-induced APBs.

Microstructure - Property Relationships

11:45 Invited
Plasticity-enhancement in Ultra-fine Grained Steel by Deformation-induced Twinning and Twining:
Bruno De Cooman1; Pohang University of Science and Technology
A new class of ductile ultra-high strength materials with an ultra-fine microstructure, has been developed. The ductility enhancement is achieved by a combination of the twinning-induced plasticity (TWIP) effect and the transformation-structure induced plasticity (TRIP) effect, which occur in succession during straining. The application of this TWIP+TRIP mechanism to low alloy, ultra-fine grained, multi-phase steel, is shown to result in an ultra-high strength and a large tensile ductility. In the present contribution, the physical metallurgy of the ductile ultra-high strength TWIP+TRIP steel will be presented. The compositional and microstructural requirements will also be discussed in detail. A model for the strain hardening in TWIP+TRIP steel, based on the dislocation density evolution during straining, will be shown to predict the mechanical properties.

12:15 Effect of Carbon Content on the Mechanical Properties in 0.1C-5Mn Martensitic Steel:
Toshio Hanamura; Shiro Torizuka; National Institute for Materials Science
The effect of carbon on mechanical properties in a 5Mn-2Si steel has been investigated. In general tendency of strength-total elongation balance, when strength increases the total elongation of the identical steel decreases. However, in the martensite structure with different carbon content in 5Mn-2Si composition, when strength increases with increasing carbon content, the corresponding total elongation stays almost constant. The martensite steel is generally believed that when their strength is high, their ductility is rather poor. In contrast, this, the 5Mn-2Si steel exhibits excellent total balance properties. With increasing the C level farther more, however, the ductility starts to decrease. This change in mechanical properties as a function of carbon content is to be discussed with martensitic steels with the conventional composition of 1.5Mn-0.3Si.

12:30 Study of the Influence of Phase Transformations on Mechanical Behaviour of Austenitic Stainless Steel (316Nb):
William Jolly1; Caroline Toffolon-Mascal1; Thomas Guibert2; Pierre Wident1; Bernard Marin3; Lucien Allais4; François Buy5; Sylvain Ringeval1; Eric Suzer1; François Cortial1; Philippe Petit1; CEA-Saclay; CEA-Valduc; DCNS Research; Hubert & Duval
Stabilized austenitic stainless steels (316Nb type) are usually used for components exposed to significant thermal-mechanical stresses in complex environments, mostly in the chemical, nuclear and oil industries. Different phases can be found in the austenitic matrix: retained austenite, sigma phase, primary and secondary NbN(NC). Depending on the cooling rate applied after high temperature heat treatment, the microstructure of these steels can evolve leading to a “signalmisation” of the 8 ferrite. In the present work, the influence of phase transformations on mechanical properties has been studied by means of microstructural characterization by TEM and microscope measurements, SEM, TEM and WDS observations, and mechanical testing. At last, the use of CALPHAD tools such as DICTRA and MatCalc, have allowed modelling the phase transformations.

12:45 Transition Carbide Formation in a 0.2C-1.54Mn-1.48Cr-1.30Si (wt. pct) Quenched and Partitioned Steel:
Daniel Coughlin1; Dean Pierce2; Joon Seo3; Amy Clarke1; Emmanuel De Moor4; Kester Clarke1; Los Alamos National Laboratory; ASPPRC, Colorado School of Mines
Understanding the formation of transition carbides and their effect on microstructure and mechanical properties is important for the development of advanced high strength steels. Quenching and partitioning (Q&P) is a process path that can be used to create microstructures with retained austenite for ductility and martensite for strength. Q&P relies on the partitioning of carbon from martensite to austenite, but the formation of γe carbides consumes carbon that could otherwise be used to stabilize austenite. Advanced microscopy techniques were used to characterize the microstructure and determine the type of transition carbides present. Additionally, differential scanning calorimetry (DSC) was used to analyze phase transitions in the heat-treated material and determine the austenite phase stability. Compositions were selected to analyze the effect of C, Mn, and Ni content on transition carbide formation and austenite phase stability.

Pearlite

14:00 Invited
Pearlite Revisited:
Ingo Steinbach1; Ruhr-University Zener’s model of pearlite transformation in steels can be viewed as the prototype of many microstructure evolution models in materials science. It links principles of thermodynamics and kinetics to the formation of the microstructure. In addition it solves a very practical problem: How the hardness of steel is correlated to the conditions of processing. Although the model is well established since the 1950s, quantitative explanation of growth kinetics is still a matter of debate. The presentation will shortly review the classical model of pearlite transformation. Zener’s conjecture of maximum entropy production will be annotated by modern theoretical and experimental considerations of a band of stable (sometimes oscillating) states around the state of maximum entropy production. Finally, several mechanisms are investigated quantitatively be field-phase simulations which must be active together to reproduce the observed growth kinetics of pearlite.

14:30 Divergent Pearlite in a Fe-C-Mn-Al Quaternary System:
Maria Martin-Aranzadi1; Sha-Du Tsai1; Robert E. Hicks2; Jonathan Poplewsky1; Jer-Ren Yang3; Esteban Urones-Garrote1; R. Rementeria1; Carlos Capdevila1; CENIM-CIC; Department of Materials Science and Engineering, National Taiwan University; Materials Science and Technology Division, Los Alamos National Laboratory; Oak Ridge National Laboratory; Centro Nacional de Microscopía Electrónica (CNME), Universidad Complutense de Madrid
The roles of Mn and Al during the isothermal growth of partitioned pearlite under non-steady state conditions are analysed by comparing the phase compositions of austenite, ferrite and cementite (γe-M-ε-M) in the three phase field in the Fe-C-Mn and Fe-C-Mn-Al systems. The goal is to study the kinetics and thermodynamics when divergent pearlite is obtained in both ternary and quaternary systems. Transmission electron microscopy, energy dispersive X-ray spectroscopy, and atom probe tomography (APT) measurements across the γ-ε-Mε and γe-M-ε-Mε interfaces were compared to theoretical values obtained by Thermocalc software to study the LE conditions across the interfaces at different isothermal decomposition times and to establish whether a precursor phase forms under the Negligible Partitioning Local Equilibrium (NPLE) or the Partitioning Local Equilibrium (PLE) modes for both Mn and Al alloying elements. APT was conducted at the Center for Novel Materials Science, which is a DOE Office of Science User Facility.
14:45 Elastic Strain Generated by Pearlitic Transformation: Nobuo Nakada1, Norimitsu Koga2, Toshiohito Tsuchiya1; Setsuo Takaki2; Kyushu University; 2Yokohama National University

Pearlite is the diffusional transformation product formed via eutectoid transformation in steel and has a two-phased fine lamellar structure composed of ferrite and cementite. G.J. Shiflet et al. reported that lattice misfit between both phases is so significant that interfacial structures, i.e. microscopic steps and misfit dislocations, are introduced at the lamellar interfaces during pearlitic transformation. However, the microscopic description of the system is very complicated, and TEM reveals that the misfit strain does not seem to be completely accommodated by the interfacial structures, and thus mostly remains as elastic strain in pearlite, leading to an obvious crystal rotation. In addition, EBSD/ Wilkinson method, which is able to map the distribution of local elastic and plastic strains separately, shows that each pearlite colony has a different anisotropic elastic strain field. As a result, it is thought that the formation of pearlite colony contributes to uniform the transformation elastic strain field in pearlite.

15:00 Cementation Assisted by Electric Current: Patrice Chantrenne1; Damien Fabrègue1; Michel Perez2; INS Lyon

To study the influence of the current on the diffusion of interstitials, an ARMCO iron sample is placed between the two graphite punches of a Spark Plasma Sintering facility. The current between the punches is managed to regulate the temperature of the sample. Above 910°C, the ferrite transforms into austenite and carbon only diffuses into austenite. Below 910 °C, carbon diffuses in ferrite which promotes austenite. The microstructure of the samples etched and micro-hardness is measured along the diffusion direction. Results are compared to carbon concentration predicted thanks to a model taking into account of the Fick’s law, the solid phase change and the influence of the electric field. The latter phenomenon shifts the carbon atoms. Comparison between experiments and simulations is used to identify the carbon drift velocity. It is thus possible to get a better insight on the phenomena taking place in a SPS device.

14:30 Lattice Coupled Grain Growth with Low-angle Grain Boundaries: Kevin McReynolds1, Kuo-An Wu2, Peter Voorhees1; Northwestern University; 2National Tsing Hua University

Grain growth is generally driven to minimize the interfacial energy. However, for low-angle grain boundaries the requirement that lattice planes be continuous across the boundary gives rise to a coupling between the normal motion of the grain boundary and the tangential motion of the lattice. We show through simulations using the phase-field crystal model, that for a circular grain embedded at a symmetric planar tilt grain boundary this coupling gives rise to a rigid body translation of the lattice as the grain shrinks. The process is mediated by significant climb of the dislocations in the boundary in a mechanism that involves bulk diffusion of vacancies from the trailing edge to the leading edge of the crystal. The implications of these results on the motion of partially coherent two-phase interfaces will be discussed.

14:45 Molecular Dynamics Study of the Migration Kinetics of Asymmetric Grain Boundaries: Sherr Hadian1; Blazi Grabcowski1; Christopher Race2; Jörg Neugebauer1; Max-Planck-Institut für Eisen Forschung; 2The University of Manchester

Classical molecular dynamics (MD) simulations are commonly used to explore the migration of grain boundaries. Our previous research on low sigma symmetric boundaries has shown that at conditions of low driving forces as found in actual experimental setups and when going towards system sizes exceeding those commonly employed in MD a novel mechanism becomes operational that is based on mesoscopic island nucleation. In the present study we extend our earlier high temperature simulations on symmetric equilibrium boundaries to the majority of experimentally observed moving boundaries. We introduce defects by deviating the boundary plane from a symmetric one to a highly asymmetric one and the simulations show how the fundamental atomicistic mechanisms change as the nucleation driven motion shifts towards a step propagating one.

15:00 Multi-scale Quantum Mechanical Calculations of Solute-grain Boundary Interaction: Laimi Hübner1; Blaz Grabcowski1; Matthias Militzer1; Jörg Neugebauer1; Jörg Rottler1; University of British Columbia; Max-Planck-Institut für Eisenforschung

Solutes at interfaces significantly affect phase transformation and grain growth kinetics, but density functional theory (DFT) treatments are restricted to special high-symmetry interfaces. To maintain quantum mechanical (QM) accuracy near solutes and facilitate general interfaces, we propose QM/molecular mechanical (MM) coupling. We perform this coupling by decomposing the system into a small QM region and a much larger MM region, which are elastically coupled. Since DFT codes for metals use a plane wave basis set with periodic boundary conditions, variation of the QM region using vacuum clusters creates deeply penetrating electronic perturbations. Thus, we introduce new "tiker" atoms, replacing the vacuum surface with a less severe interface. We study the binding of solutes to a high symmetry grain boundary (GB) in Al which can be validated against periodic DFT calculations, allowing critical evaluation of errors. We then apply the method to solutes at a general GB, beyond DFT's reach.

14:00-00 Invited Crystallographic Analysis of Martensite and Bainite Structures by SEM / EBSD Method: Goro Miyamoto1; Tadashi Furuhara1; Tohoku University

There has been increasing attention to martensite and Bainite steels in high strength steels. It is well known that martensite and Bainite ferrite (BF) hold a near K-S orientation relationship (OR) with parent austenite and 24 variants can be formed in a single austenite grain. Since inter-variant boundaries act as obstacles against deformation and fracture, understanding of crystallography of those microstructures is essential. The present author has been performed in the past. However, predictive modeling is discussed.

14:30 Effect of Lamellar Orientation on the Plastic Deformation Behavior of Pearlitic Steel: Yoshikiko Teshima1; Makoto Kosaka1; Nobuo Nakada1; Nepon Steel & Sumitomo Metal Corporation; 2Kyushu University

Pearlitic steel has a hierarchical microstructures, consisting of pearlite colonies in which the orientation of lamellar structure is almost identical, and pearlite blocks in which the crystal orientation of ferrite is nearly the same. This complicated microstructures make it difficult to analyze the deformation process of the pearlitic steels, thus the role of each microstructure on plastic deformation has not been fully understood. In this study, we have investigated the local strain distribution along with the deformation behavior at the early stage of plastic deformation. We have performed the local strain distribution measurement with DIC (digital image correlation) method, and corresponding microstructures were analyzed with SEM-EBSD technique. It has been found that the identical local strains were measured within single colony, and larger strains are generated at a colony, where the Schmidt factor of its ferrite is large and its lamellar orientation is close to 45 degrees to the tensile axis.

14:45 Study of Carbide Precipitation During Tempering of Martensite in Fe-Cr-C Alloys: Ziyong Hou1; Peter Hedstrom2; Di Wu2; Joakim Oydbyst1; KTH Royal Institute of Technology; 2Northeastern University

Precipitation hardening is one of most effective strengthening mechanisms in steels, and much research has been performed in the past. However, predictive modeling of precipitation is still a challenge and in the present work, precipitation of carbides after tempering of martensitic Fe-Cr-C alloys up to 1000°C has been investigated. Experimental measurements using electron microscopy and modeling using a Langer-Schwarz approach has been conducted. The importance of a proper definition of the initial microstructure for predictive modeling is discussed.

15:00 Coupled APT, EBSD, FIB and NanoSIMS Techniques for Investigation of Boron Segregation in Steels: Claire Debarra1; Frédéric Danox1; Didier Blavette1; Laurence Chevalier1; David Gobin2; Thomas Sourm4; Nathalie Gobin3; Fabien Guevilly1; GPM CNRS - UMR 6634; 2GPM CNRS - UMR 5664; 3AMMIS - MERCI EA 83829; 4Asco Industries CREAS; 5LEM3 CNRS - UMR 7239

Atom Probe Tomography is a key approach to investigate phase transformation and interfacial segregation at the nanometer scale. This presentation, a correlative...
Hillert’s (1980) vision in comparing thermodynamics studies of early-stage solute-cluster formation in this strength is characterized with a few Gleeble interrupted prediction, it is thus important to be able to model the However, RS at final temper could lead to some distortions. 

Nicolas Distributioni in 7XXX Aluminum Alloy Thick Plates Prediction of Quenching-Induced Residual Stress 14:30 Simon Barker 1; 1Novelis Global R&T Center; 2Novelis Switzerland SA; 3The University of Waterloo Steel:\n
Bainite MONDAY PM ROOM: NORDIC SESSION CHAIR: MICHAEL KIRKA, OAK RIDGE NATIONAL LABORATORY 14:45 Solid-Solid Phase Transformations During Casting of Plutonium: Adam Farrall1; Jeremy Mitchell1; Terence Mitchell1; Deniece Korzekwa2; Tark Saleh3; Cameron Knapp1; 1Los Alamos National Laboratory Plutonium possesses six solid allotropes, displaying a wide range of unusual behaviors. Large volume changes, negative thermal expansion in some phases, and an assortment of low-symmetry crystal structures yield a wide variety of behaviors during cooling from high temperatures. Density changes approximately 20% from the lowest density phases to the highest, resulting in significant deformations in the part. A majority of this deformation involves mainly orthorhombic or 2 different monoclinic crystal structures, resulting in the largest deformations in the phases least able to deform without cracking. This talk will address mechanisms related to these phase transformations, mechanical mechanisms of transformations in this material, focusing on the relationships between homologous temperatures in alloptic materials, deformation mechanisms, phase transformation mechanisms, and microstructural changes due to annealing during casting. Control of microstructures to suppress cracking via process control will be related to these fundamentals.

15:00 Effect of Heating Rate on the Phase Transformation of Zirconium Alloys: Accidental Basis Accidents: Toan Nguyen1; Javier Romero1; Antoine Ambard1; Michael Preuss1; João Quinta da Fonseca1; 1The University of Manchester; Westinghouse Electric Company; 2Électricité de France R& D 

The effect of heating rate on the phase transition temperature and phase fraction evolution was studied in two industrial Zr alloys: recrystallized ZIRLO® and cold-worked Zircaloy-4. An electro-thermal-mechanical tester was used to heat the materials at rates similar to the rates experienced during in loss-of-coolant accidents (LOCA) in nuclear fuel assemblies. The aim was to determine how these fast rates affect the kinetics of the transformation and the final texture of the different materials, which is relevant to material degradation during LOCA. By using experimental resistivity-strain analysis, it was found that fast heating, in the range of 10-100ºC/s, increases transition temperature and lowers 8 fraction at a given temperature. After a complete α→β transition from upper to lower of bainite.

15:15 Break

Non-Ferrous Alloys MONDAY PM ROOM: NORDIC SESSION CHAIR: MICHAEL KIRKA, OAK RIDGE NATIONAL LABORATORY 16:00 Investigation of Bainite Formation in a Chemically Inhomogeneous Medium Carbon Spring Steel: Constantinou Goulaou1; Pina Mecozzi2; Jilt Sietsma3; 1Materials innovation institute (M2i)/ Delft University of Technology; 2Delft University of Technology 

The effect of chemical inhomogeneity on the isothermal bainite formation is investigated in medium carbon low silicon spring steel by dilatometry and microscopy. The analysis of the microstructure at different times during the transformation shows that chemical segregation of substitutional alloying elements resulting from casting strongly affects the bainite formation by relaxing the transformation kinetics and limiting the maximum achievable bainite fraction. The effect of prior austenite grain size and Cr-rich carbide precipitation in the segregation bands is investigated, and compared with the findings in homogenized material. A physically based model is used to simulate bainite formation and the mechanism of nucleation and growth is discussed. The calculated difference in nucleation rates between the enriched and the depleted areas is not by itself sufficient to explain the microstructures obtained and thus significant influence of growth on bainite formation is observed, which indicates that a diffusional transformation mechanism is taking place.

16:15 Role of Cementite in the Formation of Bainite in 0.3 mass% C Steels: Jiaping Yin1; Mats Hiltén1; Annika Borgenstam1; 1KTH Royal Institute of Technology 

The role of cementite in the transformation of austenite to bainite has been studied in three 0.3 mass% C steels, with 0.5 mass% Si, 0.5 mass% Mn and both 0.5 mass% Si and 0.5 mass% Mn, respectively. Samples have been isothermally heat treated from the austenite finish temperature down to below the martensite start (Ms) temperatures and characterized using Light Optical Microscopy and Scanning Electron microscopy. The role of cementite in the bainitic transformation has been followed and the influence of cementite on the evolution of the bainitic morphology and on the growth rate of acicular ferrite is discussed. Attention has also been paid to the role of cementite on the transition from upper to lower of bainite.

16:30 Ultrafast Granularization of Lath-like Bainite in FeNiC Alloys During Isothermal Holding: Menenm Ben Hayd Samia1; Sébastien Alia2; Nathalie Gey2; Lionel Germain2; Kangying Zhu1; JULEM1; JU1; JLEM2; ArcelorMittal Research Center/Mazières les Metz 

Evidences of a fast and unexpected lath-like bainite «granularisation» during isothermal holdings will be reported. The phenomenon is characterized by improved angular resolution EBSD and TEM, and is observed in a FeSn50.13C alloy transformed at 380°C (above Ms) after an austenitic soaking. The granularisation process starts once the initial lath bainite transformation is over (lower and upper bainites) after 1 min and is characterized by an evolution of the ferrite matrix morphology and microtexture and by a carbide ripening process. During subsequent holdings (typically 30 min), variant coalesced zones develop and rapidly grow within paquets, at the expense of highly misoriented laths (60º). The resultant low misorientation angle boundaries then progressively recover and carbide films precipitate on former packet boundaries. This explains the mechanical properties decrease. The associated driving forces will be discussed. This texturing mechanism occurring with slower kinetics in more conventional FeMnNiC alloys could contribute to bainite classification.

16:45 Break

Bainite MONDAY PM ROOM: ALPINE A-B-C SESSION CHAIR: KESTER CLARKE, LOS ALAMOS NATIONAL LABORATORY 15:30 Invited Certain Aspects of the Bainitic Transformation in Steel: Annika Borgenstam1; 1KTH, Royal Institute of Technology 

A review of certain aspects of the bainitic transformation in steel based on the diffusional theory will here be given. Underlying thermodynamics, kinetics as well as microstructure evolution will be reviewed including the effect of temperature and alloy composition. The thermodynamic barrier needed and its physical nature will be discussed together with modelling and experimental measurements of growth rates of acicular ferrite, the change in morphology with temperature and composition both with respect to ferrite and cementite, the transition between upper and lower bainite and the fact that bainite can form below Ms. The effect of the symmetry in the Fe-C phase diagram will also be considered.
15:30 Invited

Atomistic and Continuum Modeling of Diffusion Controlled Growth of Facetted Interfaces: Peymann Sadı1; Jeffrey Hoyt2; 'McMaster University

The kinetics of many solid-solid and solid-liquid phase transformations are governed by the diffusion controlled lateral motion of steps along a facetted interface. Despite the importance of the step flow mechanism the velocity of facetted interfaces is not completely understood. In this work we employ the boundary element method to model the composition profile and velocity of an infinite periodic array of steps along a solid-liquid interface and assume that due to convection, a boundary layer of a specified thickness exists at the interface. In addition, a multiple scale analysis is utilized to derive an analytic expression for the growth of a stepped interface in the case of a solid-solid interface where no convection is present. Finally, the continuum results are compared to molecular dynamics simulations of facetted Si111 growth in Al-Si liquid alloys and the transition from attachment controlled to diffusion controlled growth is discussed.

16:00

C2-NEB: The Nudged Elastic Band Method with Two Climbing Images, Validated on the Martensitic Transformation in NiTi Shape Memory Alloy: Nikolai Zarkevich1; Dianne Johnson2; 'Aires Laboratory

The nudged-elastic band (NEB) method is modified with concurrent two climbing images (C2-NEB) to find a transition state (TS) in complex energy landscapes, such as those with serpentine minimal energy path (MEP). If a single climbing image (C1-NEB) fails to find the TS, C2-NEB finds it with higher stability and accuracy. However, C2-NEB is suitable for more complex cases, where C1-NEB misses the TS because the MEP and NEB directions near the saddle point are different. Generally, C2-NEB not only finds the TS but guarantees that the climbing images approach it from the opposite sides along the MEP, and it estimates accurately the three images' highest-energy one and its climbing neighbors. C2-NEB is suitable for fixed-cell NEB and the generalized solid-state NEB (SS-NEB). We validate the C2-NEB method on the solid-solid phase transformations in NiTi, and find agreement with experiment.

16:15 Invited

From Nanoscale to Second: Bridging the Time Gap in the Atomistic Dynamics of Complex Materials with the Kinetic Activation-Relaxation Technique: Normand Mousseau1; Laurent Beland2; Peter Brommer3; Fawad El-Mellouhi4; Jean-François Joly5; Gawonou N’Tosiaou4; Oscar Restrepo3; Mickaël Trochet1; 'Université de Montréal; 2Oak Ridge National Laboratory; 3University of Warwick; 4Qatar Environment and Energy Research Institute; 5Carleton University; 'Texas A&M University at Qatar

Understanding atomistic diffusion and relaxation mechanisms remains one of the main challenges of materials science. How can we follow the microscopic motion of atoms on times scales relevant to describing age, crack propagation and self-assembly? With the advent of faster computers and the development of a new class of algorithms, we are now starting to bridge this time gap in complex materials, opening the door to the numerical study of crucial, but long neglected problems. In this talk, I will present the kinetic Activation-Relaxation Technique (k-ART), an off-lattice kinetic Monte Carlo algorithm with on-the-fly catalysis building, a method able to follow atomistic kinetics of highly defective and disordered materials over more than 10 decades in time, reaching the second time scale and more. I will show recent applications to carbon diffusion in iron, relaxation of Si on bombarded silicon, defect diffusion in amorphous materials and more.

16:45 Break

In-situ Techniques I

15:30 Invited

Stabilization of bcc Fe by Magnon-phonon Interactions: Brent FutI; Lisa Mauger2; Fritz Körnmann2; Blazie Grabowski3; Matthew Lucas3; Jing Munoz2; Sally Tracy2; Bissawanath Dutta4; Tilman Hickey3; Jörg Neugebauer4; 'California Institute of Technology; 'Max-Planck-Institut für Eisenforschung

Magnon densities of states (DOS) were measured for bcc Fe between 300 K and 1184 K using nuclear resonant inelastic x-ray scattering. All phonons shifted to lower frequencies with temperature, but the low transverse modes shifted especially rapidly above 700 K, showing an unusual nonharmonic behavior that followed the thermal trend of the magnetic entropy. This excess phonon shift made a contribution of 35 meV/atom to the free energy at 1100 K. A new ab-initio approach for quantitatively assessing effects of magnon-phonon interactions and lattice expansion showed that for some phonon branches, the magnon-phonon interaction is in order of magnitude larger than the inelastic x-ray scattering at thermal expansion or anharmonicity. The magnon-phonon interaction makes a surprisingly important contribution to the thermodynamic stability of bcc Fe.

16:00

Differential Scanning Calorimetry as a Powerful Tool for Investigation of Solid-Phase Transformations in Heat Affected Zones: Zainab M. Sheta1; Benjamin Mikereit1; Marco Starkin2; Olaf Kellner3; Christoph Schick2; 'University of Rostock; 'University of Southampton

During the recent years, we developed advanced techniques to analyze solid-phase transformation by Differential Scanning Calorimetry (DSC) in a very wide dynamic range. Our lab today covers the entire heating and cooling rate range of technical but also physical interest — up to eight orders of magnitude for inorganic materials (0.001 K/s – 10,000 K/s). This talk will introduce the Kinetic Activation-Relaxation Technique (k-ART) for crystallographic analyses allowing thermodynamic and enthalpy change determination with high precision. The k-ART is an off-lattice kinetic Monte Carlo algorithm with on-the-fly catalysis building, a method able to follow atomistic kinetics of highly defective and disordered materials over more than 10 decades in time, reaching the second time scale and more. I will show recent applications to carbon diffusion in iron, relaxation of Si on bombarded silicon, defect diffusion in amorphous materials and more.

16:15

Control of Phase Transformation During Heat Treatments Based on DSC Experiments: Philipp Schumacher1; Stefan Pogatscher2; Olaf Kellner1; Marco Starkin3; Christoph Schick1; Volker Möhles1; Benjamin Mikereit1; University of Rostock; 'ETH Zurich; 'University of Southampton; 'RWTH Aachen University

Phase transformation in Al-Si alloys during cooling from solution annealing was investigated with advanced DSC techniques in a wide cooling rate range (2 K/s–0.001 K/s). Applying the k-ART and the TEM, we show that quench-induced Si particles of different shape and size can precipitate. The dependence of formation enthalpy on cooling rate and temperature is modelled, providing a consistent physical description of precipitate volume fraction and solute Si amount during cooling. This allows control of phase transformation via precise heat treatments and thus allows generation of well-defined microstructural states. Thereby, samples having an equal amount of solute Si but different precipitation states could be tested in order to investigate the influence of different precipitation types on the mechanical behaviour. A big advantage of this method is that the strengthening contribution of precipitates can be determined without the need to assume any - potentially inaccurate - superposition law between particle and solute strengthening.

16:30

Rotation of Single Crystal Cu Nanopillar Revealed by In-situ Electron Diffraction: Jian-Min Zuo1; Min-Jun Zuo2; 'University of Illinois at Urbana-Champaign

The crystal rotation and slip behavior during compression in bulk samples are well-described by Taylor rotation model and Schmid's law. However, when sample sizes are reduced to the micron or nano scale, whether the classical geometrical model could be applied is still under debate. In this study, in-situ electron diffraction experiment is performed in a transmission electron microscope to study the crystal rotation in Cu single crystal nanopillar under compression. The evolution of diffraction pattern is used to track the crystal rotation behavior and to predict the primary and critical slip systems by using Quantitative Electron Diffraction software to fit diffraction patterns. Results show that Cu single crystal rotates during compression. If it undergoes double slip on the geometrically predicted slip system, followed by single slip behavior. These detailed information are helpful to understand the deformation behavior of nanopillars under compression.

16:45 Break

TRIP Materials

15:30 Invited

Development of “Steels Like” Titanium Alloys Combining High Strength, High Strain Hardening and Improved Ductility: Jeffrey Hoyt1; 'McMaster University; 2Southampton

Titanium alloys are attractive for industrial applications, due to their remarkable strength/density ratio and corrosion resistance. However, major drawbacks arising from low plasticity (<20%) and a lack of strain hardening are still limiting their potential in advanced applications when compared to steels. This work aims at designing a new family of Ti-Cr and Ti-V titanium alloys with improved mechanical properties. These alloys show an extremely high ductility (45% of plastic deformation) accompanied by both a high strength and a very high work hardening rate. Extensive microstructural characterization revealed a complex sequence of deformation mechanisms consisting in activation of internal mechanical twinning accompanied by and assisted stress induced precipitations. In this talk, design strategy and chronology of deformation mechanisms will be highlighted in order to understand the improvement of the mechanical behaviour. Future directions towards the development of a new family of metallic materials will be discussed.

16:00

The Interaction of Martensitic Phase Transformations in MMC Based on TRIP-steel with Zirconia Particle Reinforcement: Harry Berek1; Christian Weigt2; Christer Anzwe1; 'TU Bergakademie Freiberg

A new class of metal-matrix composites (MMC) consists of stainless steel showing transformation induced plasticity (TRIP) and magnesium partially stabilized zirconia (Mg-PSZ). Both components exhibit martensitic phase transformations during deformation, thus generating the potential for improved mechanical properties. The MMC can be produced in the form of cellular materials as foams and honeycombs. They enable different light weight applications. This paper describes the experiments of the martensitic phase transformations within steel and zirconia during deformation. Investigations based on in situ x-ray computed tomography (XCT) were performed. Local phase analysis was performed by electron backscatter...
diffraction (EBSD). A correlation between the degree of local deformation and the local martensitic phase transformation was found within the ceramic reinforcement. There are maxima of deformation and martensite formation within the steel at steel-ceramic boundaries. Nevertheless the transformation of the steel starts at a higher deformation level in comparison to the ceramic.

16:15 Invited

Metastability of Austenite in High Strength Steels Associated with TRIP Effect: Xuejun Jin;
Jiao Tong University

Economically manufactured Advanced High Strength Steels (AHSS) are increasingly demanding to satisfy the requirements of better structure materials for comfortable life and sustainable development. “Third Generation” of AHSS shows strength-ductility combinations significantly better than showed by the first generation AHSS (ferrite-based microstructure) but at a cost distinctively less than required for second generation AHSS (austenite-based microstructure). Considerable amount of austenite is attained through the combination of delicate composition design and sophisticated process control, which gives rise to a better mechanical performance assisted by transformation induced plasticity effect. Here, metastability of austenite is evaluated and discussed with respect to external loading or temperature change. Factors such as heterogeneous composition, grain size and surrounding constrains controlling the metastability of austenite have been studied in Quenching-Partitioning treated steels, Medium-Mn steels and Trip dual phase stainless steels. A few models are compared and applied to evaluate metastability of these newly developed AHSS.

16:45 Break

Plenary 2

MONDAY PM ROOM: EMERALD BALLROOM
SESSION CHAIR: HATEM ZUROB, MCMASTER

17:00 Plenary

Importance of Phase Transformations in Development of Modern High Strength Steels: Tadashi Furuhara;
Tohoku University

Fundamental and applied research in structural steels attracts much attentions recently. In development of modern high strength steels, importance of strength and ductility/toughness balance is increasing and more advanced and sophisticated controls of microstructure formed during phase transformations are utilized particularly. In the presentation, two major topics in high-strength low-alloy steels are discussed; 1) nano-sized precipitation of alloy carbide accompanied during ferrite transformation, i.e., interphase precipitation, which establishes high yield strength, moderate work-hardening and high local elongation in low-carbon ferritic sheet steels, and 2) substructure and transformation kinetics of bainite which should contribute to improvement of toughness of plate steels. In such design of microstructure, importance of various aspects in phase transformations, i.e., thermodynamics, kinetics and crystallography, will be emphasized.
Preliminary Statement

The kinetics of the austenite decomposition even in lean steels has been studied for many years as it is surprisingly difficult to construct a consistent model which takes into account the effects of the change in crystal structure and more importantly the effects of element partitioning at the moving austenite-ferrite and the austenite-bainite interface. Existing models make different assumptions regarding the degree of element partitioning but are equally capable of describing the experimental data for simple linear cooling. At Delft we developed the cyclic partial transformation concept to magnify the effect of the solute partitioning and to discriminate between various models. Extension of the concept to the austenite-bainite transformation appears to be independent of the cooling rate.

10:45

Solid Solution Formation Rules and Crystal Structure Indicators on High Entropy Alloys: Isaac Toda-Caballero; Pedro Rivera-Diaz-del-Castillo; University of Cambridge

High Entropy Alloys (HEAs) are multicomponent systems incorporating several elements in a nearly equiatomic constitution. The contents of each solute can typically vary between 5 and 35 at%. The high entropy associated to mixing several elements can inhibit the formation of intermetallic phases in favour of FCC or BCC solid solutions. Existing rules for predicting HEA formation are at an incipient form, generally not offering information on the crystal structure. In this work, the interatomic spacing, as well as bulk moduli, remain within the lattice parameters of FCC or BCC HEAs, occurring. Additional, several samples were studied by transmission electron microscopy to gain a detailed insight into the microstructures before and after tempering and to depict their differences.

11:15

Break
compositions were compared with the experimental data decomposition line and specific heats for various alloy moments, elastic modules, Grüneisen’s parameter and electronic specific heat coefficients, the average magnetic Methodology was developed to calculate the solubility Heat of bcc Fe-Cr Alloys Using Physical – Empirical rules for predicting HEAs has been achieved by analysing statistical analysis on the reliability of the complete set of conventional Calphad databases. OpenCalphad provides a new models and their integration into software tools for materials simulations. This presentation describes the progress made in development of the OpenCalphad code and databases. The goal of OpenCalphad is to develop high quality software for thermodynamic calculations and databases with parametric physical models of the pure elements as basis for multicomponent databases as well as conventional Calphad databases. OpenCalphad provides a highly structured tool that can be used, together with kinetic models, in microstructure and continuum simulations.

10:45 Invited Advanced Small-angle X-ray Scattering for Quantifying Complex Precipitation Kinetic Pathways: Alexis Deschamps; Frédéric de Geuser; Grenoble Institute of Technology; 3Grenoble INP – LAPP
Small-angle X-ray Scattering, used with X-rays or neutrons, enables a rapid quantification of precipitate microstructures at the nanoscale. This technique is particularly well adapted to use in-situ during thermal or thermo-mechanical treatments, or for scanning samples with heterogeneous microstructures. This presentation will give an overview about the capability of such experiments to provide insight on the kinetics of precipitation in complex situations in different alloy systems: quantifying the morphology evolution of plate like precipitates and particularly the transition between lengthening and thickening (Al-Cu-Li), validating precipitation models by in-situ kinetic data in isothermal and non-isothermal situations (Al-Li-Mg and Fe-Si-Ti), understanding the coupling between plastic deformation and concurrent precipitation (Al-Zn-Mg-Cu), understanding the precipitation kinetics in severely plastically deformed materials (Al-Zn-Mg-Cu), mapping heterogeneous microstructures in welds (Al-Cu-Li)

10:15 Thermo-mechanical Simulation Coupled with Synchrotron X-ray Scattering: A Unique Tool to Explore and Develop Materials: Antonio Ramirez1; Leonardo Wu2; Guilherme Faria3; Thais Alonso3; Leiron Palermo1; 1LNano
The development and optimization of materials and processes involves always the use of cost-effective characterization and modelling techniques. Among those, intense x-ray synchrotron beamlines present the possibility to study materials under near to application conditions in real time. When such photon sources are combined with powerful thermo-mechanical physical simulators, the possibilities to study fundamental phenomena and rapidly develop/optimize materials are enormous. This was the strategy used to design and built the x-ray scattering and thermo-mechanical simulation installation (XMS) of LN Nano/LNLS-Braga. This possibility to simultaneously submit the sample to a well-controlled and reproducible strain/stress and temperature conditions using a customisable Gleeble® system while approaching its crystallographic characteristics by x-ray diffraction have made possible to study the fundamentals of phase transformations and to optimize processing conditions for several materials. The capabilities of such unique installation will be presented along with selected examples of fundamental studies on metallic alloys.

11:00 Calculation of the Miscibility Gap and Specific Heat of bcc Fe-Cr Alloys Using Physical – Empirical Models: Dmitry Vasilyev1; Aleksandr Udvolsky2; Blaauw Institute of Metallurgy and Materials Science, Russian Academy of Sciences
Methodology was developed to calculate the solubility curves, the spinodal line and temperature dependencies of specific heats of alloys; including one-two phase states in a frame of physical – empirical models, which use physical properties of alloys: Delbye and Curie temperatures, the electronic specific heat coefficients, the average magnetic moments, elastic modules, Grüneisen’s parameter and thermal expansion coefficients - as input parameters. The results of calculated solubility curves as well as the spinodal line decomposition line and specific heats for various alloy compositions were compared with the experimental data and the calculated results obtained by other researchers.

11:15 Break
Subsequent annealing caused progressive size increase and, crucially, morphological changes: ellipsoidal(Inr) near-cuboidal(64 hrs) cuboidal(256 hrs). Furthermore, after only 1 hr of annealing, the phase was substantially depleted in V, which exhibiting martensitic transformations with interface. Possible factors contributing to the morphological and compositional evolution of α at lower temperatures and α-assisted nucleation and growth of a precipitates at higher annealing temperatures will be discussed.

10:15 Interplay between Microstructure and Phase Transformation Kinetics during Thermal Transformation from 16 sp²-Hybridised BN under Extreme Conditions: Christian Schimpf; Marcus Schwarz; Christian Lathe; Eduard Schubert; David Rafaiji; TU Bergakademie Freiberg; 2GFZ Geoscientific Research Centre for Geosciences

The kinetics of the high pressure/high temperature (HP/HT) phase transition from hexagonal to cubic boron nitride were studied by means of laboratory and in-situ X-ray diffraction under HP/HT conditions using a multi-anvil press. Hexagonal graphic BN precursors (h-BN) were characterised with respect to their microstructure (crystallite size, microstructure defects) using the profile analysis of X-ray diffraction lines. The real structure of the samples significantly affects the phase transition kinetics and product. Kinetic parameters of the phase transition were determined in-situ at high pressure. Experimtally, quantitative results have shown that basal plane corrugations in h-BN assist the direct transformation to c-BN without the formation of intermediate wurtzitic BN (w-BN). Contrary, defect-poor h-BN transforms to c-BN via w-BN, thereby showing more sluggish and growth rate. A complementary analysis using TEM and XRD (in-situ and laboratory) was applied to reveal microscopic driving forces of the phase transition mechanisms.

10:30 Phase Transformations in Electrodeposited Cobalt-phosphorus Coatings: Srimat Vijayan1; Na Luo; Mark Andersson1; 1Rutgers University

Nanostructured Electrodeposited Co-P alloy coatings have been identified as attractive alternatives to electrolytic hard chrome coatings due to their superior corrosion and wear resistance, and the more environmentally friendly electroplating bath formulations involved. Three different types of Co-P coating microstructure can be formed depending on the P content: crystalline, hybrid and amorphous. The hybrid structure forms at intermediate P contents, comprises a nanostructured mixture of crystalline and amorphous phases, and gives optimized fatigue strength. This report a study on the stability of the phases and microstructures in DC-plated Co-P coatings with 0-15 wt % P by comparing the as-deposited coating with subsequent thermal exposure. A combination of differential scanning calorimetry, x-ray diffraction and transmission electron microscopy techniques have been used to reveal the character and sequence of the phase transformations that occur upon heating as a function of P content.

10:45 Solid-state Reactive Diffusion between Sn and Iron Family Metals: Masanori Kajihara; 2Tokyo Institute of Technology

Solid-state reactive diffusion between various metals with low-melting and high-melting temperatures is experimentally examined in our research group. For the reactive diffusion between Sn and iron family metals in the temperature range of 433-473 K, only the most Sn-rich Sn-Fe alloy is considered to have a layer with visible thickness, though there exist several stable compounds in this temperature range. The layer growth is controlled by vertical segregation of Sn in X-ray, which indicates the occurrence of subsequent thermal exposure. A combination of differential scanning calorimetry, x-ray diffraction and transmission electron microscopy techniques have been used to reveal the character and sequence of the phase transformations that occur upon heating as a function of P content.

11:00 Break

11:45 Quenching & Partitioning Heat Treatment on a Ductile Iron: Competition between Martensite/Austenite Carbon Partition and Bainite Reaction - Mechanical Properties: André Melotto; Arthur Nishikawa; Hélio Goldenstein; Edwin Kroke; David Rafaja; 1TU Bergakademie Freiberg; 2GFZ Geoscientific Research Centre for Geosciences

In this work the kinetics and microstructural evolution during Quenching & Partitioning (Q&P) heat treatment applied on a ductile cast iron (DGI) was studied. Heat treatments were conducted in oil and salt baths and by means of dilatometry, allowing kinetics measurements. Additionally, evolution of phase fractions and lattice parameters were followed by means of in situ X-ray diffraction conducted at the XTMS experimental station facilities at Brazilian Nanotechnology National Laboratory (LNANO). Real time temperature evolution based on the accelerated kinetics of competitive reactions and changes on austenite lattice parameter was obtained based on those results providing evidences for two main mechanisms of austenite carbon-enrichment: martensite carbon partitioning and bainite reaction. Microstructural characterization was performed by Scanning Electron Microscopy and Transmission Electron Microscopy (TEM). It was able to produce tailored microstructures composed by tempered martensite, carbide-free bainite and carbon-enriched stabilised austenite.

12:00 Quenching & Partitioning Heat Treatment on a Ductile Iron: Competition between Martensite/Austenite Carbon Partition and Bainite Reaction - Mechanical Properties: André Melotto; Arthur Nishikawa; Hélio Goldenstein; Edwin Kroke; David Rafaja; 1TU Bergakademie Freiberg; 2GFZ Geoscientific Research Centre for Geosciences

In this work, the mechanical properties and stability of austenite of a ductile cast iron after processing using the quenching and partitioning (Q&P) route was studied. Heat treatments consisted on heating the material to 880°C for 2 hours followed by quenching in oil at 140 and 27°C. The retained austenite was then isothermally directly reheated to 300 and 375°C (partition treatment) for different times between 15 to 120 minutes. Mechanical properties were characterized by tensile and impact strength tests. Fracture surfaces were studied by scanning electron microscopy. The transformed austenite upon plastic deformation in the range from 0 to 20% thickness reduction of the samples was analyzed. The retained austenite and induced martensite after rupture was characterized using X-ray diffraction with Rietveld refinement. It was observed that the austenite thickness stays mostly stable even after plastic deformation.

12:15 Mossbauer Spectroscopy Investigation of Transition Carbides in Partitioned and Partitioned Steel: Mathew Pearce; Daniel Coughlin; Don Williamson; Kester Clarke; Amy Clarke; John Spear; Emmanuel De Moor; Colorado School of Mines; Los Alamos National Laboratory

Quenching and partitioning to quenched and austenite stabilized austenite stays mostly stable even after plastic deformation.

13:00 Dissolution Versus Morphological Evolution of Residual δ-Ferrite in Model Austenitic Stainless Steels: Mahmoud Saeidi; Yves Du Terrail Couval; Catherine Tassini; Jessica Detacoulo; Muriel Véron; Jean-Denis Miticheux; E. Rigal; APERAM; 1Univ. Grenoble Alpes; 2Univ. Grenoble Alpes; 3CEA Grenoble

The dissolution kinetics of residual δ-ferrite was studied in a cast Fe-17.3Cr-9.4Ni austenitic stainless steel ingot by means of heat treatments at temperatures lying between 780 and 1300°C. The experiments show that the ferrite fraction transiently increases at early stages of the transformation, until reaching a maximum value, after which the dissolution starts driven by Cr and Ni diffusion. The dissolution rate undergoes a slight decrease at the intermediate stage of the transformation; this slowdown is attributed to the complex microstructural features such as martensitic lath and δ-ferrite interlath interface energy leading to a morphological change of the ferrite. To overcome the complex microstructural features such as martensitic lath and δ-ferrite interlath interface, several geometries have been produced using austenitic and ferritic Fe-Cr-Ni alloys, allowing a better description of the different stages of the phase transformations. Experimental results are compared to a 1D finite-difference modeling.
12:45 Molecular Dynamics Simulation of the Effects of fcc/bcc Interfaces on the Nucleation and Growth of Martensite in Iron: Xiaoqin Ou; Jill Sietsma; Maria Santomina Navarro; Tu Delft.

Molecular dynamics simulations have been used to study the effect of fcc/bcc interfaces in the Nishiyama-Wasserman (N-W) orientation relationship on the fcc-to-bcc transformation at 300 K in pure iron. Simulations show the growth of the original fcc phase in the initial configuration as well as the nucleation and growth of new bcc grains inside the original fcc phase. During growth, heterogeneity and homogeneity bcc nucleation both pin the propagation of the original bcc/fcc interface. In some locations, neighboring newly-nucleated bcc plates merge into a single bcc grain. The fcc phase transforms to bcc phase by a predominantly martensitic mechanism.

13:00 Diffusion and Diffusion-controlled Transformations in -talk and N- to hbermetals: Atomic Modelling: Rafal Abdank-Kozubska; Andrzej Biborski; Miroslaw Kozlowski; Piotr Sowa; Sylwia Brodacka; Christof Grebennik; Veronique Pierron-Bolmes; Jolanta Janczak-Rusch; Elena Lochenko; Alexander Evertz; Irina Belova; Graeme Murch; Jagiellonian University in Krakow; 2Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology; 3Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504; 4EMPA, Swiss Federal Laboratories for Materials Science and Technology; 5University Centre for Mass and Thermal Transport of Inorganic Materials, School of Engineering, The University of Newcastle Callaghan.

Self-diffusion, decomposition, precipitation, chemical ordering and surface segregation in bulk and nanolayered intermetallics have been modeled at the atomic scale using hybrid Monte Carlo – Molecular Statistics algorithms. Three particular results are reported: (i) The experimentally observed discontinuous transformation from “in-plane” to “off-plane” L10 variant in [001]-oriented FePt nano-layers modeled with Analytical Bond-Order Potentials (ABOP); (ii) The configuration of the eutectic mixture of Ag and Cu precipitates in nanolayered Ag-40at.%Cu modelled with many-body potential derived for Ag-Cu within the Second-Moment Approximation; (iii) Vacancy thermodynamics, self-diffusion, and “order-order” kinetics modeled by means of Semigrand Canonical Monte Carlo and Kinetic Monte Carlo simulations in B2-ordering A-B system mimicking Ni-Al. Experimentally observed relationships between the activation energies for ordering and self-diffusion in NiAl are reproduced and its origin is elucidated. The study is extended upon AB nanolayers where an interplay between surface-segregation and ordering is revealed.

13:15 Lunch and Poster Session

Theory of Displaceable Transformations

TUESDAY AM
ROOM: CALLAGHAN
SESSION CHAIR: DANIEL SCHWARTZ,
LOS ALAMOS NATIONAL LABORATORY


Using high-resolution transmission electron microscopy (HRTEM) and atomistic simulations (density function theory and molecular dynamics), we explored zero-shape phase transformation mechanisms that occur in hexagonal close packed Ti, Zinc-blend AlN, and Wurtzite InAs. A face-centered cubic titanium (fcc-Ti) was characterized in polycrystalline titanium where the two phases have the orientation relation <0001>|Ti<001> and <10-10>|Ti<1100>. We discovered that the fcc-Ti band forms via a pure-shuffle mechanism and migration of phase boundary via a shear-shuffle mechanism or a pure-shuffle mechanism. Zinc-blend AlN nanolayer was characterized in Al-AlN-TiN trilayers. Zinc-blend AlN transforms to wurtzite AlN during mechanical loading through collective glide of three Shockley partial dislocations as one unit that has a net zero Burgers vector and corresponds to a zero-shape strain. The same transformation mechanism was also characterized in InAs nanowires. I will report on zero-shape phase transformation mechanisms and discuss potential application in designing nanostructured materials.


Anomalous precursor effects are observed in cubic austenite phases prior to martensitic transformations, which are difficult to explain from conventional phase transition theories. Based on incomplete phonon softening that generally occurs above martensite start temperature, a Grüneisen-type phonon theory of martensitic precursors is developed. The theory considers phonon free energy contribution and addresses the effects of deformation-dependent incompletely-softened low-energy phonons on the structural, thermal, acoustic and elastic behaviors of pre-martensitic cubic crystals on the same physical footing of thermal expansion. It shows that martensitic precursor effects are natural consequences of anharmonic lattice dynamics in cubic crystals that undergo incomplete phonon softening. In-situ 3D phonon diffuse scattering and Bragg reflection experiments using high-energy synchrotron X-ray single-crystal diffraction are performed to test the theory. Exotic domain behaviors are observed in pre-martensitic austenite phases, which are fundamentally distinct from usual ferroelastic domain switching behaviors and are explained from phonon point of view.

12:45 Invited Continuous Martensitic Transformation and Invar and Elinvar Anomalies: Dong Wang; Liangxiang Zhang; Xiaobing Ren; Yanzhi Wang; Xin Jiao Tong University; National Institute for Materials Science; Ohio State University.

Martensitic transformation (MT) is a typical first-order diffusionless solid state phase transformation accompanied by a global shear strain at martensitic start temperature. Long-range elastic interactions dominate the microstructural evolution, with strong autocatalysis leading to an avalanche of self-accommodated strain domains (martensitic variants) via nucleation and growth. Such transformation characteristics are too sharp and nonlinear for certain applications. By creating martensitic embryos with a broad distribution of degrees of maturity and hence of different MT start temperatures, suppressing the autocatalyst, and regulating the spatial extent of domain growth via random fields from point and extended defects, we show that this sharp MT can be rendered continuous. Accompanying such a continuous MT, there could be many special properties, including superelasticity of nearly zero hysteresis, nearly zero thermal expansion (Invar anomaly), and low and temperature-independent elastic modulus (Elinvar anomaly) over a broad temperature range. The simulation predictions agree well with experimental observations.
Ferrous Austenite

TUESDAY AM ROOM: NORDIC SESSION CHAIR: MASATO ENOMOTO, IBARAKI UNIVERSITY

11:45 Invited
Some Metallurgical Issues Concerning Austenite Conditioning in Microalloyed Steels Processed by Near-net-shape Casting and Direct Rolling Technologies: Jose Rodriguez-Ibarbe1; Beatriz Lopez2; 1CEIT
As steel grades with higher strength/ductility requirements combined with smaller total reductions are required, austenite conditioning during hot working of as-cast microstructures becomes a key step that needs to be properly analyzed. If this conditioning prior to transformation is not well achieved, in the final microstructure coarse high angle boundary crystallographic units can be present which impair toughness. The complexity of this austenite conditioning has increased due to the displacement from single to multiple microalloying additions (usually Nb combined with other elements such as Ti, Mo or V) and to the development of new hot rolling configurations and rolling strategies with smaller reductions. It is worth emphasizing that these microalloying combinations can affect the softening-strain induced precipitation interactions associated with Nb microalloying. This manuscript analyzes some of the microstructural features that should be taken into account during austenite conditioning, with special emphasis in Ti-Nb and Nb-Mo microalloyed grades.

12:15 Austenitization Kinetics of Medium Mn Steels during Intercritical Annealing: Haiwen Luo1; University of Science & Technology Beijing
Medium Mn steels which usually contain 5-10 wt.% Mn are the promising candidate for the 3rd generation automotive steels as they exhibit an excellent combination of strength and elongation. The key production process of these steels is intercritical annealing, during which part of ferrite shall transform to austenite. Austenitization kinetics determine the amount and stability of austenite formed intercritically and then retained after cooling, which accounts for the improved tensile properties via TRIP effect. The austenitization kinetics and partition of the solutes between ferrite and austenite during intercritical annealing were not only measured experimentally but also simulated numerically. We found a discrepancy between the measured and simulated results on the partition of Mn, and then discussed the possible reasons.

12:30 Austenitic Decomposition and Properties of Mo-Nb Containing Press Hardening Steels: Fatih Fazel1; Colin Scott1; 1CanmetMATERIALS
Press hardening steels with strength exceeding 1.5 GPa enable significant down gauging of the structural parts of lightweight vehicles without compromise of crash performance. Austenite decomposition of blank sheets during forming operation controls microstructure and crashworthiness of fabricated parts; particularly the fraction and microstructural features of martensite which depend on alloy composition and forming parameters. Modified 22MnB5 steels with Mo-Nb addition were developed for improved press hardenability and enhanced crash performance. Dilatometric study and microstructural analysis were carried out to assess the role of processing parameters, i.e. forming temperature, applied strain and thermal path. Dynamic recovery of austenite during forming and its subsequent softening upon die cooling were analyzed to understand the interaction between austenite deformation and decomposition. Further, hat-section parts were fabricated to provide specimens for tensile and three-point bend tests. The transformation behaviour of the developed alloys and the interplay among microstructure-processing-properties are discussed in details.

12:45 Microstructures and Mechanical Properties of High Strength Medium Manganese Steel: Xiaolong Yang1; Yunbo Xu2; Ying Zou1; Xiaodong Tan1; Zhiping Hu1; Yongmei Fu1; Di Wu1; 1Northeastern University
With the development of microalloyed steels, the excellent combination of high strength and high ductility becomes a target in modern industry. Due to the low price of manganese and excellent mechanical properties, the medium manganese steels are attracted much more attention recently. Based on TMCP and UFC technology, the microstructures and mechanical properties of medium manganese steel were studied in this paper. The hot-rolled medium manganese steel was treated by reheating quenching process. The mechanical properties of medium manganese steel were measured by tensile and impact test, and microstructures were observed by optical microscopy (OM), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The excellent mechanical properties were obtained in this study, and relationship between microstructures and mechanical properties was further investigated in order to acquire a good combination of high strength, high ductility and excellent impact toughness.

13:00 In Situ Study of Austenite Reversion Kinetics during Intercritical Tempering of a 12Cr-6Ni-2Mo Supermartensitic Stainless Steel: Julian Escobar1; Guilherme Faria1; Leonardo Wu1; Paulo Roberto Mei1; Antonio Jose Ramirez2; 1State University of Campinas; 2Brazilian Nanotechnology National Laboratory
With the development of microalloyed steels, the excellent combination of high strength and high ductility becomes a target in modern industry. Due to the low price of manganese and excellent mechanical properties, the medium manganese steels are attracted much more attention recently. Based on TMCP and UFC technology, the microstructures and mechanical properties of medium manganese steel were studied in this paper. The hot-rolled medium manganese steel was treated by reheating quenching process. The mechanical properties of medium manganese steel were measured by tensile and impact test, and microstructures were observed by optical microscopy (OM), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The excellent mechanical properties were obtained in this study, and relationship between microstructures and mechanical properties was further investigated in order to acquire a good combination of high strength, high ductility and excellent impact toughness.

13:15 Lunch and Poster Session
in the first stage is attributed to enhanced dislocation multiplication and impingement caused by precipitates. Equal strain hardening behavior is due to the balanced effect of dynamic recovery and dislocation entangle.

P-A4: Effect of Cooling Rate after Solution Treatment on Phase Separation in Fe-Cr Alloys: Xin Xu1; Peter Heidström1; Joakim Odqvist1; ’KTH Royal Institute of Technology

It is known that the solution treatment of bcc Fe-Cr alloys will affect subsequent low temperature aging and phase separation kinetics. There are several factors contributing and their individual effect is not clear. Hence, in the present work we have tried to isolate and study the effect of the cooling rate after solution treatment on the phase separation kinetics in Fe-Cr alloys. The alloys were cooled at different rates after solution treatments and subsequently aged. The microstructure was characterized and mechanical properties were measured. The effect of cooling rates on the kinetics of the phase separation during subsequent aging, and the resulting microstructure and mechanical properties is discussed.

P-A5: Isothermal Decomposition of Austenite below Ms and during Tempering on a C-Si Steel: José da Cruz Junior1; Dagoberto Santos1; Arthur Nishikawa2; Hélio Goldemstein1; ‘Metalurgical, Materials and Mining Engineering Department of the Federal University of Minas Gerais; 2Department of Metallurgical and Materials Engineering of University of São Paulo

Experimental investigations were performed on the formation of ferrite-martensite structures in a steel during isothermal heat treatments below the martensite start (Ms) temperature, in the range of 200–270°C. After the isothermal heat-treatment, the same steel was subjected to tempering at various temperatures (350–450°C). Isothermal and non-isothermal dilatometry experiments were performed to characterize the kinetics of phase transformations during the initial austenite decomposition and during the subsequent tempering heat treatment.

P-A6: The Structure Property Relationships Governing Zone-Boundary Formation in Austenite: Michael Hoerner1; Mark Eberhart1; John Speer1; E. Damm1; Colorado School of Mines; 1TinkenSteel Corporation

Austenite grain size and austenite boundary motions play an important role in ferrous phase transformations and property control. Solutes are known to interact with austenite grain boundaries, but the nature of these interactions is not well understood. To understand these interactions, ab-initio density functional theory calculations have been performed on a number of grain boundaries with varying cohesive energy/bond strength. The binding energy of solutes to the boundary has been determined. In low symmetry environments traditional parameters that drive site segregation, such as site volume, have been difficult to calculate. Analysis of the changes in the local charge density that are caused by the introduction of solute atoms has been performed in the present work. This analysis was found to provide a meaningful way to understand the origin of solute-boundary binding energy in low symmetry boundaries.

P-A7: Phase Field Modeling of the Austenite-ferrite Transformation in Fe-C-Mn Alloys: Hao Chen1; Benjamin Zhu1; Matthias Millitzer1; University of British Columbia

Three different approaches for considering the effect of Mn on the austenite-ferrite interface migration have been coupled with a phase field model (PFM). In the first approach (PFM-I), only long range C diffusion is considered while Mn diffusion, C and Mn diffusion are considered in the second approach (PFM-II). In the third approach (PFM-III), C diffusion is considered in competition with Mn diffusion. C diffusion due to Mn diffusion inside the interface. PFM-I, PFM-II and PFM-III are all applied to simulating the isothermal transformation and the cyclic transformation in Fe-C-Mn-C alloys. PFM-II and PFM-III predict both bainite growth retardation phenomenon experimentally observed during cycling transformation whereas PFM-III can only replicate the stagnant stage but no growth retardation and PFM-I predicts neither the stagnant stage nor growth retardation. This study suggests a significant role of Mn redistribution near the interface on reducing transformation rates.

P-A8: Austenite Stability in Low Density Steels: Ian Zuazo1; Aurelien Bauche1; Patrick Barges1; Xavier Garat1; ’ArceorMittal

High aluminium steels of the FeMnAl system are an alternative to current automotive steels due to a higher strength coupled to a density reduction of 10% and higher. In the two-phase austenite-ferrite (Duplex) family, the stability of austenite plays an important role on mechanical behaviour. In this alloys TRIP behaviour is observed to depend strongly on annealing parameters (temperature and time) that modify austenite: grain size, partitioning, internal structure, etc. In addition sub-zero cooling down to liquid nitrogen leads to mixed structures where the apparition of martensite, enhanced by the presence of aluminium in an otherwise highly alloyed and stable austenite, also depends on annealing parameters. These aspects will be discussed in relation with the resultant mechanical properties from room temperature to sub-zero testing.

P-A9: Precipitation in Strip Cast Austenite: Adam Taylor1; Peter Hodgson1; Nicole Stanford1; ’Deakin University

Precipitation behaviour of a strip cast model austenitic alloy (Fe-25Ni-0.17Bn-0.14Mn-xC wt.%) was investigated. This particular alloy was chosen as it retains its austenitic structure on cooling to room temperature and thus allows the precipitation behaviour in austenite during the strip casting process to be studied directly. The fast cooling times associated with strip casting process results in a different microstructure when compared to the conventionally cast material. These rapid cooling rates can also result in chemical segregation and the formation of solute clusters and nano-precipitates. The unique precipitation behaviour of this alloy was studied utilising a combination of atom probe tomography (APT), transmission electron microscopy (TEM) and scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS).

P-A10: A Model for the Growth Rate of Bainitic Ferrite: Lindsay Leach1; Anikka Borgendurdt1; John Ågren1; Lars Hjöland1; ’KTH Royal Institute of Technology

The appeal of bainitic steels lies in their immense potential for improved mechanical properties as is evident in the good combination of strength and toughness they exhibit, a development which can be facilitated by computational tools. The aim of this work is to develop a predictive model for the formation of bainite. At this point, it is solely the ferrite component of bainite that is considered. A model for the lengthening rate of bainitic ferrite has been developed. The critical conditions of formation and thermodynamic driving forces are used to delineate thermodynamic barriers. The growth kinetics has been conducted within a diffusional framework and a maximum lengthening rate concept has been applied. It is demonstrated that under these conditions, the growth rates of bainitic ferrite can be predicted to a sufficient extent thus laying the foundation for further development of a quantitative model to predict the degree of transformation.

P-A11: Nano-sized Precipitates in an Fe-13Cr Alloy Formed Under Oxidizing Water Vapor: Leonardo Andrade A. Mosquera1; Bert Nolte1; Fernando Rizzo1; 1BAD; 2PUC Rio de Janeiro

Oxidation of a Fe-13Cr alloy under water vapor at 600°C produced a zone of nano-sized precipitation underneath the oxide scale formed on iron boride and John spinel. The precipitated particles present an orientation relationship to the ferritic matrix. The precipitates have a lamellar morphology with main axes parallel to [001]-ferrite direction. The majority of the precipitates also show a fixed orientation relationship to the ferritic matrix. EDS and EBSD were used to characterize the oxide layer. The precipitates were investigated by transmission electron microscopy and energy extracted by FIB to target an area previously characterized
by EBSD, consisting of the base material, the precipitation zone and the spinel layer. Energy filtered selected area imaging and EDS in the scanning (S)TEM mode were also employed in the characterization of the specimens.

P-A12: Experimental and Numerical Analysis on Transformation from Martensite to Austenite during the Intercritical Annealing of 13Cr-5Ni Steel: Lu Liu1; Zhe-Gang Yang2; Chi Zhang1; Yuan Xia1; Pengcheng Song1; 1Rzeszow University of Technology; 2AGH, University of Science and Technology; 3Tsinghua University

Microstructure evolution from martensite to austenite and partitioning behavior of alloying elements during the intercritical annealing at solidus temperature 550°C to 700°C with different durations at a heating rate of 10°C/min in a 13Cr-5Ni steel were examined experimentally and analyzed numerically by Thermo-Calc and DICTRA. Several microstructural changes were observed:

- The increased heterointerface density strongly affects the misorientations between the phases, additional alloying with 4 at% Ge
- The increased heterointerface density increases the volume fraction of austenite at room temperature after intercritical annealing firstly increased with the annealing temperature, exhibiting a maximum at 625°C and then decreased at higher temperatures. Additionally, the volume fraction of austenite at room temperature, which was determined by using EBSD, showed a decrease from 625°C to 825°C with increasing duration of the intercritical annealing. Formation of austenite was controlled by diffusion of Ni in martensite.

P-A13: Hierarchical Optimization of the Structure and Properties of Semiconducting 8-Fe2Si, which result in a competitive thermoelectric material. Edelstob decomposition e-Fe2Si, e-Fe + 2Si results in Si nanorods embedded in 8-Fe2Si. The increased heterointerface density strongly reduces thermal conductivity. To further increase performance, we simulated simultaneously engineered misorientations between the phases, additional alloying with 4 at% Ge has been attempted by arc melting. This produces coarse eutectic lamellar structures of Si1-xGex and a-FeSi2 upon solidification, with a non-equilibrium Bi2O3 phase present. However, melt-spinning the alloy markedly decreases the lamellar length scales to the nanoscale regime, and eliminates Fe3Si. Eutectic equilibrium has not been reported in this region of the Fe-Si-Ga phase diagram, and we are beginning to map out the liquidus surface. This provides an opportunity to engineer microstructures from the combined eutectic/eutectoid decomposition process, and how this affects thermoelectric properties.

P-A14: In situ Investigations of Partitioning Mechanisms in Q&P Steels by Synchrotron Diffraction Experiments: Szabóber Álfré1; Guillaume Grandell1; Jean-Christophe Heil1; Michel Soler1; Frédéric Danoux1; Mohamed Gouné1; 1Institut Jean Lamour; 2ArcelorMittal Mazères Research SA; 3GPM; 4ICMIB

Quenching &Partitioning is a new annealing route proposed to produce the third generation of Advanced High Strength Steels. It relies on the generation of a mixed martensite and austenite microstructure by an interrupted quench (Quench-Temperature annealing), which is produced by a bi-velocity (Darken) method. The Kirkendall effect is used to maximise the total surface energy reduction per vacancy emitted. We explain the measured void shrinkage by a pseudo-Kirkendall type mechanism modified to take into account electron beam irradiation. This provides an explanation for the presence of a specific, non-equilibrium void shape before shrinkage starts.

P-A15: The Frenkel Effect during Diffusion Process: Bartek Wierzb2; Patrycja Wierzb2; Wojciech Skibinski1; 1Rzeszow University of Technology; 2AGH, University of Science and Technology

In this paper numerical description of the reactive diffusion process including Frenkel effect is shown. The vacancy generation and void evolution is discussed in terms of numerical simulations. The proposed approach based on the generalized Darken approach where the volume velocity is essential in defining the local material velocity at non-equilibrium. The void formation in TiN-Al diffusion system is experimentally discussed and modeled.

P-A16: Competition between Kirkendall, Frenkel and Backstress Effects during Diffusion Process: Wojciech Skibinski1; Bartek Wierzb2; Stanisław Wedrychowicz2; 1AGH University of Science and Technology; 2Rzeszow University of Technology

In this work the relation between Kirkendall and backstress effects induced in the diffusion process is discussed. Both effects are caused by the difference in diffusion coefficient of Kirkendall and Frenkel plane shift is simulated and experimentally verified. Several simulation methods are discussed – trajectory, velocity curve and entropy density. This approach is based on the bi-velocity (Darken) method which combines the Darken and Brenner concepts proposing that the volume velocity is essential in defining the local material velocity at non-equilibrium.

P-A17: Mechanisms of Void Shrinkage in Aluminium: Zhaozhong Zhang1; Tianyu Liu1; Andrew Smith1; Nikolai Medvedovich1; Nahid Nazifi1; Laure Bougeais1; 1Department of Materials Engineering, Monash University; 2School of Physics, Monash University; 3Monash Centre for Electron Microscopy, Monash University

Voids in aluminium can significantly affect materials performance. An important question is: why do they shrink? We performed in-situ annealing in a high-resolution transmission electron microscope and found that void shrinkage is not monotonically driven from a non-equilibrium to an equilibrium shape and then shrinks progressively keeping its equilibrium shape until its collapse. This phenomenon can be explained through a surface energy analysis: the void shrinks so to maximise the total surface energy reduction per vacancy emitted. We explain the measured void shrinkage by a pseudo-Kirkendall type mechanism modified to take into account electron beam irradiation. This provides an explanation for the presence of a specific, non-equilibrium void shape before shrinkage starts.

P-A18: Growth of Compounds during Reactive Diffusion between Sn-base Alloys and Conductor in Binary Mg-Sc System: Makoto Inomoto1; Naiming Liu1; Eva Rosker1; William Soffa1; Jerry Ando2; Yuji Sutou 2; Junichi Koike 2; 1Tohoku University; 2AGH, University of Science and Technology; 3Tsinghua University

In this study, aging behavior of Sn-based compounds containing spherical AlTi particles was studied. Spherical AlTi intermetallic compound particles were prepared by gas atomization method. A 13Cr-5Ni steel strip with a range of 75-150 μm and 150-212 μm were sintered with pure aluminum particles by spark plasma sintering (SPS), where volume fraction of AlTi particles within the composites was fixed to be 10 Vol.%. When the composites are aged at elevated temperature, the spherical AlTi particles are divided into smaller parts. This is because the AlTi particles prepared by gas atomization method are poly-crystal.

P-A19: Growth of Compounds during Reactive Diffusion between Sn-base Alloys and Conductor in Binary Mg-Sc System: Makoto Inomoto1; Naiming Liu1; Eva Rosker1; William Soffa1; Jerry Ando2; Yuji Sutou 2; Junichi Koike 2; 1Tohoku University; 2AGH, University of Science and Technology

In this study, aging behavior of Sn-based compounds containing spherical AlTi particles was studied. Spherical AlTi intermetallic compound particles were prepared by gas atomization method. A 13Cr-5Ni steel strip with a range of 75-150 μm and 150-212 μm were sintered with pure aluminum particles by spark plasma sintering (SPS), where volume fraction of AlTi particles within the composites was fixed to be 10 Vol.%. When the composites are aged at elevated temperature, the spherical AlTi particles are divided into smaller parts. This is because the AlTi particles prepared by gas atomization method are poly-crystal.
The stability of these different precipitate phases, i.e. number density of fine scale precipitates compared to the due to Zn addition, will be discussed.

The nucleation ratio of the certain variant is larger in the nucleation ratio between the variants. Consequently, when in volume fraction of preferred variant strongly depends on microstructure evolution in the later stage was studied on two-step aging condition; natural aging and then subsequent artificial aging. Application of HPT processing on two-step aging condition; natural aging and then subsequent aging at 593 K decreased with natural aging.

The precipitation state in high temperature ceramic coatings and the effect of deformation on decomposition is discussed. It is then important to consider whether the effect of deformation on decomposition is however lacking and in the present work we have used a combination of atom probe tomography and phase-field modeling to elucidate these details. The effect of strain on the decomposition mechanism and the kinetics is discussed.

Displaceable Transformations

P-B1: An In-situ Method to Identify Lattice Correlations For High Temperature Ceramic Coatings: For Intelligent Systems, and University of Stuttgart, Institute for Intelligent Systems (formerly Max Planck Institute for Metals Research) and University of Stuttgart, Institute for Materials Science.

The thermally-induced precipitation of the hcp-phase from fcc saturated Cu-Ge solid solutions (in the range of 8-11 at. % Ge) was claimed in the past to be an isothermal martensite transformation exhibiting C-type transformation curves in TTT diagrams (1,2). However, the kinetics of the hcp-phase formation upon isothermal ageing were not determined until now and therefore the above statement has not been validated until now. Against this background, in the present study in-situ x-ray diffraction studies on Cu-Ge powders (with 10.8 at. % Ge) were performed at different temperatures in the range of 200-750 °C to quantitatively study the formation of the hcp lattice and thereby reveal the underlying transformation mechanism. [1] P.J. Moroz, R. Taggart, D.H. Polonis, J. Mater. Sci., 22 (1987) 639-652; [2] P.S. Kotval, R.W.K. Honeycombe, Acta Metalurgica, 16 (1968) 597-607.
P-B4: Comparative Grain-scale Characterization of Mechanical Twinning in Austenitic Steel and Beta-Ti: Matthieu Marteleur; Perrine Tanguy; Frédéric Prima; Pascal Jacquies; UCL; "Chimie-PansTech

Since its discovery by Sir Hadfield in the late 1800s and the first {

P-B5: Formation of Widmanstätten Ferrite in a C-Mn Steel at Temperatures High in the Austenite Phase Field: Claudioaldo Arauza; Rupanjit Grewal; John J. Jonas; McGill University

Compression tests were carried out on a 0.06% C-0.3%Mn-

P-B6: Phase Transformation of Nanostructured Bainite after High-strain Rate Deformation: Yu-Ting Tsai; Hung-Wei Yen; Jer-Ren Yang; Woei-Shyan Lee; National Taiwan University; National Cheng Kung University

In this research, a split Hopkinson pressure bar is used to study the microstructure evolution of nanostructured bainite at high strain rate, and the results indicate very high strength (>250 MPa) and high fracture strain (>0.3). Scanning electron microscopy results show that large blocks of nanostructured bainite sheaves are rotating and accommodating more strain. Transmission electron microscopy results show that after deformation, retained austenite thin films are heavily twinned in one major variant, with low-angle variants nanowires and some evidence of strain-induced martensite formation inside internal twins. On the contrary, blocky retained austenite component and complex phase transformation behavior, and multiple twining band and irregular-shaped martensite was found. Significant distortion structure change inside nanostructured bainitic ferrite is found by scanning transmission electron microscopy. Finally, the work-hardening rate is explained by the sequential phase transformation behavior.

P-B7: Detection of the Martensitic γ → α Phase Transformation on a Metastable Austenitic Steel, Transformation Behavior in 304 Austenitic Stainless Steel: Jarrad A. Kauzman; Abdul M. Al-Mutairi; Paul J. Junilang Liu; The University of South Carolina

Deformation-induced phase transformation in 304 austenitic stainless steel has been studied in tension at room temperature. It was found that austenite transformation sequence was 1050°C to 100°C in-situ in a Transmission Electron Microscope. The experiments were done on two types of 304 stainless steel: (i) a cold-rolled steel and (ii) stress-relieved 304 bar. The results indicated that the cold-rolled steel was observed during the cooling to cryogenic temperatures without external stress applied. The nucleation and growth of the martensitic phase developing under strain were monitored in-situ and captured on video. The processes involved in the phase transformation were studied. The presentation will report the observations done and analysis especially at room temperature.

P-B8: Influence of Quenching and Partitioning Conditions on the Microstructural and Mechanical Properties of a 0.2C Steel: Pierre Hugger; Cédric Georgé; Stéphane Gabet; Université Libre de Bruxelles; CRM Group

The Quenching and Partitioning process consists of an initial isochronal annealing or full austenitization, followed by a partitioning step in order to stabilize the austenite through carbon enrichment, leading to martensite formation. The use of specific alloying elements and the design of appropriate Q&P parameters are required to eliminate competing mechanisms such as carbide formation and austenite decomposition. In the present work Q&P heat treatments were carried out in a quench dilatometer on 0.2% C-0.4%Mn-1%Ni austenitic steel. The transformation sequence was intercritical annealing or full austentization, followed by a partitioning step in order to stabilize the austenite through carbon enrichment, leading to martensite formation. The transformation, a phenomenon called SME (Spontaneous Magnetism Emission), had previously been described during cooling at cryogenic temperatures of metastable austenite. The results were discussed in light of mechanical Barhausen Noise (MBN), X-ray diffraction and microstructures obtained before and after the tests.

P-B9: Emerging Concepts on the Microstructural and Mechanical Properties of a 0.2C Steel: Pierre Hugger; Cédric Georgé; Université Libre de Bruxelles; CRM Group

P-B10: Variant Selection of Bainite Nucleated at Austenite Grain Boundaries: Takeshi Kaneshita; Goro Miyamoto; Tadashi Furuhara; Tohoku University

Bainitic ferrite(BF) has a near K-S orientation relationship with the parent austenite and the formation of K-S equivalent variants. High angle inter-variant boundaries impede slip deformation and crack propagation. Therefore, variant pairing of neighboring BF is a key to determine the mechanical properties of BF. In BF steel with more than 0.2% C, especially martensite transformation, carbon partitioning and austenite decomposition were evaluated. The microstructure evolution was characterized using SEM, XRD and EBSD. The tensile properties of selected samples were measured. The mechanical properties are shown to be highly dependent on phase volume fractions and the stability of austenite during deformation.

P-B11: Surface Effects on Martensitic Phase Transformation, a Simultaneous In Situ XRD and Dilatometry Study: Guilherme Faria; Julian Escobar; Antonio Ramirez; Brazilian Nanotechnology National Laboratory

Martensitic transformation temperatures are largely dictated by this transformation nucleation driving force. In FCC to BCC/BCT martensitic transformations, one of the driving forces is the increase of the surface energy, given the difference in atomic densities between the initial and final phases. At the surface of metallic samples, there is a direction in which the newly formed martensite develops at this surface, where the region the strain energy term will be smaller than at the core, and that the transformation will happen at different temperatures. In this work, this difference is assessed through simultaneous in situ X-ray diffraction and laser dilatometry. Transformation temperatures determined by both techniques for the same specimen had very small differences show up to 140°C. Anisotropic elasticity calculations allow the qualitative determination of the evolution of the surface martensite stress state during the test.

P-B12: On the Martensitic Transformation of AISI D2 Tool Steel through Cryogenic Cooling: Hadi Ghasemi; Abdolrahman Jahanzadeh; Tom Leveaque; Ecole de Technologie Superieure; Ecole de technique superieure; DK SPEK Company

In this research, high resolution BÀHR dilatometer DIL805 (AVD) was utilized to study martensitic transformation in D2 tool steel (0.3% C and 12% Cr) with 1.5 K/s above critical cooling rate to obtain full martensitic microstructure. Austenitizing was carried out at 1300K for 20 min then continuous cooling until 173 K was applied. The dilatometry diagrams revealed two distinct behaviors: 1) regular behavior where a single change in the slope of the curve is observed and associated with martensitic transformation; 2) an atypical behavior where another inflection point is appeared in the curve. For the regular behavior section of the curve an original equation is proposed which accurately describes the martensitic transformation and could be used for predicting such transformations in similar steels. An analysis is proposed for the atypical behavior which is based on the occurrence of dynamic straining of austenite during austenitization.

P-B13: Understanding the Role of Prior Austenite Grain Boundaries on the Transformation Kinetics: Ashwath M. Ravi; Jilt Sietsem; Maria J. Santofimia; Delft University of Technology

Prior austenite grain size (PAGS) is one of the key factors influencing the transformation kinetics in martensitic steels. Previous studies indicate that austenite grain refinement increases the nucleation rate which generally results in acceleration of bainite kinetics. These studies also indicate, on the other hand, that PAGS influence on overall transformation kinetics. In this work, the kinetics of the bainite formation during isothermal treatments in low silicon steels is investigated. Information regarding the fraction of bainite which evolves solely due to grain boundary nucleation as well as the fraction of bainite which evolves solely by auto-catalytic nucleation retrieved from dilatometry experiments. Using this approach, an attempt to provide a deeper insight into the role of PAGS on the transformation kinetics as well as on auto-catalytic nucleation is carried out.

P-B14: Elastocaloric Effect in the Fe-31.2Pd (at.%) Single Crystal: Fei Xiao; Xuejin Jin; Takashi Fukuda; Zhaoxu Gu; Shuxian, Shanghai Jiao Tong University; Osaka University

In typical shape memory alloys exhibiting an obvious first-order martensitic transformation, significant elastocaloric effects appear only in the parent phases. However, we report here that a significant elastocaloric effect appears both in the parent and martensite phases in an Fe-31.2Pd (at.%) alloy, which exhibits a weak first-order martensitic transformation. When a compressive stress of 200 MPa applied in the (001) direction was removed, the specimen exhibits an adiabatic temperature decrease of more than 1.5 K in a wide temperature range of between 175 K and 250 K. The refrigeration capacity is calculated in this temperature range to be 5 MJ/m².

P-B15: Functional Properties of SMAs Based on Shape Memory Alloys Containing Finely Dispersed Precipitates: Philipp Kooß; Peter Kadetz; Malte Vollmer; Johannes Guenther; Christoph Somsen; Yuki Chutl pajakó; Hans Maier; Thomas Niendorf; Tu Freiberg; Ludwig-Maximilians-Universität; Ruhr-Universität Bochum; Tonsk State University; Leibniz Universität Hannover

Shape memory alloys (SMAs) are promising candidates for the development of transforming and shape-memory devices. This is mainly due to their higher work output compared to other functional materials. Established SMAs have been largely used in numerous industries. In this regard, iron based SMAs (Fe-SMAs) are able to
overcome these issues since established processing routes from steel industries are well suited for fabrication of Fe-SMAs. Recent promising Fe-SMAs, such as FeNbCoAlX and FeMnNiAl show up to 13% reversible strain which makes them interesting for actuation and damping devices. However, cyclic instability is the key issue preventing Fe-SMAs from widespread applications. Thus, this study investigates the cyclic stability in Fe-SMAs in order to identify microstructural features accountable for functional degradation. In-situ testing, electron microscopy and neutron diffraction was used to correlate between the phase transformation and microstructural features.

P-B16: In Situ SEM Observations of Nucleation and Growth of Thermelastic Martensitic Transformation in Shape Memory Alloys: Yohei Soejima1; Takayuki Miyoshi2; Tomonari Inamura3; Minoru Nishida1; Kyushu University; 1Tokyo Institute of Technology

The nucleation, growth, forward and reverse transformation processes of thermelastic martensite in polycrystalline Ti-Ni, Cu-Al-Mn and Ni-Mn-Ga shape memory alloys have been investigated by in-situ SEM cooling and heating observations. The clear information was obtained by electron channeling contrast images with back scattered electrons. For instance, the characteristic strain contrast associated with martensite formation was clearly visualized in the residual particle phase. Homogeneous nucleation was observed in Ti-Ni alloys. The homogeneous nucleation in Ti-Ni alloy was confirmed by FIB/SEM serial sectioning. For polycrystalline Cu-Al-Mn and Ni-Mn-Ga alloys there was no microstructure memory effect of martensitic phase in the three alloys upon thermal cycles. The interaction between habit plane variants clusters of B19' martensite in Ti-Ni alloys is also presented. The evidence of full effect in in-situ TEM observations will be provided.

P-B17: High Temperature TiPd Shape Memory Alloys Systems: Application of Thermoelastic Deformation: Thomas Waltz1; Mitsuhiro Matsumura1; Michael Kerbel1; Ajit Panigrahi2; 1University of Vienna; 2Kumamoto University

TiPd high temperature shape memory alloys show a transformation between the B2 austenite and the B19 martensite. Ti-50at.%Pd was subjected to high pressure (HPT) to study its impact on the martensitic phase transformation. HPT samples were analysed by X-ray diffraction using standard refinement methods. Considering possible lattice structures of TiPd (B2, B19, B19′ and L30) the positions of most of the peaks agree with B19 while intensities indicate (partial) disorder or a strong texture. Additional peaks agree with a L10 lattice structure. Heating in a differential scanning calorimeter yields an exothermic signal at a temperature of about 425°C that might arise by ordered (or amorphous) TiPd. Additional peaks also recover in a growth direction prior to the onset of the B19 to B2 reverse transformation. Therefore the martensitic transformation occurs at a transformation temperature as in the undeformed alloy.Financial support by the Austrian COMET program is gratefully acknowledged.

P-B18: Two-Way Shape Memory Ni-Ti Alloys with Small Transformation Hysteresis Prepared by Rapid Solidification and Constrained Ageding: Xiao Ma1; Yuanquan Li1; Shan Shan Cao2; Xinping Zhang2; 1South China University of Technology; 2University of Pittsburgh

A simple yet effective method for fabricating Ni-Ti alloys with two-way shape memory behavior and a small transformation hysteresis is reported. Ni-Ti button ingot was prepared by vacuum arc melting, and the molten master alloy was sucked into a water-cooled copper mould under vacuum condition to obtain rapidly solidified stripe. The stripe was then subjected to the thermal under constraint condition in specially designed moulds of different shapes bringing about series of initial bending strains. Results showed that both the aging temperature and dwelling time have significant influence on phase transformation behavior and two-way shape memory effect of Ni-Ti alloy. Deformation features of the Ni-Ti alloy stripes during cooling and heating were characterized, which are well corresponding to the forward and reverse phase transformations respectively. The small transformation hysteresis characteristic of the Ni-Ti alloy stripe makes it a promising candidate for fabricating artificial joint spacer.

P-B19: Effect of Austempering Strain on Martensite Start Temperature: Binbo He1; Wei Xu2; Minxin Huang1; 1The University of Hong Kong; 2ArcelorMittal Global R&D Gent

Austempering is generally believed to decrease the martensite start (Ms) temperature. However, a recent experiment found that Ms temperature firstly increased at small strain and then decreased at large strain. This interesting finding may be explained by a strain-induced metastable transformation, which is attributed to an austempering-induced martensite. The strain-induced Ms temperature was measured, both in real time and at different strain levels. The results indicated that austempering strain significantly increased Ms temperature. This strain-induced Ms temperature increase led to an increase in austempering temperature.

Advances in Experimental Techniques

P-C1: Microstructural Evolution of a Severe Plastically Deformed Austenitic Stainless Steel: Using Precession Electron Diffraction: Yaakov Idell1; Jorg Wiezorek2; 1National Institute of Standards and Technology; 2University of Pittsburgh

The nucleation, growth, forward and reverse transformation processes of thermoelastic martensite were used. The nucleation, growth, forward and reverse transformation processes of thermoelastic martensite. Ti-50at.%Pd was subjected to high pressure (HPT) to study its impact on the martensitic phase transformation. HPT samples were analysed by X-ray diffraction using standard refinement methods. Considering possible lattice structures of TiPd (B2, B19, B19′ and L30) the positions of most of the peaks agree with B19 while intensities indicate (partial) disorder or a strong texture. Additional peaks agree with a L10 lattice structure. Heating in a differential scanning calorimeter yields an exothermic signal at a temperature of about 425°C that might arise by ordered (or amorphous) TiPd. Additional peaks also recover in a growth direction prior to the onset of the B19 to B2 reverse transformation. Therefore the martensitic transformation occurs at a transformation temperature as in the undeformed alloy. Financial support by the Austrian COMET program is gratefully acknowledged.

P-C2: Atomic Structure and Bonding of the Interfaces between Gold Nanoparticles and Epitaxially-Regrowth Oxide Substrates: Wei Zhou1; Paolo Longo2; Mai Zhang1; Xia Li1; Xinping Zhang2; 1Shanghai Jiao Tong University; 2Gatan

Equipped with aberration correctors and an electron energy-loss spectrometer, transmission electron microscopy allows the study of chemical composition and bonding information at atomic resolution, and thus becomes the ideal tool to investigate the interfacial complex, which usually includes a few monolayers with intricate atomic structures. By applying the above advanced techniques, we investigated a few unique metal/oxygen interfaces, complex oxides and gold nanoparticles and oxide substrates, such as TiO2 and MgAl2O4. The clarification of these atomic structures provides deep insights in the understanding of the abnormal epilayer growth of a previous stable substrate (e.g. TiO2 and MgAl2O4) under gold nanoparticles. In addition, this can also shed the light on the understanding of the strong interaction between metal/nanoparticle and oxide substrates, such as Au-TiO2 and Au-MgAl2O4.

P-C3: Misfit Induced Changes of Lattice Parameters in Two-Phase Systems: Coherent/Incoherent Precipitates in a Matrix: Maryam Akhlaghi1; Tobias Stein1; Sai Ramudu Meka3; Andreas Leineweber1; Eric Muller2; Max Planck Institute for Intelligent Systems; 1Max Planck Institute for Intelligent Systems; 2Max Planck Institute for Intelligent Systems and Institute for Materials Science, University of Stuttgart

Precipitate volume fractions, local strain fields, etc. is relevant data on these precipitates remains a problem due to the configuration of Ni4Ti3 samples varies inside the ARSMA. In these samples they can appear. In the present work we have applied approach will be combined with in-situ TEM tensile testing to observe the strain evolution and its variant selection due to the different precipitate configurations.

P-C4: In Situ Characterization of Precipitation and Dissolution in an Al-Zn-Mg-Cu Alloy by Electrical Resistivity Measurement: Fulio Jiang1; Halem S. Zurbu1; Gary R. Purdy1; Hui Zhang2; 1Hunan University; 2McMaster University; 3Austrian COMET Center for Interdisciplinary Research and Technology; 4Max Planck Institute for Intelligent Systems, 5Max Planck Institute for Intelligent Systems and Institute for Materials Science, University of Stuttgart

Electrical ac modulation of precipitation induced or thermal-induced misfit led to large changes in crystallography. Formulate for calculation of such misfit induced lattice-parameter changes are presented. In this study, the aggregate of phase precipitation and dissolution for the occurrence of either coherent or incoherent deterioration by matrix and second phase particle. Experimental data and theoretical predictions agree well for various cases available in the literature.

P-C5: Transmission Electron Microscopy Study of Microstructure Evolution in Cryotreated AISI D2 Tool Steel: Hadi Ghareeri Naima1; Mohammad Jahan1; Tom Levasseur2; 1University of Ottawa; 2Ecole de technologie superieure; 3DK SPEC Company

After austenitization at 1300 K, samples of D2 tool steel were cooled down to 175K. The evolution of the microstructure was studied by transmission electron microscope (TEM). Field-emission gun scanning electron microscope (FEG-SEM) was also used to investigate other microstructural features. Thanks to the precision and accuracy of the sample preparation and 3D imaging capability, it was possible to distinguish the complex microstructure of the investigated alloy, which was comprised of carbides, alholomorphic ferrite, Widmanstatten ferrite, acicular ferrite, and mainly bainite instead of traditionally expected martensite. The obtained results are compared with the “life microscope” approach and the precipitate microstructure obtained when a cooling rate of 50 K. s-1 is used.

P-C6: Ni-Ti, Investigation in an ARSMA Using ASTAR Orientation Imaging Microscopy and Phase Mapping: Xiayang Yao1; Yuanquan Li1; Shan Shan Cao2; Xiao Ma1; Xinping Zhang2; Dominique Schuyven3; 1The University of Hong Kong; 2ArcelorMittal Global R&D; 3University of Antwerp; 4South China University of Technology

Applications of Ni-Ti-based shape memory alloys strongly depend on the existence and arrangement of nano- or micron-sized Ni-Ti precipitates, produced by an appropriate ageing. Obtaining quantitative and statistically relevant data on these precipitates remains a problem due to their small size and the four orientation variants in which they can appear. In this study, we have applied the new technique of automated crystal orientation and phase mapping, now available in a TEM and able to reach nanoscale resolution, to samples prepared for all-round shape memory applications (ARSMA). In these samples the configuration of Ni-Ti samples varies inside the material and quantified data on grain sizes and orientation, precipitate volume fractions, local strain fields, etc. is indispensable for further development of the material. This approach will be combined with in-situ TEM tensile testing to observe the strain evolution and its variant selection due to the different precipitate configurations.
Titanium alloys are used in a wide variety of high performance applications where the high strength, high stiffness, and good corrosion resistance of titanium are beneficial. The mechanical properties of titanium alloys are strongly related to microstructure developed during thermo-mechanical processing. In this study, our final goal is to determine the relationship between the texture of the beta phase and final microstructure and properties. In particular, the deformation plays a significant role in determining the transformation of C and B in steels, and the consequences can be related to grain size. The objective of this work is to in-situ monitoring of microstructure evolution during thermo-mechanical treatment. In this technique, the deformation, full-potential (FP) KKR method has been used to calculate the lifetime of a metastable state with large system-size. We obtained the 3D critical nuclei with large volume in order to establish the validity of the LUMet technique. The main asset of austenitic stainless steels of HP type (Fe3Ni-C, containing Nb, Ti and Si) is their long-time ability to support high (1000 °C) temperatures. Their mechanical resistance is mainly due to the presence of semi-coherent carbide precipitation, especially NbC and MC. The kinetics of carbides co-precipitation has been studied experimentally (SEM, TEM) and modelled by Thermocalc / PRISMA software at different temperatures (600 – 950°C). Experimental analysis was used to identify physical parameters necessary for modelling; especially, the interface energy values for both NbC and MC, carbides, hardly available from literature, could be deduced from our TEM quantitative analyses. We have shown that at 700°C, values of gamma NbC = 0.26 mJ/m² and gamma M6C = 0.22 mJ/m² lead to a satisfactory description of co-precipitation kinetics in terms of particle mean size. Yet, the gamma values are strongly dependent on temperature, as well as the M6C equilibrium composition is. More than a hundred nanometers is obtained after quenching to room temperature. The Ms of the retained austenite is lower than room temperature and the TRIP effect is thus exhibited. By tuning the annealing temperature and time, the Mse of the austenite was adjusted approaching to room temperature, aiming to obtain best mechanical properties from the TRIP effect. The microstructure was simulated using Thermo-Calc and DICTRA, and Mse was predicted by a thermodynamic model. Both results showed good agreement with experiments.
The electronic spectra and atomic structures for the metal and oxygen environments were determined. Theoretical approaches for predicting these structures are calculated using density functional theory and projected augmented wave method as implemented in VASP package. In many cases the symmetric point defect configurations are found to be unstable against a symmetry-breaking distortion via the Jahn-Teller mechanism. An enhanced stability of titanium dumbbells is obtained for sub-stoichiometric TiC, where the dumbbells form clusters with the carbon vacancies. Possible migration pathways for point defects and their clusters in TiC are explored. The obtained electronic and phonon spectra of point defects, as well as their formation and migration energies, can be useful in spectroscopic characterization and atomistic modeling studies of TiC.

P-D8: Tracking Fe Solid Solution Level through the Whole Processing Route of Commercial Purity Aluminum Alloys: Guangxi Li1; Pavol Kordáň1; 1Royal Institute of Technology (KTH), Stockholm, Sweden

It has been found in the commercial purity aluminum alloys, the solid solution level of Fe has a profound effect on softening kinetics. In this paper, a through process modeling approach is employed to predict the Fe solid solution level during casting, homogenization heat treatment, hot rolling and annealing. The models' predictions were compared with the reported experimental results. It was expected this exercise could identify the missing links for the existing through process chain model framework to make reliable through process predictions of microchemistry evolution.

P-D9: Cation Ordering in Cuprice, CuOH: Yunguo Yang1; Claudio Louzada1; 1Brasília University, Brazil

CuOH is a solid solution of cuprous hydroxide, whose structure was established in computational studies of Cu–O–H compounds and rationalized as a hybrid between the structures of cuprite Cu2O and ice-VII H2O. In contrast to O–H compounds and rationalized as a hybrid between the structure was established in computational studies of Cu–OH are also reported. It was assumed (but not proved) that all the possible predictions on microchemistry evolution.

P-D10: Phase Field Crystal Simulation of Dislocation Annihilation Mechanism of Grain Boundary under Strain at High Temperature: Yun Jin1; 1Guangxi University

In this work, the annihilation process of subgrain boundary(SGB) and splitting of low-angle grain boundaries(SGBs) during plastic deformation near but below the melting point were simulated using the phase field crystal model. In this work we have calculated the nucleation and the annihilation of dislocations by gliding, which will result in the change of Burgers vector of dislocation and the exchange of the topological model to martensitic phase transformations, and also the generation of new dislocations and occurrence during annealing, and more specifically during recrystallization. Isolating the individual phenomenon and analyzing its effect through experimental analysis is a very hard task to achieve, if not impossible. In this research, we propose a new approach of modeling phase transformation based on nonlinear diffusion equations taking strains generated by defects. The results show, that the distribution of the interiors near the crack tip has a quite complicated character and the hydrogen distribution has qualitatively different character as compared with carbon distribution.

P-D11: An Analysis of the Thermal Properties of Metals: New Application of the Cluster Variation Method: Yasunori Yamada1; Tetsuo Mohri1; 1Tokohu University

Cluster Variation Method (CVM) is an efficient statistical tool to describe phase equilibria of a given system. The original formula was proposed by late Prof. Kikuchi, and he calculated phase transition behavior of ising model. We proposed a new approach to calculate the free energy of phonon. The advantage of the present scheme is that we do not have to calculate many samplings of the dispersion relation as conventional phonon calculations, and then we diagonalize only a small number of matrices which are defined by interatomic force constants for each cluster. Thery, we analyzed the thermal properties of metals.

P-D12: Simulation of Impurity Atom Segregation Formation in the Vicinity of Dislocations and Crack Tips: Alexander Nazauroz; Alexandre Mikheev; 1National Research Nuclear University (MEPhI); 2Moscow State University of Design and Technology

We use new equations for the interstitial impurity diffusion fluxes under strain to study impurity atom redistribution in the vicinity of crack tips or dislocations taking account the strain generated by mentioned defects. Two levels of equations are applied which are defined as follows: the first level, which we have developed a model in the framework of molecular static method taking into account an atom environment as near the interstitial site as for the saddle-point configuration. The saddle-point configuration is determined based on nonlinear diffusion equations taking strains generated by defects. The results show, that the distribution of the interiors near the crack tip has a quite complicated character and the hydrogen distribution has qualitatively different character as compared with carbon distribution.

P-D13: Evaluation of Parameters Influencing Recrystallization: A Simulation Study: Panthea Seperhardt1; Shahrzad Esmaeili1; 1Santa Clara University; 2University of Waterloo

Mechanical properties of polycrystalline materials are highly dictated by size and distribution of their grains. Thermomechanical processing, consisting of a cold-deformation process followed by an annealing treatment is a common technique to manipulate grain structure characteristics. Proper control of grain structure evolution requires deep understanding of the phenomena occurring during annealing, and more specifically during recrystallization. Isolating the individual phenomenon and analyzing its effect through experimental analysis is a very hard task to achieve, if not impossible. In this research, we propose a new approach of modeling phase transformation based on nonlinear diffusion equations taking strains generated by defects. The results show, that the distribution of the interiors near the crack tip has a quite complicated character and the hydrogen distribution has qualitatively different character as compared with carbon distribution.

P-D14: An Atomic and Mesoscopic Investigation of Nb Precipitation in NbZr Alloys: Maeva Cottura1; Emmanuel Clouet1; 1CEA

Nobium-containing zirconium alloys are currently used in nuclear power plants. Our goal is to understand Nb precipitation under irradiation and its consequences on the alloy behavior. Under irradiation, coherent niobium precipitates (b.c.c. structure) presenting a platelet shape lying in the basal planes appear in the Zr matrix (h.c.p.). In the present work, a novel criterion for determining the (Fe,Ni) grains was 8 nm. This new criterion for determining the (Fe,Ni) grains was 8 nm.

P-E1: Formation of Nanocrystalline (Fe,Ni,Co) Phases on the Sheet under High-Temperature Induced by Ball Collisions: Sergey Romankov1; Yun Chang Park2; Jeong Mo Yo1; Dong Jun Shin1; 1Chonbuk National University; 2National Nanofab Center

Surface severe plastic deformation induced by repeated ball collisions has recently received great attention because of its simplicity and efficiency. One of the main problems associated with ball treatment is impurities introduced into the material from the grinding media used in the milling process. However, contamination can be favorable and provide a new approach for the fabrication of nanocrystalline composite materials. In the present work, a source of Ni and Fe contaminations was deliberately introduced into the ball treatment process. We demonstrated that Ni and Fe contaminations could be used for preparing nanocrystalline magnetic alloyed steel sheets. During processing, Ni and Fe fragments were transferred and alloyed to the surface of a Ti sheet by ball collisions. The combined effects of the deformation-induced plastic flow and mechanical intermixing resulted in the formation of the (Fe,Ni) phase. The average size of the (Fe,Ni) grains was 8 nm.

P-E2: In Situ High Temperature Synchrotron Studies of Ceramics: Wintail Krives1; Pankaj Sarin1; Ryan Hagerty1; Zlatanir Apostolov2; Robert Hughes1; Zachary Jones1; 1University of Illinois at Urbana-Champaign; 2Royal Institute of Technology

Phase transformations in oxide ceramics can occur at exceedingly high temperatures up to 2,000°C and are often an important route by which the material properties are changed. However, it is difficult to study these transformations in situ. In this work, we discuss a new technique using synchrotron radiation. The experimental results were used to model and predict the behavior of these materials under extreme conditions.
The ECAPed specimens were again aged at 623 K, rare earth tungstates (3Ln 2O3•WO3) to 1350°C and rare earth reconstructive transformations have been observed in the ~860°C as well as the tantalates and niobates. Several weld trials. The thermal histories were then selected to vary experimentally measured temperature-time histories from then cooled using relevant conditions obtained from high Nb content and differing C content were austenized are welded. In this study, three experimental steels of gain insight into the optimal composition of steels which is of interest to quantify the decomposition products to through the heat-affected zones of Nb-bearing steels. It rolling and welding passes. However, Nb dissolved upon production of HSLA steels for the formation of carbonitrides Niobium is a common micro-alloying addition in the high temperature studies have been made of the displacive, and (hkl) d-spacings as a function of temperature. In situ fitting method, from which are extracted lattice parameters. Structural and mechanical properties of a Cu-3.15 mass% Ti alloy processed by a combination of heat treatment and thermo-mechanical treatment. We then examine the co-preservation phenomenon of Cu and Fe in an Al-Cu-Fe system. The precipitation kinetics are investigated with in-situ Small Angle X-Ray Scattering and Transmission Electron Microscopy. The corrosion behaviour is explored with metastable pitting tests on ex-situ samples. We demonstrate that DSC results in a significant improvement with metastable pitting tests on ex-situ samples. We demonstrate that DSC results in a significant improvement of the corrosion properties of these alloys thus enhancing their recyclability.

Industrial Applications

P-F1: Investigation of Nano-scale Precipitation Phenomena in Al-Fe and Al-Cu(Fe) Alloys Processed Via Direct Strip Casting: Thomas Donit1; Rajeev Gupta2; Ross Marceau1; Nicole Stanford1; Peter Hodgson1; Deakin University; 2University of Akron

The recycling of Al-Cu(Fe) alloys is often limited due to an increase in impurity content such as Fe during re-processing. Direct strip casting (DSC) is an emerging technology that shows tremendous potential to improve the recycling of these alloys. We demonstrate that the extremely rapid solidification (>1000°C/s) during DSC permits the retention of Fe in solid solution above equilibrium concentration. We first reveal that dissolved Fe results in significant precipitation strengthening in a binary Al-Fe alloy when submitted to subsequent thermo-mechanical treatment. We then examine the co-preservation phenomenon of Cu and Fe in an Al-Cu-Fe system. The precipitation kinetics are investigated with in-situ Small Angle X-Ray Scattering and Transmission Electron Microscopy. The corrosion behaviour is explored with metastable pitting tests on ex-situ samples. We demonstrate that DSC results in a significant improvement of the corrosion properties of these alloys thus enhancing their recyclability.

P-F2: Synergic Effects of Aging and Severe Plastic Deformation on Strength of a Cu-Ti Alloy: Shoda Ichij1; Tomotaka Miyazawa1; Toshiyuki Fujii1; Hiroyasu Horie1; Kazuki Kammuri1; Toshiyuki Omo1; 1Tokyo Institute of Technology; 2JX Nippon Mining and Metals

Structural and mechanical properties of a Cu-3.15 mass% Ti alloy processed by a combination of heat treatment and severe plastic deformation were investigated. Cylindrical shaped specimens were solution-treated and quenched into liquid nitrogen. The solution-treated specimens were aged at 723 K for 10 h and then were severely deformed by equal channel angular pressing (ECAP) for 4 Passes. The ECAPed specimens were again aged at 623 K, 673K, and 723 K for up to 8 h. A modulated structure along the (100) direction was found to be developed by aging. Grain refinement and twin formation occurred simultaneously during ECAP. The maximum hardness of 385 Hv was obtained from the ECAPed specimen after the secondary aging at 673 K for 30 min. It was found that the aging prior to ECAP gives a dominant contribution to the strength of the alloy.

P-F3: The Effect of Niobium on Austenite Decomposition for High Strength Linepipe Steels: Isaac Robinson1; Thomas Garcon1; Warren Poole1; Matthias Mittler1; 1University of British Columbia

Niobium is a common micro-alloying addition in the production of HSLA steels for the formation of carbonitrides that restrict recrystallization and grain growth during hot rolling and welding passes. However, Nb dissolved upon heating has been found to increase the hardenability of the steel via solute drag during austenite decomposition. These coupled effects produce a range of strength and toughness through the heat-affected zones of Nb-bearing steels. It is of interest to quantify the decomposition products to gain insight into the optimal composition of steels which are welded. In this study, three experimental steels of high Nb content and differing C content were austenitized then cooled using relevant conditions obtained from experimentally measured temperature-time histories from weld trials. The thermal histories were then selected to vary prior austenite grain size, precipitation/solution condition of Nb, and cooling rate during austenite decomposition.

P-F4: Toughening of High Strength Low Alloy Steel by Averaging and the Production of Yield Strength 900 MPa Grade Steel Plate: Zhaodong Li1; Xinjun Sun2; Zhigang Yang3; QiQiong Yang4; 1Central Iron and Steel Research Institute; 2Tsinghua University

Instead of off-line quenching and tempering (QT), on-line controlled rolling was employed to improve the toughness of low alloy steel with yield stress (YS) exceeding 900 MPa. Low carbon content ensured a high level of upper shelf energy, while ultratine martensite block transformed from pancaked austenite decreased ductile-to-brittle transition temperature and compensated the strength loss due to carbon reduction. Two mechanisms for the refinement of martensite block were proposed: One was the austenite grain refinement in the direction of thickness, and the other was the self-accommodation of martensite variants due to austenite grain hardening. In the plant trial of the YS900 MPa grade low alloy steel plate, more than 200 J of Charpy V-notch impact absorbed energy at 233 K was obtained by the on-line toughening process, which was much higher than that by the traditionally QT treatment.

P-F5: Deformation Substructure of Austenite Evaluated by Crystallographic Reconstruction and Its Influence on Microstructure Inheritance in Low Carbon Steels: Elodie Bouscar1; Nathalie Gey2; Lionel Germain1,2; Menenn Ben-Hay-Slam1;3; Sebastian Cobo2; David Fontaine1,3; 1Laboratoire d’Etude des Microstructures et de Mécanique des Matériaux, CNRS, Université de Lorraine, Ile du Saulcy; Metz, F-57045 CEDEX 1, France; 2Arcoromittal Maizières Research SA, 57283 Maizières-lès-Metz Cedex, France; 3Laboratory of Excellence for Design of Alloy Metals for Low-mass Structures (D’AMAS’ Labex), Université de Lorraine, France

Hot deformation of austenite in carbon steels is known to influence the microstructure of the transformation product [1]. However, contradictory conclusions rise up from the literature: Growth of martensite and bainite packets has been reported as well as refinement of the transformation product or formation of a granular structure. Actually the major problem relies on the lack of knowledge concerning the substructure of deformed austenite as the phase transformation prevent its direct observation. In this contribution, we apply our crystallographic reconstruction tool MERENGUE 2 [2] to evaluate the hot deformed substructure of a 0.06%C-2.4%Mn grade steel. The result shows interesting insight to analysis the complexity of the quenched microstructure. [1] N. Yu Zolotarevskii et al, Metal Science and heat treatment, vol.55,N°9-10, 2014 [2] German L., Gey N., Mercier R., Blanpain P., Humbert M., Acta Materialia (2012) 60, pp 4551-4562
Microstructural evolution during phase transformation is significantly dependent on the characteristics of nucleation and growth phenomena which is exploited by different manufacturing processes to tune effective properties through various microstructural changes. In this talk, we present a phase field model using Fourier spectral method with optimized approach for concurrent nucleation and growth to study microstructure evolution. The model handles both interface limited and diffusion limited growth and accommodates homogeneous and heterogeneous nucleation process. The nucleation and growth characteristics are dictated by the processing condition variations such as thermal history and external stresses which in turn determines the driving force for the transformation. We discuss the optimization strategies which were undertaken to address the modeling of the problem and present some results in the form of time dependent nucleation and growth rates and the characteristic microstructural outcomes such as grain size distribution as function of the processing conditions.

16:00
Application of the Extended GEB Model to Predict the Shape and Fraction Evolution of Ferrite as a Function of the Transformation Temperature for a Lean Steel Containing 1.9 w.t. % Mn: Zn yan1, Wei Xu2, Zhi-Dang Yang, Sibybrand van der Zwaag1, 2Faculty of Aerospace Engineering, TU Delft

In this work, the austenite-ferrite transformation in Fe-0.25Cr-0.35Mn alloy is studied on Gibbs-Energy-Balance considerations at the moving interface. Plate-lengthening, plate-thickening and isotropic growth is calculated. Growth with a plate-like morphology leads to the fastest reduction in Gibbs energy when the transformation takes place at 500°C and 600°C. On the contrary, isotropic (i.e. spherical) growth is preferential at 620°C. The concept, stasis for thickening of single plate is put forward. The conditions for the single bainitic shear stasis correspond nicely to the conditions for macroscopic stasis.

16:15 Break

Crystallography

TUESDAY PM
ROOM: CALLAGHAN
SESSION CHAIR: JIAN WANG, LOS ALAMOS NATIONAL LABORATORY

15:00 Invited
FCC-BCC Martensitic Transformations: Let’s Roll the Iron Atoms: Cyril Cayron1, EPFL

It is assumed that face centered cubic (fcc) to body centered cubic (bcc) martensitic transformations result from combinations of shears: the Bain distortion (1924) has been complemented by (shape and lattice) shear components in the phenomenological theory, and the physical models of Kurdjumov and Sachs (1930), Nishiyama (1934), or Bogens and Burgers (1964) are based on discontinuous shears and shuffles. We recently proposed a new model in which the distortion occurs directly without any ad-hoc assumption. The iron atoms move continuously as rolling balls from fcc to bcc positions in Pitsch, Nishiyama or Kurdjumov-Sachs orientations. The analytical matrices of distortion depend only on one parameter, and they are naturally decomposed into a product of Bain and a rigid body rotation. Surprisingly, they are not of shear type. This model permits to qualitatively discuss some microstructural characteristics of martensite such as the habit planes, microcrystal rotations, variant grouping etc.

15:30
Phase Field Modeling of Spinal Decomposition Fe-Cr Based Alloys: Thomas Barkat1, John Agrén2, Joakim Oddy3, Lars Hoglund1, 1KTH Royal Institute of Technology; 2KTH Royal Institute of Technology

In ferritic steels, especially with high Cr content, gets mixed with ferrite and cementite are allowed to intermix on a length scale of a pearlite grain. The “diffuse pearlite” recovers the local equilibrium phase fraction of ferrite and cementite without resolving the lamellar structure. An alternative approach allows to take into account the curvature and anisotropy. We will discuss the model assumptions and also give simulation examples for industrial applications, e.g. phase transformation in the heat affected zone in welding.

15:45
Optimisation Strategies for Phase Field Model of Concurrent Nucleation and Growth: Ramanarayan Harinathanpati1, Pawel Pulukiewicz1, David T Wu2, 1Institute of High Performance Computing Agency for Science, Technology and Research, Singapore

The crystallographic of intervariant boundary planes distribution in the latent martensite has been measured as a function of lattice misorientation...
In Situ Observation and Crystallographic Analysis of Martensitic Transformation in Low-carbon and Low-alloy Steel: Shoichi Nambu 1; Jyutaro Ogura 2; Junya Inoue 1; Toshihiko Koseki 1; 1The University of Tokyo

The development of a martensitic structure in a low-carbon and low-alloy steel was investigated using in-situ observation and crystallographic analysis, including the nature of variant selection. A low-carbon and low-alloy steel (Fe-0.18C-1.5Cr-3Ni) was prepared. After polishing the observation surface, the sample was heated up to 1623 K and then immediately gas quenched. During cooling, the changes in surface morphology were detected by conical laser scattering microscopy. The samples subjected to in-situ observation were also analyzed by EBSD. The results demonstrated that the initial stage of transformation involves the partitioning of the austenite grain into packets, along the growth direction of the transformation associated. The variant selection during transformation is not random, but is affected by the relationship between the shape deformation direction and the free surface.

Effect of Ms Gradient on Variant Selection of Lath Martensite in Ni Steel: Yutaka Kawanami 1; Jyutaro Ogura 1; 1The University of Tokyo

The effect of the gradient of the driving force for martensite transformation on the variant selection in lath martensite was quantitatively investigated by means of electron backscatter diffraction (EBSD) analysis in conjunction with in-situ conical laser-microscope observation. A diffusion couple composed of 22%Ni and 30%Ni ultra-low carbon steels was heat-treated at 1473K for several hours and then immediately gas quenched. During cooling, the changes in surface morphology were detected by conical laser scattering microscopy. The samples subjected to in-situ observation were also analyzed by EBSD. The results demonstrated that the initial stage of transformation involves the partitioning of the austenite grain into packets, along the growth direction of the transformation associated. The variant selection during transformation is not random, but is affected by the relationship between the shape deformation direction and the free surface.

Evolution of Microstructure during Tempering and Its Influence on the Mechanical Behavior of 2.25Cr-1Mo Bainitic Steel: Sylvain Dépinoy 1; Caroline Toffolon-Mascetti 1; Anne-Françoise Gougues-Lorenzon 1; Ernst Kozeschnik 1; Bernard Marini 2; François Roch 1; IAEA; 2Mine Research Laboratory; 3Vienna University of Technology; 4AREVA

This work focuses on the effects of heat treatments on the microstructure and consequently on the mechanical properties of a forged 2.25Cr-1Mo bainitic steel, and in particular on tempering conditions between 650°C and 725°C for times up to 24 hours. Carbide precipitation sequences have been investigated by means of quantitative synchrotron-based X-ray diffraction and complementary techniques reveal the nano-scale structural changes that occur and clarify the progression of microstructural evolution. These observations provide a comprehensive insight into martensite tempering in 4340 steel and insight into the location of alloying elements with respect to carbides. Such new perspectives will contribute to a better understanding of next generation steel alloying and processing concepts.

A New Martensitic Creep Resistant Steel Strengthened by MX Carbonitrides with an Extremely Low Coarsening Rate: Wei Yan 1; Ke Yang 2; Yoshiaki Toda 3; Sybrand van der Zwaag 1; 1Deutsches Eisenhüttenmuseum; 2Institute of Materials Research, Chinese Academy of Sciences; 3National Institute for Materials Science

An integrated computational alloy design approach based on thermodynamics and thermokinetics, a precipitation coarsening model and a genetic algorithm optimization routine is presented. This approach is applied to the design of a novel martensitic creep resistant steel strengthened by tailored MX carbonitrides which exhibit an extremely low coarsening rate. The model takes into account the gradients in the thermodynamic potentials at the precipitate-matrix interface and the diffusion coefficients of alloying elements involved. The experimental alloys quenched to a martensitic state and a high end commercial reference martensitic steel P92 are subjected to a fixed ageing temperature of 650°C for different times up to 1000 h. The microstructure evolution and resulting hardness at the intermediate stage are studied. Experimental results show that the newly designed steel displays a much slower decrease in hardness with time compared to that of P92, owing to the extremely low coarsening rate of the MX precipitates.

15:45
16:00
16:15 Break

Ferritic Martensites

TUESDAY PM
ROOM: NORDIC
SESSION CHAIR: EUGEN RABKIN, TECHNION

15:00 Invited
A New Look at Martensite Tempering in 4340 Steel: Alain Almudi 1; François Lesueur 2; Daniel Goughlin 1; Paul Gibbs 1; Dean Pierce 2; Bjorn Clausen 2; 1Colorado School of Mines; 2The University of Oxford

Quenching and tempering of medium carbon, low-alloyed steel martensites produces a wide range of useful mechanical property combinations. Although martensite in steels has been extensively studied over the century, opportunity still exists to further understand the subtle microstructural changes (e.g., carbon redistribution, transition carbide and/or cementite formation, and austenite decomposition) that occur during tempering with advanced characterization techniques. Here we characterize the location and distribution of carbon and other alloying elements in 4340 steel with atom probe tomography after quenching and tempering using a combination of small-angle x-ray scattering and 3D atom probe tomography. The number densities of G phase precipitates formed approach the highest densities of solid state precipitates observed in any alloy system.
Phonon field models have been widely employed to study the phonon-mediated transport properties of materials. However, the experimental verification of these models is often challenging due to the inherent complexity of phonon dynamics. In this talk, we will discuss recent advances in the development of experimental techniques for characterizing phonon transport in complex materials, including the use of advanced neutron scattering experiments and picosecond coherent spectroscopy. We will also present new theoretical insights into the role of phonon polaron formation in electronic transport.

16:05 Break

Ferroelectric & Magnetocaloric Materials

TUESDAY PM ROOM: CALLAGHAN
SESSION CHAIR: JEREMY MITCHELL, LOS ALAMOS NATIONAL LABORATORY

16:45 Invited
Formation of Monoclinic Nanodomains at the Morphotropic Phase Boundary of Ferroelectric Systems: Xiaogin Ren; Dong Wang; Yuzhui Wang; Xiaobing Ren; Xi'an Jiaotong University; The Ohio State University

The monoclinic (M) phase reported recently in ferroelectric solid solutions having compositions at the morphotropic phase boundary (MPB) between the tetragonal and rhombohedral phases could be responsible for the extraordinary piezoelectric properties of these materials, and its existence is under scientific debate. In this work we show by computer simulation that using a sixth order Landau free energy polynomial with small polarization anisotropy at the MPB and taking into account electroelastic and electrostatic interactions a new monoclinic structure consisting of M phase nanodomains is formed within a composition or temperature range enclosing the MPB. It is found that the M phase, even though unstable according to the Landau free energy, is stabilized by the long-range elastic and electrostatic interactions. A new phase diagram containing the M phase is established based on the simulation results.

17:15 Defect Strength and Strain Glass State in Ferroelastic Systems: Dong Wang; Duchao Yu; Yipeng Gao; Yu Wang; Xiaobing Ren; Xi'an Jiaotong University; The Ohio State University

It has been shown both experimentally and by computer simulations that stress-carrying defects can change a normal continuous strain glass transition into a first-order martensitic transformation on the other hand. We show in this paper that there exists a critical value of defect strength relative to the strength of MTs for creating a strain glass state. Using 14Ba55Ni51.5 as an example, we show that the equivalent Von Mises strain caused by anti-site defect with random distribution is 7/69 times of that created by the stress-free transformation strain of Martensitic phase in order to produce an R/B strain glass state. This finding may shed light on developing new strain glasses of much larger transformation strains for broader applications through defect engineering.

17:30 Origin of Monoclinic Distortion in Nanodomained Ferroelectrics: Liwei Geng; Yongming Jin; Yu Wang; Michigan Technological University

Monoclinic phases and nanoscale domains are commonly observed in ferroelectric solid solutions near morphotropic phase boundaries. In this work we employ complementary computational tools, namely, first principles density functional theory and phase field model, to investigate the interrelations between these two phenomena. We show that monoclinic distortion is a natural and essential consequence of nanodomains in ferroelectrics. Combining density functional theory calculations and phase field simulations, we demonstrate that the monoclinic distortion has an electrostatic origin due to the internal electric field, which is generated by the electric double layer of bound charges associated with polarization gradient across domain walls, and the monoclinic distortion increases with decreasing domain size. Thus, monoclinic phases are nanequilibrium “nanophases” in nanodomain ferroelectrics. Based on this finding, a morphotropic phase boundary-based phase diagram is constructed, where nanophases of monoclinic distortions are sandwiched between conventional rhombohedral and tetragonal phases, in agreement with recent experimental observations.

17:45 Analysis of Phase Decomposition in Al-Zn and Al-Zn-Cu Alloys by Phase Field Method: Victor Lopez-Hiriart; Erika Avila-Davila; Maribel Saucedo-Munoz; Jose Villegas-Cardenas; Arturo Ortiz-Marchal; Instituto Politecnico Nacional (ESIQIE); Instituto Tecnologico de Pachuca; Universidad Politecnica

The application of phase field method, based on the Cahn-Hilliard equation, was investigated to simulate the early stage of phase decomposition of Al-Zn-Cu alloys at different temperatures ranging from 400-600 °C. The results indicate that the initial phase decomposition is initiated by the growth of the alloy near the eutectic compositions. These results provide insights into the phase field method's ability to model the decomposition of alloys at high temperatures in near-eutectic compositions.
increases, the phase transformation temperatures tend to decrease. This study aims at considering the influence of the degree of order or the level of residual stresses on the shift of transformation temperatures. This understanding could help to improve the overall efficiency of refrigeration devices, in particular by allowing an optimal grading of the magnetocaloric material.

17:45 Invited
Improved Magnetocaloric Performance of Polycrystalline Ni2MnGa Alloys Subjected to Isobaric Thermal Cycling by Introduction of Preferred Orientation: Michael McLeod1; Bhaskar Majumdar1; Sven Vogel1; Donald Brown2; H. Matthias Reiche3; 1New Mexico Institute of Mining and Technology; 2Los Alamos National Laboratory

Magnetocaloric materials take advantage of large changes in magnetic entropy that accompany ferromagnetic to paramagnetic transitions, to bring about refrigeration in the solid state. Both experimental work and theory suggest that the magnetocaloric effect is greatest if a structural transformation (e.g., martensite to austenite) occurs simultaneously with the magnetic transition. It has been observed that there is as much as 80% increase in magnetocaloric performance when samples are subjected to thermal cycling between the austenite and martensite phase under constant compressive stress. The rationale is that the favorable twin variants would permit easier alignment of magnetic domains, and thereby produce greater magnetization in the ferromagnetic martensite state.To answer the influence of the texture on the improved properties after isobaric cycling, we utilized neutron texture analysis of samples after treatment as well as during in situ texture measurements at temperatures between room temperature and 100°C to simulate the thermal cycling.

18:15 Break

Microstructure Development in Steels I

TUESDAY PM ROOM: NORDIC SESSION CHAIR: PETER HODGSON, DEAKIN UNIVERSITY

16:45 Invited
Mechanism of Ultra-fine Microstructure Formation during Ultrafast Annealing of a Medium-Mn Steel: Artem Arlawar1; Mohamed Goun1; Alain Hazotte1; Olivier Bouaziz2; Frédéric Kegel3; 1ArcelorMittal/Université de Lorraine; 2ICMCB, CNRS UPR 9048; 3LEM3, Université de Lorraine, CNRS UMR 7239, 1ArcelorMittal Research and Development

The medium Mn steels are a topic of interest from both practical and scientific point of view. Many studies were focused on the microstructure characterization, but only some of them addressed the mechanisms of austenite formation and stabilization. Hence, there are still remaining questions regarding the link between the obtained austenite fraction and stability and the austenite formation including both the morphological and kinetics aspects. In this work, different ART annealing treatments were performed on a cold rolled 0.1C – 4.7Mn (wt.%) steel. SEM and TEM observations as well as XRD and magnetic measurements were done to characterize the resulting microstructures. Microstructure evolution was analyzed as a function of soaking time: precipitation and dissolution of cementite; austenite nucleation, growth and stabilization. The experimental observations were compared with the predictions from thermodynamic calculations. Based on the obtained results, a mechanism of austenite formation and stabilization during ART annealing is proposed.

17:15 Retained Austenite Fractions in Medium Mn Steels with Varying Mn, C, Al, Si and Cr after Intercritical Annealing: Emmanuel De Moor; Singpong Kong; John Speer; 1ASPRC Colorado School of Mines; 2Colorado School of Mines

Medium manganese steels are being vigorously issued for automotive applications requiring high strength and formability. Retained austenite fractions predicted to be stable at a given intercritical annealing were calculated for such steels with varying Mn, C, Al, Si and Cr additions, as the basis for designing a series of experiments. The austenite formation and stabilization of each phase at the intercritical temperature were obtained under the assumption of ortho-equilibrium solute distribution using Thermo-Calc® with two databases. The fraction of martensite transformed during quenching was calculated based on the austenite chemical composition. The effects of alloying additions on the retained austenite fraction with varying annealing temperature are reported and discussed in terms of four critical phase transformation temperatures. Selection of experimental steels designed based on this approach is compared with the model results.

17:30 Effect of Mn and C Segregation on the Microstructure Development of Q&P Steel: Fandeck Hay Akbar2; Kees Kwakemaak3; Jilt Sitensia4; Maria Santofimia4; 1Deft University of Technology

Optimum mechanical properties in Quenching and Partitioning (Q&P) steels are reached by adequate austenite stabilization and a limited fraction of fresh martensite. Theoretical understanding of the Q&P process has allowed the design of alloys and thermomechanical parameters to reach the desired microstructures in steels with homogenous chemical compositions. However, homogenous chemical compositions are rarely the case in industrial steels. This research is focused on the microstructural development during the Q&P process of a 0.3C-1.6Si-3.5Mn (wt. %) steel with an inhomogeneous chemical composition by applying in-situ EPMA, SEM and EBSD techniques. It was found that during the initial quenching of the Q&P process, the Mn/C-poor regions transform to martensite and thin films of austenite are stabilized via C-partitioning process. However, relatively large blocks of austenite, which form in Mn/C-rich regions, have low chance to become stable and might transform to fresh martensite during final quenching, which is detrimental for ductility.

17:45 Ultrafast Heating of Advanced High Strength Steels: Roumen Petrov1; Athina Poup1; Doreen De Knijn1; Leo Kestens1; 1Ghent University

Microstructure, texture and the tensile properties of a 70% cold rolled advanced high strength steel with microstructure of ferrite and pearlite were studied after reheating with different heating rates and subsequent quenching. Sub-size tensile samples were reheated with rates of 10, 150, 500 and 1000°C/s to temperatures below Ac1, between Ac1 and Ac3 and above Ac3 and subsequently quenched without isothermal soaking and with isothermal soaking of 30 s and 60 s. By following the microstructure and texture changes it was found that after reheating with 500°C and 1000°C the recrystallization was suppressed and the alpha-gamma phase transformation starts in non-recrystallized or partially recrystallized matrix. Significant grain refinement and increase of both tensile strength and elongation was observed in the samples after ultrafast heating and subsequent quenching without isothermal soaking. The isothermal soaking erased the grain refining effect of the ultrafast heating even if it was as short as 30s.

18:00 Bainite Formation Kinetics and Properties of an Ausformed 0.7wt% Carbon Plate: James Saragosa1; Fateh Fazel2; Jason Lo1; Gianluigi Bott01; 1Carnett Materials, 2McMaster University

Carbide-free bainite formed below 275°C consisting of nanoscale bainitic ferrite and retained austenite demonstrates strength beyond 2GPa; so-called super bainite. A modified super bainite alloy with 0.7wt% carbon and cobalt addition was designed to achieve faster bainite formation and improved toughness. Dilatometric study was carried out to measure transformation start time, rate and final fraction of bainite and to optimize processing conditions. Different thermo-mechanical cycles varying ausforming parameters, transformation temperature and time were carried out using pilot-scale facilities to produce prototype plates. Microstructure and properties, namely tensile and Charpy impact toughness of the plates, for various processing conditions were assessed. Electron backscattered diffraction microscopy was used to characterize the effects of ausforming on bainite morphology and variant selection. Guidelines for alloy design and processing of super strong bainite plates with adequate toughness are discussed based on thermodynamic and kinetic concepts.

18:15 Break

Plenary 4

TUESDAY PM ROOM: EMERALD BALLROOM SESSION CHAIR: LONG QING CHEN, PENN STATE UNIVERSITY

18:30 Plenary
Cluster Variation Method as a Theoretical Tool for the Study of Phase Transformation: Tetsuo Mohri1; 1Tohoku University

Cluster Variation Method (CVM) has been applied to various phase transformation studies. The free energy within CVM is approximated by a finite set of cluster probabilities, and the larger the basic cluster is, which is the largest cluster considered in the entropy, more accurate result one can obtain. The computational burden associated with the introduction of larger basic clusters has been relieved along with the development of high performance computers. Major application of the CVM is the first-principles phase equilibria calculations including the stability analysis in k-space leading to the concept of spooral ordering. The extension of the CVM to time domain has been attempted in two directions. One is the atomistic kinetics study based on Path Probability Method, and the other is CVM-PTM study which leads to multiscale calculations. Recent development of Continuous Displacement CVM opens up a possibility of unified study of reative and displacive transformations.
Diffusional phase transformations have been extensively studied and modeled in relatively simple situations where they occur as a unique phenomenon, in isothermal treatments in a macroscopically homogeneous composition field. This sound corpus of knowledge can be used in more realistic situations where several transformations compete, and where long range diffusion occurs. Examples of such situations will be taken to illustrate the potential of physically based modeling to treat quasi-industrial situations. The coupling of allotropic phase transformations and precipitation, the precipitation kinetics in a long range chemical flux, the coupling between grain growth and precipitation and the occurrence of abnormal grain growth, the coupling between precipitation recovery and recrystallization will be applied to the understanding of microstructure generation in microalloyed steels, to defect generation in forgings and extrusions, and to annealing kinetics in dissimilar welds.

Austenitization

11:30 Invited Effect of Heating Rate and Microstructural Scale on Austenitization: Kestler Clarke1; Amy Clarke1; Robert Hackenberg1; Chastity Vigil1; Christopher Van Tye2; Los Alamos National Laboratory; 1Colorado School of Mines

The effect of heating rate and prior microstructure on austenitization kinetics has been evaluated for induction hardened steels with ferrite-pearlite or spheroidized initial microstructures. Initial microstructural conditions were used to vary microstructural scale. Diatomite at various heating rates was used to assess austenitization heat treatments. As-quenched hardeness were determined as a function of heating rate and maximum temperature for each microstructural condition. The initial microstructural scale and alloy composition are shown to cause significant variation in the as-quenched microstructure and material properties, particularly for the highest heating rates. Diffusion simulations support the observed microstructural and material property differences observed between the various initial microstructures and the plain carbon and alloy steel compositions.

12:00 Study of Austenitization Kinetics by In Situ Synchrotron X ray Diffraction for Different Initial Microstructures: Benoît Demaend1; Vladimír Eš1; Quentin Le Bihan1; Moukrame Dehman1; Julien Texeira1; Guillaume Gearder1; Sabine Denis1; Thomas Saurma1; Elisabeth Reby-Gautier1; 1Institut Jean Lamour - UMR 7198 CNRS - Université de Lorraine; 2MINES ParisTech; 3Ascometal - CREAS

The formation of austenite during slow and fast heating (0.25–100°C/s) was investigated for three initial microstructures (ferrite-pearlite, bainite or tempered martensite) of low-alloy steel. New observations from high-energy X-ray diffraction (HEXRD) concern in-situ tracking of the amount of all phases: not only ferrite and austenite, but also cementite. Moreover, results reveal two kinetics regimes of austenite formation, corresponding to simultaneous transformation of ferrite and cementite, followed by progressive disappearance of remaining ferrite for each initial microstructure. While this is well known for ferrite-pearlite, it is not yet documented for bainite and tempered martensite. In addition, lattice parameters evolution were characterized. These measurements reveal a non-linear evolution with temperature for the retained austenite in the initial bainite microstructure. Also, the time required to homogenize the austenite is examined. Microstructure evolution calculations based on a diffusion-controlled mechanism helped rationalize the differences observed between the three initial microstructures.

11:00 Break
12:15 Influence of Heat Treatment on the Stability of Austenite in a High Co-Ni Secondary Hardening Steel: Manna Gruber1; Gerald Ressl1; Manfred Wiesner2; Stefan Plüger2; Stefan Mansner2; Reinhold Ebner2; Materials Centre Linz Forschung GmbH; 2Böhrer Edelstahl GmbH & Co KG

In high Co-Ni steels thin layers of austenite have beneficial effect on toughness properties. As the positive influence on toughness is rather related to reverted austenite than to retained austenite layers, this work presents an experimental study corroborated with thermodynamic simulation to describe the differences between reverted and reformed austenite and their evolution during tempering. To this end chemical composition and the phase fractions of reformed and reverted austenite and martensite were characterized by atom probe tomography and transmission electron microscopy at different stages of tempering. Additionally, correlation of these experimental findings with microstructure simulations allowed a more detailed understanding of austenite evolution. The investigations revealed that the composition of retained austenite remained unchanged during tempering because of diffusional inability of austenite on the one hand and that the reverted austenite was mainly formed as a result of nickel diffusion in martensite towards the retained austenite layers.

12:30 The Growth of Austenite from Martensite during Continuous Heating in a Fe-0.1C-2Mn Steel: Koutaro Hayashi1; Toshinobu Nishibata1; Masato Enomoto2; 1Nippon Steel & Sumitomo Metal Corporation; 2Ibaraki University

The growth of austenite from martensite during continuous heating was studied at a heating rate of 28 °C/s in an Fe-0.1C-2Mn alloy. Under the assumption that austenite precipitated at martensite lath boundaries with a 200 nm thickness, the planar growth of austenite/martensite interface was simulated by DICTRA. The volume fraction of austenite determined by dilatometry was more detailed than to retained austenite layers, this work presents an experimental study corroborated with thermodynamic simulation to describe the differences between reverted and reformed austenite and their evolution during tempering. To this end chemical composition and the phase fractions of reformed and reverted austenite and martensite were characterized by atom probe tomography and transmission electron microscopy at different stages of tempering. Additionally, correlation of these experimental findings with microstructure simulations allowed a more detailed understanding of austenite evolution. The investigations revealed that the composition of retained austenite remained unchanged during tempering because of diffusional inability of austenite on the one hand and that the reverted austenite was mainly formed as a result of nickel diffusion in martensite towards the retained austenite layers.

12:45 Growth of Austenite:Ferrite Boundaries at a Late Stage of Austenitization in an Fe-0.1C-3Mn-1.5Si Alloy: Ran Wei1; Masato Enomoto2; 1International Research Institute for Steel Technology, Wuhan University of Science and Technology; 2Ibaraki University

The growth of austenite at a late stage of austenitization was studied with focus on the possible shrinkage of austenite which was discussed in a previous paper [R. Wei et al, Acta Materialia, 61(2013): 967]. The overall volume fraction of austenite which nucleated at martensite lath boundary did not decrease by holding at longer times than previously. The result of STEM-EDX analysis in an Fe-0.2C-5Mn alloy that a high Mn concentration region formed near the boundary in austenite essentially stopped. The conditions in which the boundary to the inside Mn-lean region after the growth of austenite lends support to this observation. The shrinkage high Mn concentration region formed near the boundary in austenite remained unchanged during tempering because of diffusional inability of austenite on the one hand and that the reverted austenite was mainly formed as a result of nickel diffusion in martensite towards the retained austenite layers. The re-austenitization from spheroidized microstructure during intercritical annealing was studied in a Fe-0.1C-3.5Mn alloy, in which the cementite is enriched with Mn. The austenite grains dominantly nucleate at the intergranular cementite but not at the intragranular cementite. The austenite growth is accelerated by increasing annealing temperature. The simulation by DICTRA, assuming local equilibrium condition, reproduces the austenite growth kinetics at various tempering temperatures. The predicted C and Mn activity profiles show that, when the cementite Mn content is high, the austenite growth is essentially composed of two stages: a partitioning growth controlled by Mn diffusion in ferrite, and a stage controlled by Mn diffusion in austenite for final equilibration. The partitioning growth results in homogeneous carbon distribution within austenite, which is supported by NanoSIMS carbon mapping. A parametric study predicts that if the cementite Mn content is sufficiently decreased, the initial negligible-partitioning growth controlled by carbon diffusion in austenite becomes significant.

12:15 Phase Field Modeling of Cyclic Phase Transformations in Low-carbon Steels: B. Jiang1; H. Chen1; Matthias Militzer1; 1University of British Columbia; 2Tsinghua University

A phase field model has been developed to describe microstructure evolution during cyclic phase transformations for two low-carbon steels (Fe-0.1wt%C, Fe-0.1wt%C-0.5wt%Mn). The austenite-ferrite phase transformations are assumed to occur under negligible-partitioning condition for Mn and only long-range diffusion of carbon is considered. A Gibbs-energy dissipation model has been integrated with the phase field model to describe the stagnant stages during cyclic phase transformations. Experimental results, e.g. length of stagnant stages and the cyclic phase transformation kinetics, have been successfully duplicated with 20 phase field simulations.

12:30 Invited Element Partitioning at Reaction Interfaces in a Reactive Diffusion Setting: Spinel Layer Growth in the MgO-Al2O3 System, Experiment and Thermodynamic Modeling: Stefan Marsoner1; Peter Jordek1; Erwin Povoden-Karadeniz2; Gerlinde Huber1; 1University of Vienna; 2Institute of Physics of Materials, Academy of Sciences of the Czech Republic, 1Charles University Prague; 2Technical University Vienna

Corona structures formed by reactive diffusion are common phenomena in rocks. From their phase content, composition patterns, and microstructure the formation could be reconstructed, if the underlying processes are calibrated. We report on experimental layer growth of magnesiowüstite spinel (MgAl2O4) at periclase-cordierite interfaces, aiming at identifying and quantifying these processes. Periclase and cordierite were contacted and annealed at 1623K and ambient pressure for 5 to 160 hours. Along the contact a spinel layer formed showing corona growth. The spinel exhibits monotropic decrease in Al content from the spinel-cordierite interface to the spinel-periclase interface, where local spinel-periclase equilibrium is closely attained. In contrast, at the spinel-cordierite interface the Al content increases with run duration approaching but never attaining local-equilibrium. Based on the experimental data a thermodynamic model accounting for dissolution due to long-range diffusion, interface migration, and generation/annihilation of vacancies at reaction interfaces is calibrated.

12:45 Invited Evolutionary Microstructures, Deformation, and Fracture in Solid Oxide Fuel Cell Anode Materials: Mikko Haataja1; 1Princeton University

Energy conversion processes in solid oxide fuel cell (SOFC) materials are strongly affected by a nonuniform coupling between mass/charge transport, heat transport, and morphology at nanometer and micrometer length scales. This multi-scale multi-component system. Furthermore, under continuous operation, these complex morphologies and local compositions evolve over time in response to a multitude of physical, chemical, and mechanical cues at elevated temperatures. In the first part of my talk, I will present our recent work on quantifying coarsening kinetics of metallic particles within SOFC cermet microstructures based on large-scale in situ interface model simulations. In the second part of my talk, I will focus on the development of elastic stresses and resulting mechanical failure in SOFC cermet materials driven by re-oxidation of the metallic particles by employing a diffuse-interface fracture mechanics model within a finite deformation framework.
Displacive Transformations in Non-Ferrous Alloys

Wednesday AM | Room: Callaghan Session Chairs: Yu Wang, Michigan Tech; Yunzi Wang, Ohio State University

11:30 Invited Stress-induced Transformations During the Compression of a Ti 1033 Alloy: Manur Ahrends; Adzir Gazder; Ahmed Saleh; David Wexler; Elena Pereloma; University of Wollongong

Realisation of transformation-induced plasticity and/or twining-induced plasticity is a promising pathway to combat the low ductility of Ti alloys. Near-Ti 10V-3Al-3Fe (wt.%) alloy containing after thermo-mechanical processing different fractions of α phase was compressed to 40% reduction. Detailed microstructure evaluation was carried out using high resolution scanning transmission electron microscopy and electron back scattering diffraction. For the first time, deformation-induced β→α and β→α transformation products together with {332}<113>β and {112}<111>β twinning systems were simultaneously detected in a meta-stable β alloy with the previous phase. The effects of the strain rate and β phase stability on the preferential activation of these reactions were analysed. It was found that increasing the rate or increasing the temperature leads to a decrease in the β phase stability and twin rate. On the other hand, compared to [112]<111>β, {332}<113>β twinning was more prominent in the dominant at low strain rate and twinning fraction was enhanced with increase in strain rate.

12:00 In Situ Investigation of Plasticity Mechanisms in β-Metastable Titanium Alloys Presenting Synergetic TRIP and TWIP Effects: Matthieu Marteleur; Pascal Jacques; Frédéric Primot; Hosni Issidi; Steven Van Pletgem; Université Catholique de Louvain; Chimie-Paritext; Paul Scherrer Institute

β alloys with plasticity driven by dislocation glide suffer from a lack of work hardening, which is most of the time a major drawback. Recently, several β-metastable Ti grades have been designed to exhibit simultaneous TRIP and TWIP effects in order to increase mechanical properties of as-quenched β phase. Indeed, work hardening rates never reached before by Ti alloys seem to result from the activation of α stress-induced metastable (SIM) phase as well as from mechanical twinning with α phase precipitation. In this work, we investigate the mechanisms of β→α and β→α SIM transformation during tensile loading with in-situ synchrotron XRD, EBSD and TEM microscopy in as-quenched Ti-12 wt.% Mo alloy, as well as their own role in the global improvement of the mechanical properties.

12:15 Stability of the Two-phase Microstructure of Shocked Zirconium: Guozhi Dong; Jane E. Pargellis; Ellen Cerreta; Bjorn Clausen; Los Alamos National Lab

The microstructure of two-phase (α+e) shocked zirconium was studied in-situ during heating with high energy X-ray diffraction techniques. The volume fraction of the metastable α phase was monitored as the reverse phase transformation occurred: the start and finish temperatures being 470K and 550K, respectively, during heating at 3K/min. Phase strains were monitored and separated in terms of thermal expansion and mechanical strains due to local phase constraints. Stresses in the α zirconium were estimated using a hydrostatic component (order of -0.5GPa) and uniaxial component (order of -1GPa) along the e-axis. A high distortion was observed in both the α and e phase in the as-shocked state. The distortion of the e phase decreased preceding the reverse transformation suggesting that it is the presence of the high concentration of defects in the e phase that retarded the reverse transformation to the stable α phase.

12:30 Aging and the β-to-α Transformation in Pu-Fe Alloys: Jeremy Mitchell; Franz Freibert; Terence Mitchell; Daniel Schwartz; Los Alamos National Laboratory

Face-centered cubic β-phase plutonium that has been stabilized by very low temperature with small amounts of Ga (≤3 at. %) will transform to monocrystalline α at ~100°C. This martensitic transformation results in a very large volume contraction, has a large temperature hysteresis, and saturates at ~30% of the volume change at higher temperatures. The reverse transformation is characterized a mixed mode. By the solute diffusion across omega/beta interface. The microstructure is characterized a mixed mode.

12:45 Heating-cooling Asymmetry in the β→α Transformation in Plutonium: Clausius-Clapeyron Considerations: Daniel Schwartz; Jeremy Mitchell; Los Alamos National Laboratory

On heating, the regions of plutonium allotropic stability and phase transformation onset are well defined. Cooling behavior is quite different, and the β→α cooling transformation displays a burst character, with an anomalously large temperature hysteresis of the β→α transformation products together with {332}<113>β and {112}<111>β twinning systems. The phase structure of this phase transformation will be described in detail. Pu phase transformations were examined within the Clausius-Clapeyron relation to get information about the temperature-pressure behavior of Pu near its critical points. Compared to the other solid-state transformations in the Pu system, the Pu→α transformation displays a burst character, with an anomalously large temperature hysteresis, suggesting that a pressure-temperature mechanism may be operating to produce the burst phenomenon. The model describing will be described in detail. DC arguments do not explain why bursting only occurs upon cooling, but recent work examining the detailed atomic movements involved in the δ→α to structure provide insight into the asymmetry.

Microstructure Development in Steels II

Wednesday AM | Room: Nordic Session Chairs: Eric Jaegle; Max-Planck-Institut für Eisenforschung; Amy Clarke; Los Alamos National Laboratory

11:30 The Control of Transformation in Steels Through Conventional and Novel Processes to Produce Novel Products: Peter Hodgson; Ilana Timokhina; Hossein Beladi; Nicole Stanford; Deakin University

Steel products rely on the control of the phase evolution to develop microstructures suitable for a wide range of applications. The nature and scale of the transformation phases and the evolution of precipitates and solutes are all important in determining the strength, ductility and toughness as well as other properties. This paper will review recent work related to the control of the microstructure under conventional deformation and cooling conditions as well as the more radical conditions experienced under new processes such as strip casting. In the latter case the cooling rates during the initial phase transitions are extremely rapid and lead to unique microstructures both in terms of the nature of the phases but also in the scale of the transformed solutes. These can have a dramatic effect on downstream processing as they interact with the deformation and precipitation reactions. For instance, there are two major aims. The first is to reduce the scale of the microstructure to under ultrafine or nanoscale transformation products, while the second is to control the evolution and size and stability of the precipitates.

12:00 Advanced Experimental Approach Using EBSD to Quantify the Evolution of Precipitate Size in X80 Linepipe Steel: Jennifer Reichert; Matthias Militzer; Warren Poole; The University of British Columbia

The graded microstructure in the heat affected zone (HAZ) of state-of-the-art girth welded pipelines consists primarily of complex bainitic transformation products. The details of these HAZ microstructures depend on the welding technique and the associated thermal profiles that also affect the amount of Nb in solution as a function of the distance from the fusion line. An X80 linepipe steel has been investigated and tools were established to characterize and map complex bainite microstructures occurring in the HAZ. Electron Backscatter Diffraction (EBSD) was used to distinguish bainitic transformation products in Nb in solution solid state transformation (NBSST) from Nb in solution solid state transformation (NBSST). Thick metallographic sections displaying both Nb in solution solid state transformation (NBSST) and Nb in solution solid state transformation (NBSST) were studied using EBSD. The EBSD results showed that Nb in solution solid state transformation (NBSST) was the main mechanism occurring in the HAZ. Linepipe Steel products rely on the control of the phase evolution to develop microstructures suitable for a wide range of applications. The nature and scale of the transformation phases and the evolution of precipitates and solutes are all important in determining the strength, ductility and toughness as well as other properties. This paper will review recent work related to the control of the microstructure under conventional deformation and cooling conditions as well as the more radical conditions experienced under new processes such as strip casting. In the latter case the cooling rates during the initial phase transitions are extremely rapid and lead to unique microstructures both in terms of the nature of the phases but also in the scale of the transformed solutes. These can have a dramatic effect on downstream processing as they interact with the deformation and precipitation reactions. For instance, there are two major aims. The first is to reduce the scale of the microstructure to under ultrafine or nanoscale transformation products, while the second is to control the evolution and size and stability of the precipitates.

12:00 Microstructure Evolution During Thermomechanical Processing of a High Strength Sheet Steel: Doug Boyd; Hayley Scott; Luana Siqueira; Gagan Sidhu; Fateh Fazel; Xiang Wang; Keith Pilkey; Queen’s University; CatterMatMATERIALS; McMaster University

The formation of high strength sheet steel is sensitive to variations in the microstructure on several length scales. The goal of this research is to delineate the microstructural evolution during thermomechanical processing (TMP) of a commercial hot-rolled stretch-flangeable steel (low-C, microalloyed, 780 MPa tensile strength) to understand how microstructure development during cooling schedules were characterized by OM, SEM, and TEM, and austenite transformation kinetics were studied by deformation dilatometry. The microstructures are a complex mixture of polygonal ferrite (PF), granular bainite (GB), lath bainite (B), martensite/austenite (M/A), and ‘coarse’ (~100 nm) and ‘fine’ (~30 nm) (Ti,Nb,CN) precipitates. A pancaked (unrecrystallized) austenite condition promotes the formation of PF to higher cooling rates and the formation of GB to higher temperatures. The cooling temperature controls the relative amounts of B and M/A, as well as the type and distribution of precipitates.
Based on these insights, TMP schedules can be designed to produce desired final microstructures and properties.

12:30
Formation Mechanism of Acicular Ferrite during the Heat Treatment of High Strength Low Alloy Steel: Yongchang Liu1; Lei Shi2; Yan Chen2; Chenxi Liu2; Liming Yu1; Tianjin University

Although Acicular ferrite (AF) has been widely considered one of the most attractive candidate microstructures for HSLA steels, the formation mechanism has not been clarified up to now. It this approach, the formation mechanism of acicular ferrite was firstly discussed according to the effect of dissolution and precipitation of Nb on the subsequent phase transformations of undercooled austenite. Then the effects of different intercritical quenching and intercritical normalizing treatments of the HSLA steels were explored. It is recognized that the morphology of AF exhibits a lath-type when an intercritical normalizing treatment is adopted, instead of the formation of polygonal and acicular ferrites after a traditional normalizing treatment. Further intercritical tempering treatment would bring a fibrous and tempered AF structure. The formation mechanism of the lath-type, fibrous acicular ferrites and their morphological evolution are addressed in view of diffusion- or interface-controlled growth mechanism.

12:45
Control of Nano-scale Mx Dispersion in Grade 91 Steel through Thermo-mechanical Treatment: Benjamin Shassere1; Yukinori Yamamoto2; Sudarsanan Babu1; 1University of Tennessee; 2Oak Ridge National Laboratory

Detailed microstructure characterization of Grade 91 (modified 9Cr-1Mo, ASTM A387) steel was performed after a thermo-mechanical treatment (TMT). This process includes rolling at temperatures above or below the γ/γ phase field with varying plastic strains, followed by an isothermal aging in the α+γ phase field, which aims at enhancing very fine MX (M: Nb and V, X: C and N) dispersion in the base metal. Such pre-existing MX precipitates are expected to be stable during welding and improve the creep resistance of the fine grained heat affected zone in contrast to standard “normalization and tempering” heat-treatment. Dense MX precipitates were dispersed readily after TMT, resulting in improving cross-weld creep properties in comparison to standard heat-treated samples. The paper will discuss the competition between MX and M23C6 precipitation, as well as, their correlation to high-temperature strengthening mechanisms. Research sponsored by US-DOE, Office of Fossil Energy, the Crosscutting Research Program.

13:00
The Contribution of TEM-EELS to Understanding the Behaviour of Carbon in the Fe-C System: B. Shalchi-Amirkhiz1; Fateh Fazeli1; Chad Sinclair; Colin Scott2; 1CarnegieMATERIALS

Carbon is the most important addition element in determining the physical properties of structural ferrous alloys. Despite this, there remains much to be discovered about the basic behaviour of interstitial carbon atoms and the stable and metastable iron-carbides that form. Driven by recent improvements analytical techniques, important advances have been made in the past decade. This is particularly true for the study of carbon in non-equilibrium environments like quenched martensite, supersaturated ferrite and during cementite decomposition. Here, we provide an overview of an important analysis technique used for carbon quantification, Electron Energy Loss Spectroscopy (EELS) in the TEM. In particular, it will be shown that the near edge fine structure observed in EELS spectra can be interpreted to provide not only quantitative (i.e. atomic concentration) but also chemical (coordination number, bonding) information in the Fe-C system. Applications including martensite, Fe3Cp thin films and third generation automotive steels will be discussed.

13:15
Impulse Internal Friction Analysis of High-damping Fe-Mn Alloys: Sunmi Shih1; Won Seok Oh1; Jongbae Jeon1; Bruno De Cooman2; 1Pohang University of Science and Technology; 2Pohang University of Science and Technology; 3Korea Institute of Industrial Technology

Fe-Mn alloys are being considered for the production of automotive panels. Their high-damping properties are expected to reduce substantially noise levels and prevent fatigue failures. Their use requires the precise matching of the material's maximum damping relaxation peak with the in-service vibration frequency and temperature. The damping spectrum of high damping Fe-Mn is characterized by diffusion-controlled phase transformations, martensitic transformations and magnetic transformations. The damping properties of Fe-Mn high-damping alloys and the effect of critical alloying additions, such as carbon, were characterized by means of the impulse internal friction technique and dilatometry. The results showed that the movement of magnetic domains contributed significantly to the damping. The thermo-elastic martensitic transformation was found to coincide with the anti-ferromagnetic phase transformation. The influence of the strain amplitude on the damping of Fe-Mn alloys was studied, and effects related to interface break-away were clearly observed.
Thur 2 July 2015

Plenary 6

08:30 Plenary
Importance of Atomic Scale Modeling in Describing and Predicting Properties of Solids and Interfaces: Gogeb Sawatzky; University of British Columbia

My field of solid state physics and strongly correlated electron systems seems far removed from the real world dealt with in most of the presentations at this meeting, so one might wonder if what I have to say is of any use to this broad audience. However perhaps now that multi-scale modelling has become very fashionable also in the descriptions of construction materials maybe we can in fact learn from each other. In my world the biggest problem is to deal with strong electron correlation effects which we believe are at the source of the wide diversity of physical properties of materials involving 3d transition metal atoms and rare earth elements resulting in things like strongly localized magnetic moments, quantum spin fluctuations, high temperature superconductors, and a multitude of phase transitions involving the lattice, spin, and even the atomic quadrupole moments. Obviously atomic physics in such systems plays an equally important role to that of the translational symmetry and band structure effects. In this field the last decade has also brought in new ideas and concepts which are especially relevant for the properties of interfaces between systems such as for example a thin layer of LaAlO3 grown on top of SrTiO3 both perovskite structures and electrical large band gap insulators but resulting in an interface that is metallic and even superconducting. This has opened a huge new field of research in which interface engineering is slowly emerging as a way to generate new properties and also new potential devices. I will try to describe some of these developments and describe some of the challenges in trying to explain observed properties in which indeed also defects both extended and point defects play a very important role.

09:00 Break

Carbide Precipitation in Steels

09:45 Invited
Transmission Electron Microscopy Investigation of the Transition from Interphase-precipitated Carbides to Fibrous Carbides in Fe-Cr Steels: Jin-Ren Yang; 1National Taiwan University

For vanadium steels, the previous research work indicated that interphase-precipitated carbides were changed into fibrous carbides in localized regions of the ferrite matrix, and suggested that the most coherent regions of the ferrite/austenite interface are the most sluggish and thus have the best possibility of developing fibrous precipitate. However, the exact circumstances bringing about the formation of fibrous carbides in the face of competing interphase-precipitated carbides have not yet been clarified. In this work, through the isothermal treatments, the attempt to produce the fibrous carbides adjacent to the interphase-precipitated carbides has been achieved in vanadium-containing medium-carbon steels. Therby, transmission electron microscopy can provide direct orientation information about the transition. The transmission electron microscopy reveals that in the same ferrite matrix, the interphase-precipitated carbides can be intimately connected with the fibrous carbides. From the analysis of orientation relationships, the correlation between these two precipitation modes has been proposed.

10:15 Effect of Vanadium, Titanium and Tungsten on Secondary Precipitation of Metallic Carbides in High Temperature Austenite Modified HP Alloys: Robin Guiz; Anna Fraczkiewicz; 1; École Nationale Supérieure des Mines de Saint-Etienne

Centrally cast HP alloys (Fe-Ni-Cr-C with Nb, Ti and Si additions) were designed to endure high temperature conditions. In these materials, simultaneous precipitation of two phases in the austenitic matrix is to be considered during service: Ni3C and M(2C1-x)6. The precipitation of these phases is not yet well understood. In this study, from the dissolution of primary as-cast phases, the mechanical properties of the alloy Though, after long-time service at high temperature, these particles will be subject to coarsening, leading slowly to the weakening of the material and its severe damaging. This work aims at studying the evolution of the secondary precipitation state on chemically modified alloys, cast in the laboratory. Their compositions were chosen on the basis of results obtained with Thermo-Calc and TC-PRISMA softwares, as well as on microstructural observations. Thus, the effects of new alloy elements on the precipitation have been investigated (SEM imaging, TEM, EDS) after aging at high temperature.

10:30 Dominating Factor on the Dispersion of VC Interphase Precipitation in V-added Steels: Yongjie Zhang; Goro Miyamoto; Kunio Shinbo; Tadashi Furuhara; Tohoku Univ.

Nano-sized interphase precipitates formed at migrating ferrite/austenite (γ/α) interface during a transformation attracts increasing attention due to its excellent precipitation strengthening. However, the distribution of various factors, e.g. transformation temperature, alloying content, on its dispersion have not been clarified yet quantitatively. Therefore, the present study aimed to clarify the dominating factor(s) on VC interphase precipitation through the quantification on the number density of precipitate by using three-dimensional atom probe (3DAP). A series of V-added steels with different V and C contents were transformed at various temperatures between 873K and 993K. It is found that, compared with the migrating rate of γ/α interface, the number density of VC shows better correlation with the driving force for its precipitation.

10:45 Precipitation and Growth of Intragranular Prouectoetoid Cementite in an Ultrahigh Carbon Steel: Matthew Hecht; Bryan Webler; Yoosuf Picard; 1; Carnegie Mellon University; 2; CMU

A heat treatment for commercial 2Cr-4C ultrahigh carbon steel (UHCS) was found to result in extensive precipitation of discrete equiaxed cementite particles within the microstructure, with morphology similar to the idiomorphic cementite of the Dubé/Aaronson classification. The resultant carbide distribution indicates partitioning of carbon away from the cementite network which lines grain boundaries in UHCS. As others have shown, network breakup increases the toughness in UHCS by removing brittle pathways for crack propagation. Nucleation of cementite, studied by in-situ confocal scanning laser microscopy (CSLM), was observed around 950°C during rapid heating. Effects of varying chromium content and hold temperature were also studied to better understand the kinetics and driving force for nucleation and growth. A quantitative method for SEM and optical images was developed to help predict the network reduction needed for a given toughness level.

11:00 Precipitation Processes in High Manganese Steels: Ian Zuazo; Patrick Burgess; 1; A rectoolMittal

Further improvement of strength in high manganese steels or TWIP steels for automotive applications can be achieved via precipitation of vanadium or niobium carbides. In order to improve the understanding of the precipitation processes in this class of steels several compositions were casted with varying additions of C, V, Nb and Ni. Intragranular carbides with different morphologies and arrangements have been detected at and above 800°C in homogenized and non-homogenized samples. At the lowest temperature discontinuous precipitation is observed after long treatments times. The nature of precipitates agrees well with calculations from a new thermodynamic database developed for high manganese steels. The precipitate compositions measured via EELS and the precipitate volume fractions obtained by a chemical dissolution method have been compared with equilibrium predictions. Transitions at temperatures below 600°C are also discussed.

11:15 Break

Phase Field Modelling III

09:45 Invited
Dynamics of Phase Transformation in LiFePO4 Particles in Battery Electrode: Hui-Chia Yu; 1; Bernard Orvananos; 1; Oncu Akyildiz; 2; Katsuyo Thorold; 1; University of Michigan

Lithium iron phosphate (LFP) has been a successful material for Li-ion battery cathodes due to its enhanced safety and rate capability. For cathodes consisting of LFP nanoparticles, the current-voltage response in macroscopic electrochemical measurements exhibits a feature indicative of solid-state phase transformation during the charge-discharge process. However, the Li concentration evolution within individual nanoparticles remains to be elucidated. Thus, understanding the phase evolution in LFP nanoparticles is of great importance. Using phase field modeling, we investigated the effects of a variety of material parameters and their anisotropies on the phase morphology evolution in cathode nanoparticles, including Li diffusivities, interfacial energies, surface insertion rate, electronic conductivity, and misfit strain. The effect of conductive surface coatings on the particles was also examined. Finally, we will introduce a thermodynamic model with the simulations, which provides an explanation of recent experimental observations of highly inhomogeneous Li concentration distribution in LFP particles.

10:15 Phase Field Modeling of Sigma Phase Formation in Duplex Stainless Steel: Amer Malik; Lars Höglund; John Ågren; 1; Joakim Odqvist; 2; ‘KTH Royal Institute of Technology

Duplex stainless steels have an excellent combination of strength, toughness and corrosion resistance. However, due to their high alloy content they are prone to precipitate various undesirable phases such as sigma phase and chi phase. Even relatively small fractions of the sigma phase could drastically lower the impact toughness and resistance to pitting corrosion. In order to study the formation of sigma phase in duplex stainless steel a phase field model has been developed. The model uses thermodynamic and kinetic quantities from CALPHAD databases. Multicomponent and multiphase simulations starting from different morphologies of the austenite-ferrite matrix as well as during continuous cooling have been performed.
3D Modeling of Ferrite Transformation in Deformed-austenite Using Multi-phase-field Method and Crystal Plasticity Fast Fourier Transformation Method: Akino Yamashita1;2; Tokyo University of Agriculture and Technology

Recently, the multi-phase-field (MPF) model has been frequently used for investigating the effects of chemical composition on microstructure evolution during the austenite-to-ferrite (γ→α) transformation. In the previous study [A. Yamashita, T. Takaki, Y. Tomita, ISIJ Int., 52 (2012) 659-668], we developed a simulation model to describe the γ→α transformation in deformed austenite phase using the crystal plasticity finite element method (CPFEM) and the MPF model. Using the developed model, we investigated the effect of plastic deformation in austenite phase on the transformation behavior in 2D space. In this study, we propose a computationally efficient methodology to simulate the γ→α transformation in deformed austenite phase using crystal plasticity method on the fast Fourier transformation (CPFFT) and the MPF model. On the basis of the results, the effects of plastic deformation in austenite phase on the nucleation and growth of ferrite grain are discussed.

Kinetics of Orientational Phase Ordering near Line Defects in Crystals: Chistina Bjørk1; Ali Massih1;2; Malmö University

General properties of directed ordering of second-phase near line defects in elastic crystals undergoing phase transition are studied using the two-component time-dependent Ginzburg-Landau equation, which describes two different low symmetry phases. The corresponding potential accounts for a first-order transition and it comprises the elastic properties, the singularity that characterizes the defect and a bi-quadratic anisotropy term. The model is able to simulate the effect of line defects on phase domains is demarked. After quenching the system below its transformation point, the broken symmetry parameters in a vicininity of the defect are evaluated, and the effect of the anisotropy on the temporal evolution is analyzed. The development of topological defects, i.e. vortices, is explored and their interaction with the structural defect is examined. Finally, applications of the model to the case of phase transitions in improper ferroelectrics in light of experimental data are discussed.

Domain Pattern Evolution in Hexagonal Systems: Fei Xue1; Xueying Wang1; Yanzhou J1; Sang-Wook Cheong1; Liang Qing Chen1; Penn State University, Rutgers University

The solid phase transitions in hexagonal systems lead to fascinating domain patterns. Here we employ phase-field near line defects in the order parameter configurations of hexagonal systems using YMnO3 and Sc5O4 as examples. The improper ferroelectric YMnO3 exhibits antiphase domain structures made up of six types of domains. The domains connect with vortices and antivortices, so called “topological defects”. The vortex, antivortex, and domain walls connecting them form domain wall networks, which can be categorized into two types based on the configurations of the six types of antiphase domains. The transition between the two types is demonstrated by phase-field simulations. On the other hand, the ferroelastic Sc5O4 shows short domain walls between three domain ferroelastic variants. The three domain variants lead to the formation of three-pointed stars at different spatial hierarchies. From single-domain and phase-field simulations, we demonstrate that there are four types of domain stars and six types of star parings.

Shape Memory Alloys

THURSDAY AM ROOM: CALLAGHAN SESSION CHAIR: GREGORY ROHER, CARNegie MELLon UNIVERSITY

09:45 Invited
TEM/SEM Studies on Nucleation and Growth of Precipitates in Various Martensitic Systems: Dominique Schnyder1; University of Antwerp

The use of shape memory materials as reversible switches, superelastic wires, actuators, etc. is based on the underlying displacive martensitic transformation occurring between a high temperature high symmetry austenite phase and a low temperature low symmetry martensitic phase. In many of these alloy systems, however, the actual transformation process or even the possibility for practical applications depends strongly on the existence of precipitates formed during the material preparation, training or ensuing product application. The fundamental conditions for nucleation and growth of precipitates, which usually also include atom diffusion, thus need to be well understood to allow further improvement of these systems. In the present contribution an overview will be given of early day and model results of the characterisation of precipitation in Ni-Al, Ni-Ti, … by various TEM techniques aiming for quantification of structural and chemical parameters such as interface structures, strain fields, concentration gradients, etc.

10:15 In Situ X-ray Diffraction Studies of the Austenite-Martensite Transformation upon Load Cycling of Superelastic NiTi Shape Memory Alloys: Efthymios Poliadis1; Nikolay Zotov1; Eric Mittemeijer1; Max Planck Institute for Intelligent Systems (formerly Max Planck Institute for Metals Research), Stuttgart, Germany

Components made of NiTi shape memory alloys exhibiting superelasticity may undergo numerous stress-induced austenite-martensite transformation cycles during their service life. Consequently, it is important to understand the effect of cyclic loading on the transformation behavior of superelastic NiTi alloys and to be able to predict the change of their superelastic behavior. The effect of previous cyclic loading on the transformation behavior of superelastic NiTi (50,3 at.% Ni) was investigated by in-situ synchrotron and laboratory-based X-ray diffraction techniques to determine the effects of different conditions on load cycling up to 100 cycles in tension and compression. For each of these stress states, the strain stress curves were determined by loading and unloading at ambient temperature. It was found that with load cycling the character of the reversible austenite-martensite transformation changes from localised (via the propagation of transformation fronts) to uniform. Changes in the strain-stress curves (strain hardening, decrease of the dissipated energy) with cycling are discussed and correlated to the changes in the transformation behavior and the evolution of the martensite fraction as deduced from the diffraction analysis.

10:30 Magneto-thermo-mechanical Coupling Effects on the Dynamic Performance of NiMnGa Magnetic Shape Memory Alloy: Hungjun He1; Oana Zenaida Pascan1; Ziad Mounir1; ENSAT-PolTech

Ferromagnetic Shape Memory Alloy (FSMA) is a smart material coupling magnetic, thermal and mechanical fields that leads to many potential applications (actuators, energy harvesting, refrigeration, etc.). The FSMA is a candidate for high-frequency actuators as it provides large recoverable deformation with fast-changing magnetic fields. The existing prototypes of high-frequency FSMA actuators can work only at short periods due to temperature rise caused by eddy current and twin-boundary friction. In the experiments on the martensite reorientation in NiMnGa under magnetic fields and various frequencies, we found that the heat dissipation and the twin-boundary motion was much less than that in quasi-static loadings, but the twin-boundary friction was still the main heat source for the temperature rise. Accompanying the temperature variations, the FSMA dynamic performance shifts during the cyclic loadings. Understanding such thermo-mechanical coupling is important in academic study and engineering applications.

From Lab to Application

THURSDAY AM ROOM: NORDIC SESSION CHAIR: JOSE RODRIGUEZ-IJABE, CITE

09:45 Invited
Flying Martensite: Transformations in Materials Design: Greg Olson1;2; Northwestern University

Martensitic steels represent the first examples of successful integrated computational materials design and AIM qualification, meeting the technology acceleration goals of the national Materials Genome Initiative (MGI). Parametric design of alloy composition and process specifications employs mechanistic transformation theory in predictive control of martensitic Ms temperatures, precipitation rate constants, and critical particle size. Detailed process optimization employs efficient transformation simulators such as the CryoMART code for cryogenic treatment and the PrecipiCalc code for final heat treatment. For Ni-based superalloys, coupling of PrecipiCalc to heat transfer simulations accelerates process optimization of complex components such as aerospace disc. Under the DARPA Open Manufacturing program, accelerated optimization of additive manufacturing addresses both precipitation hardening and microstructural simulation tools play a vital role in the NIST-funded Chicago-regional ChiMAD Center for Hierarchical Materials Design in support of the MGI.
THURSDAY | 2 JULY 2015

10:15 Microstructure Evolution and Precipitation of a Low Carbon Low Alloyed Steel by the Two-step Intercritical Treatment: Chengjia Shang1; Zhengyi Xie1; Zhiqun Wang1; Wenhai Zhou1; S.V. Subramanian1; 1University of Science and Technology Beijing

Stable retained austenite (9 vol.%) and multi-scale precipitates were obtained in a 0.08C-0.5Si-0.05Mn-0.5N-0.9Cu(14)(Ni+V+Mo)(wt%) steel by the two-step intercritical treatment. The first step of intercritical annealing creates a microstructure of preliminary enriched martensite and lean alloyed intercritical ferrite. The second step of intercritical tempering is helpful for producing film-like stable reverted austenite along the reverted structure. The two-step austenite reverted transformation is associated with intercritical partition of C, Mn and the fine intercritical ferrite will be the underlying basis for the stabilization of retained austenite during the two-step intercritical heat treatment. Fine niobium-containing precipitates of size ~10-30 nm were obtained in the ferrite and retained austenite. The combination of multiphase microstructure, the transformation-induced-plasticity effect of retained austenite and strengthening effect of nanometer-sized precipitates contributes to yield strength greater than 840 MPa, uniform elongation greater than 10% and excellent low temperature impact toughness.

10:30 Direct Pearlite Spheroidisation: Industrial Dream and Laboratory Reality: Matteo Caruso1; Benjamin Pihu1; Stéphane Godet2; CRM Group; 2Univ. Libre de Bruxelles

It is well-known that cold rolling of eutectoid steels requires a prior annealing step that ensures the spheroidisation of the cementite lamellae. In this work, two potential direct spheroidisation methods are analysed: the divorced mechanism during cooling and the strain-induced spheroidisation during hot rolling. Both processes are studied in terms of microstructure and critical microstructural and thermomechanical parameters are identified. The possible scale-up to the industrial scale is evaluated with tests at the pilot scale that are critically discussed.

10:45 Development of Thermodynamic and Kinetic Model for Ferrite and Pearlite Transformation in Case Hardening Steels: Hideaki Ikahata1; Hirofumi Ito1; Kouji Tanaka1; Toyota Central R&D Labs Inc

In order to study ferrite and pearlite transformation in case hardening steels, we investigated effects of the alloy element during the isothermal phase transformation using Fe-0.2C-X(Steel, Mn, Cr) (in mass %) and Fe-0.2C-0Cr-0.8Mn-0.2-0.2Mg model steels. The progress of the phase transformation was estimated by the change of the specimen’s dilatation, and the quantification of the microstructures obtained by an optical microscope. The experimental results illustrated the importance of the negligible-partitioning local equilibrium condition caused by Mn and the solute drag effects by Mg, resulting in strong inhibition of ferrite transformation. Results also suggested partition of Cr during pearlite transformation. By implementation of these phenomena, we developed a thermodynamic and kinetic model for predicting microstructures (ferrite and pearlite) during isothermal and continuous cooling conditions, and confirmed that the model was able to reproduce the experimental results well.

11:00 Significant Age Hardening Response of BCC/HCP Dual Phase Mg-Sc Alloys: Daisuke Ando1; Yukihiro Ogawa1; Tetu Suzuki1; Yuji Satoh1; Junichi Koechi1; Tohoku University

Mg alloys have poor ductility due to their HCP structure. Meanwhile, Mg-Li alloys with above 15at.%Li have BCC/HCP dual-phase and show good ductility. However, Mg-Li alloys have poor hardness. Thus, we will propose a Mg-Sc alloys with BCC/HCP dual-phase. According to phase diagrams, a beta-Sc BCC phase exists in high Mg content and a BCC/HCP dual-phase can be obtained. It is possible to control the microstructure through thermo-mechanical or ageing treatment after beta solution treatment. If such a microstructural control is possible in Mg-Sc alloy, the mechanical properties can be drastically enhanced. In this study, the age-hardening behavior in solution-treated beta Mg-15at.%Sc alloy was investigated and we found that a very high hardening of over 200HV was obtained by ageing treatment at 473 K. Such a significant age hardening response was caused by the formation of very fine alpha phase in the beta matrix phase.

11:15 Break

Preliminary in Non-Ferrous Alloys: Aluminum Alloys

THURSDAY AM ROOM: ALPINE A-B-C SESSION CHAIR: JOSEPH ROBSON, UNIVERSITY OF MANCHESTER

11:45 Invited

Coupled Precipitation, Yield Strength and Hardening Modelling for Ferrite and Pearlite Transformations in a 6061 Aluminum Alloy: Mohammad Reza F. Gumbmann1; Frédéric de Geusser2; Daniel Nellas1; Sylvain Dancret1; 1Université Lyon - INSA de Lyon - MATEIS - UMR CNRS 5510; 2Université de Lyon - LaMCoS - INSA

In age-hardening alloys, high-temperature processes, such as welding, can strongly modify the precipitation state and thus degrade the associated mechanical properties. The aim of this talk is to present a coupled approach able to describe precipitation, associated yield stresses and kinematic/isotropic hardening for non-isothermal treatments of a 6061 aluminum alloy. The precipitation state (in terms of volume fraction and precipitate size distribution) is modelled thanks to a recent implementation of the classical nucleation and growth theories for needle-shaped precipitates. The precipitation model is validated through small strain experiments and post-mortem electron microscopy experiments. The precipitation size distribution is then used as an entry parameter of a micromechanical and kinematic/isotropic hardening of the alloy. Predicted stress/stain curves are compared to tensile cyclic tests performed with various heating conditions, representative of the heat-affected zone of a welded joint.

12:15 Kinetics of Solute Clustering in Multi-constituent Alloys: Matthias Petzet1; Alexis Deschamps1; 1Univ. Grenoble Alpes, CNRS, SIMAP

Aluminum alloys exhibit age hardening at room temperature linked to the formation of small solute clusters from a supersaturated solid solution. The kinetics and extent of clustering of the solute elements in Al-based multi-constituent alloys depends both on the interaction between the solute species and between the solutes and the quenched-in impurities. The present work is a combined effort between simulation and experiments. The precipitation model is validated through small strain experiments and post-mortem electron microscopy experiments. The precipitation size distribution is then used as an entry parameter of a micromechanical and kinematic/isotropic hardening of the alloy. Predicted stress/stain curves are compared to tensile cyclic tests performed with various heating conditions, representative of the heat-affected zone of a welded joint.

12:30 Combinatorial Approach to Investigate the Influence of Minor Alloying Elements in AlCuLi Alloys: Eva Gumbmann1; Frédéric de Geusser1; Christophe Sigil1; Williams Lefebvre1; Alexis Deschamps1; Grenoble INP; 1Univ. Grenoble Alpes, SIMAP; F-38000 Grenoble, France; 2Constellium Technology Center; 3Groupe de Physique des Matériaux, UMR CNRS 6634, University of Rouen

Al-Cu-Li alloys are hardened by the T1-phase that precipitate on {111}A planes as thin platelets. Several studies show that an effective nucleation of T1 is possible only in the presence of dislocations and minor alloying additions, particularly Ag and Mg. However, there is so far no study that determines the minimum amount of these elements necessary to achieve the described effects. We apply a combinatorial approach based on monitoring the precipitation kinetics on materials based on Al-3.5Cu-1Li, where a gradient in Ag and Mg minor alloying elements has been achieved, using time- and space-resolved Small-Angle X-ray Scattering performed in-situ during precipitation heat treatments. The obtained microstructures and size fraction of precipitates as a function of solute content and heat treatment time) allow, in conjunction with hardness measurements, to determine the critical minor solute contents and better understand their role in promoting nucleation and avoiding precipitate coarsening.

12:45 Quantitative In Situ X-ray Powder Diffraction Studies of Phases Transformations in AI Alloys: Mark Styblo; Mark Gibson1; Christopher Hutchinson2; CSIRO; 1Monash University

In situ synchrotron X-ray powder diffraction is a powerful tool for studying phase transformations in engineering alloys, which, when combined with Rietveld-based data analysis methods, allows the phase composition of an alloy to be quantified as a function of variables such as time or temperature. This approach has recently been used to gain new insights into phase transitions within two Al alloys systems. In situ isothermal aging experiments have confirmed that the decomposition sequence in Al-Cu-Mg alloys involves a metastable variant of the S (Al2CuMg) phase, and enabled the kinetics of the transformation between metastable and equilibrium phases to be investigated. In addition, continuous heating experiments have been used to investigate crystallisation pathways in Al-Ni-Y alloy systems, which have allowed that a mechanism switch from a two stage process involving α-Al, to a three stage process involving Al3Ni1 and a transient excess of Al3Ni1 with increasing Ni concentration.

13:00 On the Effect of Iron and the Precipitation Behaviour of Iron during Annealing of a Cold Deformed Commercial Purity Aluminium Alloy: Sindre Bunkløv; Lykke Nes; Knut Manz; 1Hydro Aluminium Rolled Products AS; 2Norwegian University of Science and Technology

Iron is always present in any aluminium alloy and usually as an impurity element. In commercial purity alloys the concentration of iron is typically so large that iron has a strong influence on the material properties due to its low diffusivity and low solubility in aluminium. In the present work the effect of iron in solid solution and the precipitation behaviour of iron during annealing of a cold-deformed commercial purity aluminium alloy have been investigated. Iron in solution is found to have a strong retarding effect on the softening kinetics. The resulting recrystallization texture has a distinct Cube component and some weak deformation texture components. By additional cold rolling and inter-annealing, the solute content is reduced significantly by precipitation of mainly Al3Fe and some α-AlFeSi phases. Doing so speeds up the softening kinetics by a factor of ~1000 and causes a considerable strengthening of the Cube in the recrystallized texture.

13:15 Lunch
Simulation of Ordering and Pattern Formation

THURSDAY AM | ROOM: ALPINE D-E
SESSION CHAIR: CHRIS WOLVERTON, NORTHEASTERN UNIVERSITY

11:45 Invited
Self-Organization Reactions Under Irradiation: Toward the Design of Radiation-Resistant Materials: Pascal Belloni1; Robert Averback2; 1University of Illinois
Irradiation can drive materials into non-equilibrium states, induce additional transformation, and nanoscale reorientation through self-organization. These nanostructures can impart radiation resistance by providing a large density of interface sites for point defect elimination, while at the same time improving mechanical properties. We will present two approaches that have been identified for alloys comprised of immiscible elements. In a first approach, for instance observed in Cu-Nb-W, nanoprecipitation of a highly immiscible solute (W in Cu) takes place during displacement cascade, providing a fractal-like template for the precipitation of a second and less immiscible solute (Nb). Atomistic kinetic Monte Carlo (KMC) simulations reveal that, under these conditions, nanoprecipitates can be completely resistant to thermal coarsening. In a second approach, the competition of ballistic mixing with thermal diffusion can lead to self-organized nanoprecipitates, which are thus coarsening resistant by design. KMC reveal that effective point-defect sinks can extend this nanopatterning to elevated temperatures.

12:15
Thermo-kinetic Modeling of Mg-Si Couples Formation as a Precursor to Precipitation in Al-Mg-Si Alloys: Yao Shan1; Jiri Svoboda2; Franz Fischer3; Ernst Kozezisch4; 1Materials Center Leoben Forschung GmbH, 2Institute of Physics of Materials, Academy of Sciences of the Czech Republic, 3Institute of Mechanics, Montanuniversität Leoben, 4Institute of Materials Science and Technology, Vienna University of Technology
As the first step a thermodynamic model describing the Gibbs energy of the system accounting for Mg-Si co-precipitation in an Al-Mg-Si matrix is developed. The equilibrium concentration of co-precipitates is obtained by minimizing the Gibbs energy of the system for a given temperature, chemical composition and the trapping energy, describing the decrease of energy due to Mg-Si co-precipitation which is possible to Mg-Si alloys... In the second step, the evolution equations describing the kinetics of dimer formation are derived by means of the Onsager (Ziegler) thermodynamic extremal principle. The studies based on this model, can significantly contribute to a better understanding of the early stages in nucleation of complex precipitates. The predictions of our model are compared to different approaches in open literature, such as the models of Howard and Lidiard, and of Starink et al., which use different approaches to the treatment of the configurational entropy.

12:30
Grain and Interphase Boundary Anisotropy and Growth Pattern Formation: Theory, Experiments and Numerics: Silvère Alama-Nabu1; Sabine Bottin-Rousseau2; Gabriel Faivre1; Suppyo Ghosh1; Mathis Plapp1; 1CNRS - UPMC, 2École Polytechnique
The anisotropy of the free energy of solid-solid boundaries in alloys often plays a determining role in the formation of growth microstructures during phase transformation. In a recent work, we showed that a rotating directional-solidification method, during which the crystal orientation can be varied continuously, can give experimental access to the interfacial anisotropy of grain or interphase boundaries left behind the solidification front in a polycrystal or eutectic solid. We will present an approximate theory that formalizes this statement (it refers to the local-equilibrium condition at solid-solid-liquid trinjunctions), and experimental observations of it. We also present (2D) numerical simulations of tilted lamellar eutectic growth patterns with two different methods—phase field and dynamic boundary integral—by implementing various (model-dependent) boundary conditions, without and with Hermitian-unstable orientations. They confirm the general validity of the theoretical analysis, and give an estimate of the accuracy of the above mentioned experimental method.

12:45 Invited
Ordering of Two Dimensional Strained Films: Kim Eldred, Hong Kong University of Science and Technology
In this talk I would like to discuss the ordering of ultrathin films grown on various substrates. The lattice mismatch between the film and substrate leads to strain induced patterning and phase transitions. The talk will focus on using amplitude representations of the phase field crystal model to study large scale ordering of triangular films on triangular substrates (referred to as graphene on various metallic substrates). This approach bridges the gap between atomistic details such as dislocations and large scale ordering on micron length scales.

13:15 Lunch

Characterization of Displacive Transformations in Ferrous Alloys

THURSDAY AM | ROOM: CALLAGHAN
SESSION CHAIR: DONALD BROWN, LOS ALAMOS NATIONAL LAB

11:45 Invited
Atom Probe Tomography Investigation of Carbon Segregation and Redistribution from Supersaturated Virgin Fe-C Martensites: Frédéric Danoix1; Sebastien Allain2; Mohamed Gouné3; Helena Zapolsky1;1CNRS - Université de Rouen; 2UL Nancy; 3ICMCB Bordeaux – UPR CNRS 9048
Due to its renewed importance in modern steels, numerous works have been carried out for years to explain the strength of as-quenched martensitic steels. The relation between microstructure and tensile properties is still a matter of debate, partly because fine scale microstructural defects acting as obstacles for dislocation motion are not known in details. The difficulty lies in the autotempering, which strongly depends on the cooling rate. In order to avoid it, we study virgin martensite, where carbon diffusion is almost completely suppressed before ageing. Even in such unstable martensites, different types of C segregation defects are observed, from segregations to structural defects, to homogeneous Fe-C phase separation by a spinodal mechanism. C redistribution in virgin martensite is investigated mostly by atom probe tomography, and the observed microstructures are correlated with the tensile behavior in order to better understand the influence of fine scale microstructural parameters on their mechanical properties.

12:15
Quantitative Metallography for Industrial Use on Martensitic Steels: Albin Stormvinten1; Annika Borgenstorm2; Goro Miyamoto3; Takashi Fukuda4; Tomoyuki Kakeshita3; 1Takashi Yamaguchi2; Takashi Fukuda1; Tomoyuki Kakeshita3; 2Osaka University
An Fe-Pt has ordered an L12-type structure, and the alloy with its degree of order of 0.75 exhibits a second-order martensitic transformation from an L12-type cubic structure to an L60-type tetragonal structure in the cooling process at a temperature near 90 K. We have investigated lattice strain of the Fe-Pt under compressive stress applied in the [001] direction by neutron diffraction at BL19 (TAKUMI) in J-PARC. We found that the large lattice strain of approximately 6% appears under a stress of ~280 MPa near the transformation temperature. The lattice strain drastically decreases with increasing test temperature. These results are the consequence of significant softening of elastic constant C.

13:15 Lunch
11:45 Invited
On the Characterisation of the Order - Disorder Transitions of Fe$_2$VAl-based ternary Thermoelectric Heusler Compounds: Pascal Jacques$^1$, Philippe Bellanger$^1$, Geoffrey Roy$^2$, Aude Simon$^1$, Camille van der Riet$^1$, UCL

Compounds based on Fe$_2$VAl are good candidates for large-scale devices devoted to the harvesting of low grade heat from industrial processes through the thermoelectric effect. However, their thermoelectric properties are badly influenced by disorder, especially at higher temperatures. The present study investigates order-disorder transformations in Fe$_2$VAl-based ternary thermoelectric Heusler Compounds: Pascal Jacques$^1$, Philippe Bellanger$^1$, Geoffrey Roy$^2$, Aude Simon$^1$, Camille van der Riet$^1$, UCL

An inherent problem of these compounds is the close atomic numbers of Fe and V making their atomic scattering factor almost similar for X-rays scattering. Hence, the D0$_3$ and L2$_1$ structures, corresponding to Fe-V and Fe-Al alloys, are hardly distinguishable by XRD. Anomalous scattering and neutron diffraction were combined with differential scanning calorimetry to highlight the order-disorder transformations in Fe$_2$VAl-based compounds. Based on these characterisations, specific heat treatments were defined to promote the formation of the L2$_1$ ordered phase.

12:15
A Simple Model for the Disorder/Order Transformation Preceding Fe$_4$C Precipitation in Martensite: Walter Mayer$^1$, Yoo Shin$^2$, Ernst Käzeschik$^3$, $^1$Institute of Materials Science and Technology, Vienna University of Technology; $^2$Materials Center Leoben Forschung GmbH, Leoben

We present a new theoretical approach to simulate the sequence from metastable disordered C- rich cluster formation and defect segregation to stable cementite (Fe$_3$C) precipitation in low and medium carbon martensitic steel. The freshly quenched virgin bct martensite is treated as a highly supersaturated solid solution of C in a heavily defect-loaded Fe matrix where, on tempering, a strong driving force for precipitation of carbides exists that are, however, experimentally not observed. In our model, in the first stage of tempering, C atoms either segregate to lattice defects (dislocations, grain and phase boundaries) or form Fe-rich C-clusters. These metastable configurations delay, or even suppress, the precipitation of Fe$_3$C at low temperature. Using the thermo-kinetic software MatCalc we simulate tempering, taking into account the full sequence of C trapping to dislocations, the formation of C clusters and, finally, transformation to stable Fe$_4$C carbide precipitates with an (ordered) orthorhombic crystal structure.

12:30
On the Interactions between Recrystallisation and Ordering Phenomena in Fe$_2$VAl-based Heusler Compounds: Camille van der Riet$^1$, Philippe Bellanger$^1$, Geoffrey Roy$^2$, Pascal Jacquet$^1$, Université Catholique de Louvain

Compounds based on Fe$_2$VAl are considered as promising materials to harvest low grade heat from industrial processes through the thermoelectric effect. On the one hand, conditions leading to hot ductility of this material are processed during the thermoelectric effect. However, their thermoelectric properties are greatly enhanced in the ordered state. The influence of the temperature as well as of the presence of defects was assessed. The interactions between recovery/ recrystallisation and ordering in specific temperatures ranges were characterised owing to X-ray diffraction and transmission electron microscopy.

12:45
Simulations of TDGL Equations for B2 Type Ordering with Two Step Phase Separation in Fe-Ni-Al Alloys: Ryukihi Oguma$^1$, Syo Matsumura$^2$, Minoru Doi$^3$, Satoshi Hata$^4$, Keisuke Ogata$^5$, Yukio Fukuda$^6$, Kyushu University; $^1$Aichi Institute of Technology

Present authors developed a time-dependent Ginzburg-Landau (TDGL) formulation for ordering processes of B2 and D0$_3$ in binary alloys. Coauthors have investigated domain structures and two-step phase separation of Fe-based FeNi-Al alloys. Micro-structures in the superalloys consist of B2 ordered domains and A2 disordered matrices in the first stage of phase separation. The second stage during a subsequent aging leads to formation of B2 ordered domains and A2 phase regions in the former A2 matrices and B2 domains, respectively. The evolution of 3D domain structures has been analyzed by electron tomography and imaging and energy-dispersive X-ray spectroscopy. In this work the authors have applied the TDGL formulation to this alloy system, and performed 3D numerical simulations assuming the thermal processing. The results of the simulations well reproduced the characteristics of the microstructures obtained from the observations.

13:00 Lunch

THURSDAY PM ROOM: ALPINE A-B-C
SESSION CHAIR: JIAN-FENG NIE, MONASH UNIVERSITY

14:15 Invited
Lamellar and Nonlamellar Decomposition in U-Nb: Energy Sinks and Approach to Equilibrium: Robert Hackenberg$^1$, Clarissa Tabyinskaya$^2$, Anna Libed$^3$, Heather Vol$^4$, Pauls Papin$^1$, Tim Tucker$^1$, Kester Clarke$^1$, Megan Emigh$^1$, Los Alamos National Laboratory; $^1$University of Illinois (Urbana-Champaign)

Kinetics prediction is complicated by the wide variety of thermodynamically permissible reaction paths, and the envelope of permissible paths expands with increasing supersaturation. Tracking the magnitudes of free energy changes along actual reaction paths provides important clues to understand the selection of length scales, growth rates, and phase compositions. This energy-tracking approach is applied to the diffusional monotectoid decomposition of binary Uranium-Niobium alloys. Niobium partitioning occurs over 3 stages: general precipitation (GP), discontinuous precipitation (DP), and discontinuous coarsening (DC). Each stage irreversibly consumes a portion of energy so available chemical driving force decreases. However, some energy in reversible energy sinks such as interfaces and strain. The driving forces of the DP and DC reactions are augmented by the release of energies stored in the predecessor reaction products. Diverging lamellae and nanostable state growth of DP and DC provide added complexity that will be quantified and discussed.

14:45
Competitive Continuous and Discontinuous Precipitation in Magnesium-Aluminium-Zinc Alloys and their Effect on Twinning: Joseph Robinson$^1$, University of Manchester

The magnesium-aluminium-zinc system forms the basis of the most widely used commercial magnesium alloys, such as AZ91. These alloys are age hardenable and of the most widely used commercial magnesium alloys, such as AZ91. These alloys are age hardenable and age precipitation result from a competition between coupled precipitation (CP) and discontinuous precipitation (DP), or a mixture of modes. The type of precipitation that occurs has important consequences for the mechanical properties of the alloy, with DP generally considered to be undesirable.

15:00 Aspects of Discontinuous Precipitation (DP) Reactions in Mg-7.5Cu: Shirley Northover$^1$, Peter Northover$^2$, Alison Wilson$^3$, The Open University; $^1$University of Cambridge

During the transformation of a metastable disordered C-rich cluster to a stable Mg$_3$Zn$_2$ carbide precipitation, it is well known that particular low C coincident site lattice (CSL) misorientations with respect to the grain into which they are growing. On the one hand, conditions leading to hot ductility of this material are processed during the thermoelectric effect. However, their thermoelectric properties are greatly enhanced in the ordered state. The influence of the temperature as well as of the presence of defects was assessed. The interactions between recovery/ recrystallisation and ordering in specific temperatures ranges were characterised owing to X-ray diffraction and transmission electron microscopy.

15:15
Time and Composition Resolved Precipitation Characterization and Modelling in (Cu – Cu-2%Co): Diffusion Couples: Frédéric de Geuser$^1$, 1; Pallas Papin$^1$, 1; Christopher Hutchinson$^1$, 1; Alexis Deschamps$^1$, 1; Mathieu Rest$^1$, 1UCL - CNRS - Univ. Grenoble Alpes; $^2$CSIRO; $^3$Monash University; $^4$SIMAP - Univ. Grenoble Alpes

Precipitation models such as the so called "class-model" are capable of reproducing complex situations such as anisothermal heat treatments and providing the evolution of the size and volume fraction of precipitates. They are now routinely used in particular in the design of alloys, with DP generally considered to be undesirable.

15:30
Numerical Simulation of Precipitation in Multicomponent Alloys: Manon Bonaulet$^1$, Thomas Philippe$^1$, Xavier Sauvage$^1$, Didier Blavette$^1$, "GP" - Université et Insa de Rouen - UMR CNRS 6634 - France

A model describing coupled precipitation and non-steady state growth of DP and DC provides added complexity that will be quantified and discussed.

15:45 Break

THURSDAY 2 JULY 2015
14:15 Invited
The Use of Density Functional Theory to Explore Precipitation-hardened Alloy Systems: Chris Wolverton1; Northwestern University

To fully optimize the large strengthening response of alloying additions to many metals, one would like to understand the energetic, stability, and morphology of precipitate phases as well as be able to predict solutions of new precipitation-hardened alloy systems. These types of materials discovery and alloy design processes may be greatly aided by the use of computational methods, particularly those atomistic methods based on Density Functional Theory (DFT). In this talk, I will present an overview of recent applications of DFT for a variety of alloy systems and precipitates. Examples will be shown for known and predicted precipitate phases in a variety of systems (e.g., Mg-, Al-, and Co-based).

14:45 A Hierarchical Computational Thermodynamic and Kinetic Approach to Discontinuous Precipitation in the Fe-Ni-Cr-C System: Fengfang Du1; Robert Rawlings2; Alexander Land2; Sean Gibbons1; Saurabh Bajaj2; Andrei Ruban3; Levente Vitos1; Patrice Turchi3; Raymundo Arroyave1; Texas A&M University; Los Alamos National Laboratory; Lawrence Livermore National Laboratory; California Institute of Technology; Royal Institute of Technology

Uranium-niobium alloys decompose via discontinuous precipitation (DP) over a broad span of aging conditions, adversely affecting properties. The growth kinetics, lamellar spacings, and Nb partitioning magnitudes have been measured, but the thermodynamic and kinetic underpinnings of the transformation specific transformation characteristics and reaction paths, vis-a-vis the monoclinic reaction, are not fully resolved. In this work, a hierarchical computational thermodynamic and kinetic approach was carried out to investigate DP. The hierarchical approach started with density functional investigations of ground-state formation energies of bcc-uranium-niobium. The estimated energetic data was then utilized as an imposed first-principles constraint to improve the consistency of CALPHAD thermodynamic and, subsequently, kinetic assessments of uranium-niobium. Phase-field simulations were then carried out to study DP’s microstructure evolution using the assessed CALPHAD thermodynamic and kinetic underpinnings with accuracy on different physical/length scales, which validated the present theoretical contributions to a better understanding of DP in uranium-niobium alloys.

15:00 Simulation of Simultaneously Occurring Coupled Inward Diffusion and Internal Precipitation: Mingyu Jung1; Sai Ramudu Meka1; Bastian Rheingans5; Eric Jan Ruban2; 1Northwestern University

Precipitation from homogeneously supersaturated solid solutions is more or less well understood. However, the precipitation occurring upon inward diffusion of one of the solutes, leading to depth-dependent degree of solute supersaturation, has not been modeled with accuracy. This is attributed to the difficulty in coupling the simultaneously occurring processes of internal precipitation and inward diffusion. To this end a model was developed which describes coupling of the inward diffusion of an element I into a substrate and the simultaneous precipitation, i.e. nucleation, growth, and coarsening, of a compound M, with as alloying element initially dissolved in the substrate. The model was applied to the gaseous nitriding of iron-based alloys, incorporating the role of elemental nitrogen and ammonia dissipation kinetics at the surface of substrate. The simulation results, e.g. the variation with depth of the precipitate-size distribution, show good agreement with experimental results.

15:15 Invited
Modeling the Interaction of Precipitation and Recrystallization during Hot Deformation of Microalloyed Steel: Heinrich Bukten1; Pavel Sherstnev1; Ernst Kuzeschnik2; Vienna University of Technology; Leichtmetallzentrums Hannover

Recrystallization is a phenomenon where the polycrystalline microstructure of metallic materials is entirely rebuilt after plastic deformation and subsequent thermal treatment. Nowadays, the kinetics of recrystallization is an important consideration, in particular, on coarsening of precipitates located at the recrystallization front and subsequent release of the pinned recrystallization front, are lacking. In the present work, we introduce a new modeling approach that describes this phenomenon of recrystallization stop by precipitation and continuation of recrystallization due to precipitate coarsening in the surrounding thermo-kinetic simulation. The computational treatment is verified against experimental data from literature, where good agreement is achieved.

15:45 Break

Martensitic & Bainitic Transformations in Steels I

14:15 Invited
Effect of Free Surface on Martensitic Transformation in Individual Retained Austenite Grains: Mingyu Huang3; The University of Hong Kong

The stability of retained austenite depends on the chemical composition, morphology, grain size and hardness of the matrix. In this work, we focus on cyclic transformation of displacive reverse martensite transformation during cooling. It was reported that there is a volume fraction of retained austenite that is not converted to martensite after a few cycles. This fraction could be attributed to the creation of potential nucleation sites in martensite/austenite interfaces. The aim of this study is to determine whether the presence of a small volume fraction of retained austenite affects the nucleation kinetics of the subsequent transformation. This kinetic effect may be attributed to the creation of potential nucleation sites in martensite/austenite interfaces. The model was applied to the gaseous nitriding of iron-based alloys, incorporating the role of elemental nitrogen and ammonia dissipation kinetics at the surface of substrate. The simulation results, e.g. the variation with depth of the precipitate-size distribution, show good agreement with experimental results.

14:45 3-dimensional Microstructural Observation of Butterfly-type Martensite in Fe-Ni-Cr-C Alloy by Serial Sectioning Method: Hisashi Sato1; Kousuke Fujimoto2; Tomoyuki Tanaka3; Yoshimi Watanabe1; Nagoya Institute of Technology

Butterfly-type martensite is formed at formation temperature between lath-type and lenticular-type martensite. Although the butterfly-type martensite has more complicated shape compared with other types, 3-dimensional shape and its crystal orientation distribution are not clear. In this study, microstructure of butterfly-type martensite in Fe-18Ni-5Cr-0.5mass%C alloy was investigated by serial sectioning method and electron backscatter diffraction (EBSD). The butterfly-type martensite in the Fe-Ni-Cr-C alloy consists of two martensite needles and has butterfly-like shape. Moreover, angle between these needles of the butterfly-type martensite is about 140°. Habit plane of the butterfly-type is mainly close to (225) of austenite matrix. Furthermore, large orientation gradients are formed in martensite and austenite phases around tip of the martensite needle. Based on the crystal orientation distribution and the 3-dimensional image of the butterfly-type martensite, growth process of the butterfly-type martensite is discussed.

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Microstructure & Alloy Design

14:15 Invited
The Distribution of Grain Boundary and Interface Plane Orientations in Transformed Microstructures: Hossein Belad1; Gregory Rohrer2; Deakin University; Carnegie Mellon University

The properties of interfaces depend not only on the lattice misorientation, but also on the interface plane orientation. Extensive studies of grain boundaries led to the conclusion that in systems evolving by grain growth, the relative areas of different grain boundary planes are inversely correlated to their relative energies. In other words, the low energy grain boundary planes make up a larger part of the population than the higher energy grain boundary planes. The hypothesis of this work is that the interface plane orientation distribution in transformed microstructures depends not only on the lattice misorientation, but also on the interface plane orientation.

14:45 Development of High Strength High Entropy Alloys (HEA) Based on CoCrFeMnNi System: Anna Frackiewicz1; Michal Mráz2; Matheu Lencz1; MINES St-Étienne

HEA (high entropy alloys) are a new challenge in the field of modern metallurgy. Since the concept was first proposed by Cantor and Yeh (2004), numerous different structures and chemical systems have been investigated. Among them, the FeCrNiMnCo system offers the most interesting set of properties. In this work, different alloys from the FeCrNiMnCo system have been studied. Starting from a computer composition, modifications of chemical composition have been proposed on the basis of Thermonic calculations. The so-chosen alloys have been cast and forged or rolled. Beneficial effects of chemical composition modification are shown: for an optimal proportion of the five elements, at room temperature, yield strength above 800 MPa with a fracture elongation of 35% could be obtained in alloys still that conserve a ductile austenitic structure even at L2N temperature. The microstructure and deformation mechanisms leading to such exceptional mechanical behavior will be discussed.

15:00 Alloy Design and Processing Routes for Novel High Modulus Steels: Hauke Spring1; Rosana Aparicio-Fernandez2; Jyoti Achari2; Han Zhang1; Zhengcong Baron2; Aleksander Kostka2; Dierk Raabe1; Max-Planck-Institut für Eisenforschung GmbH

Metal-matrix-composites show great potential for future light weighting due to the possibility of significantly improving the stiffness/density ratio compared to established metallic materials. Fe-based composites, termed high modulus steels (HMSs), are of special interest due to the high Young’s modulus and the multitude of phase transformations. However, a major challenge for the development of HMS remains the embrittling effect induced by the relatively low ductility of the unreinforced matrix material. Diffusion bonding, gas pressure bonding and pressureless sintering are the main techniques used for making HMS sheets. In this work, the influence of processing parameters on the microstructure and mechanical properties of HMS is investigated.

15:15 Further Developments in Rapidly Solidified Al-Mn-Ce Alloys: Francisco Cuury1; Claudio Boffaroli1; Walter Botta1; Claudio Kiminami2; Michael Kaufman2; Universidade Federal de São Carlos; Colorado School of Mines

Rapidly solidified Al-Mn-Ce alloys were previously reported to form fine quasicrystals dispersed in an Al matrix and were of interest as high specific strength Al alloys. In recent work, the Al-Mn alloys containing varying amounts of Ce were chill cast in a copper mold and then subjected to different heat treatments. The phases formed in the as-cast samples and after different heat treatments were identified using x-ray diffraction, scanning and transmission electron microscopy. The results are in contrast to the literature report in that no quasicrystals were observed in the ternary system but that the Mn concentration evolutes as a function of the cycle number.

15:30 Precipitation in Ultrafine Grained Aluminium Alloys Processed by Severe Plastic Deformation: Xavier Sauvaud1; Anna Nasedkina2; Elena Bobrik2; Maxim Minakov3; Ruslan Valeyev4; University of Rouen, CNRS; 1IPAM-USATU

In this presentation, it is proposed to review the influence of large levels of deformation on precipitation mechanisms and kinetics in aluminium alloys. The motivation of this research is the application of severe plastic deformation processes to combine ultrafine grained structure and nanoscaled precipitates to achieve high strength alloys. Differences in the atomic mobility and provides favourable nucleation sites. Such segregations and dynamic precipitation have an influence on grain refinement mechanisms but also on the ageing hardening behaviour. It will be shown that deformation induced vacancy and solute drag by moving boundaries are the main mechanisms controlling microstructure evolution and thus final properties.

15:45 Break

Precipitation: Crystallography, Morphology and Kinetics

THURSDAY PM ROOM: ALCAN A-B-C SESSION CHAIR: ELENA PERELOMA, UNIVERSITY OF WOLLONGONG

16:00 Invited
New Progress on Precipitation Crystallography Based on GMS Distribution and Evolution Simulation: Wenzhong Zhang1; Zhushan Dai2; Tsinghua University

Transformation crystallography, as a fundamental aspect for understanding of phase transformations, has been investigated with two approaches. One is based on the patterns of good matching site (GMS) for a general system. A precise orientation relationship (OR) may produced by such a system. The structure within a GMS cluster to form. The shape within a GMS cluster indicates a matching lattice correspondence. The shape and distribution of the clusters suggest the geometry for the possible interatomic interactions based on periodic boundary and atomic simulations. Evolution of crystallographic features at early stage of precipitation in a Cu-0.0% alloy was simulated, which shows that the N-W-OR for a small coherent precipitate, and it jumps towards the K-S OR discontinuously upon generating a dislocation loop during the precipitation process. The habit plane orientation is evolved toward the one corresponding to a local minimum of interfacial energy. The simulation results agree with the available experimental results.

16:15 Atomic Resolution Investigation of Nitride Transformation and Amorphous Interfaces in Steel: Hilmar Danielsson1; Technical University of Denmark

9%Cr high temperature martensitic steels used for power plant applications rely upon long term creep strength, where M may by V, Nb or Ta. Increasing Cr content to 12% for better oxidation resistance provokes the precipitation of a new precipitate type, CrMNN, which replaces the FeCrMNN and improves the creep strength. Investigation of the CrMNN nucleation using HRTEM shows it is a transformation rather than a nucleation event. The CrMNN was shown to be amorphous phase and evolves from the matrix by chemical composition and crystallography into CrMNN. Observations of the interface between NbTa nitrides and the ferrite showed the presence of an amorphous shell a few nm thick enveloping the precipitates, separating the two crystalline phases. The shell had the chemical composition of the nitride and was observed to crystallize under the electron beam when removing the matrix.

16:45 On the Shape Strain of Plate-shaped Transformation Products: Jian-Feng Nie1; Monash University

Crystallographic features associated with invariant plane/line strain transformations have received considerable interest in the last 60 years, and some elegant models have been developed that can describe the orientation relationships, interface orientations and interface structures. What remains to be firmly established is whether the shape change of a precipitation plate and, if so, whether the shape change can be also quantitatively described. This presentation will report on a macro model that can describe the phase transformation associated with invariant plane strain transformations. The validity of the model will be examined by selected examples.

17:00 PTCLab: A Free and Open Source Program for Calculating Phase Transformation Crystallography: Xinfu Gu; Tadashi Furuhara; Institute for Materials Research, Tohoku University, Japan

PTCLab (Phase Transformation Crystallography Lab) is a free and open source program to calculate the phase transformation crystallography. This program covers the crystallographic theories of martensitic and diffusional transformation and allows users to represent the results in stereo graphic projection. The crystallographic models treated by PTCLab include classical phase transformation models, martensite crystallography (PTMC), shear transformation products, that are traditionally classified as non-displace, exhibit in fact a remarkable shape change and that the shape change can even be a simple shear.

17:15 Hydrides Formation and Dissolution Processes in Zirconium Alloys: Crystallographic Orientation Relationships and Stability After Temperature Cycling: Egle Conforti; Xavier Feaugas1; University of La Rochelle

Hydrides have been recognized as a source of hydrogen at the alloy grain boundaries and as a means by which hydrogen can enter the alloy. In this study, the phase formation and dissolution of hydrogen in zirconium alloys is examined using TEM, SEM-EDS, and XRD in zirconium alloys as a function of different contents of hydrogen. The orientation relationships (ORs) observed between the hydride phase and the substrate were similar to those previously observed in Titanium hydrides grown on Titanium. Dislocation emission from the hydride precipitate has been directly observed using high magnification electron microscopy diffraction patterns can be also obtained by present application. PTCLab is written in python, runnable on cross platform and is distributed at https://sourceforge.net/projects/ptclab/.
Simulation of Transformation Plasticity

THURSDAY PM  
SESSION CHAIR: PASCAL BELLON, UNIVERSITY OF ILLINOIS  
ROOM: ALPINE D-E

16:00 Invited  
Phase Field Modeling and Plastic Activity: Alphonse Fine1; Pierre-Antoine Geslin2; Pierre-Louis Valdenaire2; Yann Le Bouar2; Benoît Appaolare2; 1ONERA-CNRS; 2Northeastern University

Because of the various length and time scales involved in dislocation dynamics, the modeling and coupling of plastic activity to microstructure evolution is not straightforward. We address two aspects of this problem. First, we present a multiscale modeling of climb, which is important at high temperature. We propose a new analytical expression of the climb rate of a periodically jogged dislocation. We then show how to upscale this closed-form expression to the phase field scale through an asymptotic analysis of a recently proposed phase-field model of climb.Second, we address a key issue in the theory of crystal plasticity, namely the transition between the discrete, where individual dislocations are resolved, and the continuum, where dislocations are represented through densities. We in particular focus on the underlying coarse-graining procedure and discuss its implication on the resulting correlation-induced local stresses and transport equations that control the plastic flow at the continuum level.

16:30  
General Approach to Diffusion under a Strain in Metals and Alloys: Andrey Nazarov1; Alexander Malyshev2, National Research Nuclear University (MEPhI); 2Moscow State University of Design and Technology

Our approach takes into consideration, that the strains can alter the surrounding atom configuration near the jumping atoms significantly the local magnitude of the activation barrier and a rate of atom jump. The rates of atom jumps in different directions define the flux density of the defects. Now we take into account, that strain values are different in the solute and matrix and in the rest atom position. As a result in the development of our approach the general equations for the vacancy fluxes and impurity fluxes are obtained for fcc and bcc metals. These equations give the possibility for using at low temperatures and differ sufficient from the equations that was obtained earlier. In our presentation we are going to discuss the main features of the theory of diffusion under strain, the ways of its development and its applications that are realized by computer simulation.

16:45  
Elasto-plastic Phase-field Model Based on Mechanical Jump Conditions: Daniel Schneede, Oleg Tschukin2; Abhick Choudhury1; Michael Seiber1; Britta Nestler1; 1Karlsruhe Institute of Technology; 2Karlsruhe University of Applied Science; 3Indian Institute of Science

Computational models based on the phase-field method typically operate on a mesoscopic length scale resolving structural changes of the material and provide valuable information about microstructure and mechanical property relations. An accurate calculation of the stresses and mechanical energy at the transition region is therefore indispensable. We derive a quantitative phase-field elasticity model based on force balance and Haddamard jump condition at the interface. Comparing the simulated stress profiles in a plate with a round inclusion under hydrostatic tension with the theoretically predicted stress fields and stress field calculated with Vogt/Taylor and Reuss/Sachs, we show the quantitative characteristics of the model. In order to validate the elastic contribution to the driving force of the phase transition, we demonstrate the absence of interfacial excess energy in one dimensional equilibrium condition of serial and parallel material chain as well as in two dimensional system through the Gibbs-Thomson condition.

17:00  
Influence of Plastic Relaxation on the Formation of Widmanstätten Structures: Maria Cottura1; Benoît Appaolare2; Alphonse Fine1; Yann Le Bouar2; 1LEM - ONERA-CNRS

Many metallic alloys such as steels, brass or Ti-based alloys exhibit colonies of acicular precipitates called Widmanstätten microstructures. These structures share generic features: they consist of parallel lamellae that display the same crystalline orientation and, in dislocation free conditions, they follow a highly anisotropic stationary growth process. Recently, we brought new insights on the still debated mechanism selecting the velocity and tip shape by highlighting the prominent role of the elastic driving forces. In this contribution, we proceed further by analyzing in what respect plastic activity changes or not on the different conditions. The phase-field approach recently coupled to a viscoplastic model.

17:15 Break

Martensitic & Bainitic Transformations in Steels II

THURSDAY PM  
SESSION CHAIR: DOUG BOYD, QUEEN’S UNIVERSITY  
ROOM: CALLAGHAN

16:00  
Influence of Heating/Cooling Conditions on the Martensitic Transformation in a Stainless Steel AISI 420: Microstructure and Properties: Carola Celada1; Jesus Chao1; David San Martin2; 1CENIM-CSIC

After cold forming and, to obtain the optimum strength, grade AISI 420 is given a high temperature heat treatment to transform the austenite into the Martensite. In this work, we address the problem of the austenite-to-martensite transformation in austenitic stainless steels. In particular, we focus on the austenite-to-martensite transformation at the interface. We use a thermodynamic model to describe the microstructure evolution and the austenite-to-martensite transformation.

16:15  
Martensite Formed around B2 Precipitates in Fe-Ni-Al Alloys: Tomokazu Moritani1; Hideki Fujiyama1; Yuta Tomokazu1; 1The University of Tokyo

To achieve higher-strength steels containing of martensite or bainite, it is important to control the size, morphology and the amount of those dispersive transformation products. In this study, we focus on the effect of phase-boundary phases on the martensitic transformation in Fe-Ni-Al alloys. We present a systematic investigation of the effect of phase-boundary phases on the martensitic transformation in Fe-Ni-Al alloys.
carbon steel to produce the austenite-ferrite boundary, and quenched to cause displacive transformation in the alloyed steel. It was found that martensite formed at the interface had close-packed plane or close-packed direction nearly parallel to the austenite-ferrite interface. Also, different non-metallic compound particles were embedded in steels and displacive transformation starting from the compounds was investigated with an emphasis on the crystallography and morphology of the transformation products.

17:30 Break

**Nanostructures**

**THURSDAY PM ROOM: NORDIC SESSION CHAIR: XAVIER SAUVAGE, UNIVERSITY OF ROUEN, CNRS**

**16:00 Invited**

**Phase Transformations and Plasticity in Metal Nanoparticles Obtained by Solid State Dewetting of Thin Films:** Eugen Ruban1; Dor Aniram1; Oleg Kovalenko1; Technion

We produced arrays of Fe and Fe-Au alloy nanoparticles on sapphire substrate employing the solid state thin film dewetting technique. The Fe particles exhibited an extraordinary high strength approaching the theoretical shear strength of Fe. The in-situ X ray diffraction studies demonstrated that these particles can be overheated by 200°C above the alpha-gamma transformation temperature. The transformation did occur in the particles of Fe-Au alloys, and in some of the thin Fe films during in-situ dewetting. The morphology of the two-phase Fe-Au nanoparticles was determined by the surface segregation of Au on Fe. We discuss the extraordinary strength and phase stability of the nanoparticles in terms of unifying concept of their structural perfection.

**16:30**

**Field Theory of Amorphous Nanophases:** Alexander Umansky1; Fayetteville State University

A number of very different recent experiments with nanoparticles produced very similar results. In NPs of sizes above critical the sequence of transformations is similar to that of the bulk while in NPs of sizes below the critical novel, amorphous phases appear and remain stable in significant domains of variation of the control parameters. A natural question arises: What is the origin of this phase? In a series of recent publications the author has developed a field theory of the nanophase stability, which claims that the phase that appears in NPs of sizes below the critical is a transition state between the stable bulk phases in the space of the order parameter that distinguishes between the symmetries of the bulk phases. The theory claims that the two-phase state is energetically impossible due to high "energy cost" of the phase separating interface and is replaced by the homogeneous transition state.

**16:45**

**Separation Transitions in Alloy Nanoparticles and Finite-size Scaling:** D. Custers1; Technion

Temperature-dependent chemical-order in platinum-iridium truncated-octahedron and rectangular-prismatic nanoparticles as model systems was studied using the free-energy concentration expansion method [1,2]. In order to cope with large nanoparticles, the number of concentration variables was reduced via grouping atomic sites in layers. Phase-separated nanostructures stable at low temperatures were found to transform into disordered structures at size-dependent critical temperatures, exhibiting a remarkable finite-size scaling behavior with respect to the total number of atoms. More universal fit with distinct critical exponents was found by introducing extra scaling with respect to the shape-dependent number of surface atoms. Possible surface segregation effects are currently explored. It is the first study demonstrating that alloy nanoparticles can exhibit second-order-type transitions and critical behavior in accordance with finite-size scaling theory. [1] M. Polak and L. Rubinsonov, Phys. Chem. Chem. Phys., 16 1569 (2014); [2] M. Polak and L. Rubinsonov, Surface Science Reports, 38, 127 (2000).

**17:00**

**Can Bonding Electron Distribution be Measured in a Nano-structured Material?:** Philip Nakashima1; Tianyu Liu1; Laure Bourgeois1; Joanne Etheridge1; Monash University

When rapidly quenched to room temperature from just below its melting point, aluminium can form octahedral voids of a few tens of nanometres in size, truncated with {001} facets. This geometry sets up an interesting optical scenario for convergent-beam electron diffraction (CBED) in transmission through parallel facets. The resulting CBED patterns are extremely sensitive to the three thicknesses describing the two slabs of perfectly coherent crystal and the free space that they sandwich. Furthermore, we show that by considering such a system as a layered material within the volume of the electron probe, and by implementing the multislite formalism for calculating electron diffraction patterns, we can resolve features in the bonding electron distribution surrounding the nano-void. In this manner, we attempt to make the first bonding measurements in an inhomogeneous nano-structured material.

**17:15**

**Effect of Interfacial Monolayers on Gold-assisted Growth of Crystalline Stable Substrates:** Wei Zhou1; Xin Li1; Guo-zhen Zhu2; Shanghai Jiao Tong University

We discovered the growth of crystalline oxide nanostucture from a previous stable substrate, facilitated by the presence of an Au over layer and the application of heat. The self-assemble nano-structures consist of crystalline oxide bases, epitaxially aligned gold nanoparticles, and in-between, unique thin interfacial layers with completely different crystal structures. This phenomenon has not been previously reported in any other similar metal-oxide system. By clarifying the atomic structure of these thin interfacial layers by aberration-corrected transmission electron microscopy, we believe that these interfacial monolayers, as examples of the interfacial complexion, induce the atomic transport from substrates to gold-substrate nanostructures. The unique interfacial structures can provide deep insights in the strong metal-support interaction mechanism for heterogeneous catalysts such as Au/TiO2 and Au/MgAl2O4.

**17:30 Break**

**Plenary 7: Hillert-Cahn Lecture**

**THURSDAY PM ROOM: EMERALD BALLROOM SESSION CHAIR: GARY PURDY, McMMASTER UNIVERSITY**

**17:45 Plenary**

**Coarsening of Two-phase Mixtures: From Particles to Bicontinuous Phases:** J. Thompson1; E. B. Gulsoy1; C. L. Park3; Katsuyo Thorrson2; Patr Hooijaas2; Northwestern University; University of Michigan

Two-phase mixtures can evolve with time by the diffusion of mass from regions of high to low interfacial curvature, a process known as coarsening. Through the experiments on the International Space Station, we have employed a model two-phase mixture that both satisfies all the assumptions made by theory and in which all the materials parameters needed to compare theory and experiment are known. We find that the observed exponents and amplitudes of the temporal power laws for the average particle size and number of particles per volume, as well as the particle size distributions match those predicted by theory. We thus conclude that interfacial energy driven ripening is well described by existing theory. Extensions of this theory to systems in which the coarsening domains have spatially varying curvature, such as those found following spinodal decomposition or ordering, will be also discussed.
Using microstructure as a design variable is one of the goals of integrated computational materials engineering (ICME). However, significant scientific and engineering challenges must be overcome to achieve a predictive microstructural design capability. In this talk, we will survey these issues, including calculating the atomic-scale properties of microstructural features, developing physically-based mesoscale models for microstructural evolution, connecting microstructural data to materials performance, and creating and utilizing microstructural databases and archives. The focus will be on strategies for stabilizing bulk nanocrystalline structures against low temperature coarsening, but the approaches apply more generally to understanding and predicting microstructural evolution in polycrystalline materials of all types.

10:30 Phase Transformations Kinetics of Ti-6Al-4V during Very Fast Heating: High Energy X-ray Diffraction (HE-XRD): Andi Ildar Ismail1; Moukrane Dehman1; Elisabeth Aebi-Gautier1; Benoît Appoloni2; 1ULL, CNRS-Université de Lorraine; 2LEM, CNRS-ONERA

In-situ experiments were performed to characterize the transformation kinetics during very fast heating using the synchrotron radiation facilities (HE-XRD) as well as electrical resistivity measurements. The phase amounts and the mean lattice parameter variations were characterized during continuous heating up to the single beta-phase domain with heating rates ranging from 0.25 °C/s to 200 °C/s. For both techniques, results clearly evidence a shift of the beta-phase transformation kinetics toward higher temperatures as the heating rate increases. A poor effect of the initial size of the alpha grains is characterized. In addition, at temperatures lower than 600°C, the average lattice parameter of the beta-phase shows a deviation from linearity, which amplitude depends on the heating condition. The transformation kinetics variations are discussed in regard of calculated dissolution rates. In addition, the beta-phase lattice parameter variations are analyzed in regard of internal stress relaxation or changes of chemical composition.

10:45 Influence of Phase Transformation Kinetics on Variant Selection and Microtexture Development Associated with Alpha Precipitation at Beta Grain Boundaries in a Beta Metastable Titanium Alloy: Mattheu Salit1; Lionel Germann1; Julien Teixeira1; Nathalie Gey1; Elisabeth Aebi-Gautier1; 1Institut Jean Lamour - CNRS - Université de Lorraine; 2LEM - CNRS - Université de Lorraine

The influence of phase transformation kinetics on variant selection and microtexture development associated with heterogeneous precipitation of alpha at beta/beta' variant selection and microtexture development associated with heterogeneous precipitation of alpha at beta/beta grain boundaries is studied in the Ti-11.7 beta-metastable alloy, by using dark field scanning transmission electron microscopy and selected area electron diffraction (SAED) techniques. The effect of increasing deformation on the alpha/beta' phase equilibrium is evidenced. The number of variants and microtexture parameter variations are analyzed in regard of internal stress relaxation or changes of chemical composition.

11:00 Thermal Stability of HPT-induced Omega Phase in Biocompatible Ti-16.1Nb Alloy: Ali Parighani1; Matthias Bönisch2; Thomas Waltz1; Mariana Calin1; Werner Skrotzki2; Jürgen Eckert1; 1University of Vienna; 2IFW Dresden, Dresden University of Technology

TiNb alloys are potential materials for orthopaedic implants due to their excellent biocompatibility and low Young’s modulus of the cubic β and orthorhombic α‘ lattice structures. The present work focuses on the microstructural features of Ti-16.1 wt.% Nb induced by very severe plastic deformation and subsequent annealing were systematically studied. Upon high pressure torsion, the parent α martensite transforms into a bulk nanocrystalline α-phase. The formation of the α-phase is triggered both by pressure and strain. In-situ heating experiments using synchrotron radiation show that the α-phase starts to decompose into the hexagonal α and the cubic θ equilibrium phases at a temperature of about 320°C. The phase transformation is complete at a temperature of 460°C. The pathway via an intermediate nanocrystalline α-phase provides a new processing route for the production of a bulk material with an ultrafine and equiaxed α/β phase structure. Funding by EC (ITN BioTiNet – 264635) is gratefully acknowledged.

11:15 Break

Modelling and Experiment

09:45 Invited Detailed Structure Analysis of Precipitates Combining TEM and DFT: Jasper Fins1; Sigurd Wenner2; Calin Marian3; Randi Holmestad2; 1SINTEF; 2Univeristy of Vienna; 3University of Science and Technology (NTNU)

The age-hardenable Al-Mg-Zn-Cu alloys are important as structural materials for automotive and aerospace applications. In this work, we have studied the structure of some of the precipitates, of which the plate-like β’ phase is the most important for hardening when the amount of Cu is low. Structure models including the precipitate-matrix interface, are derived from high angle annular dark field scanning transmission electron microscopy and validated with calculations based on density functional theory (DFT). Cu additions to the alloys do not affect the β’ structure. Instead, some Cu substitutes Zn sites. The level of substitution has been estimated using energy-dispersive X-ray spectroscopy. For the β’ precipitate, this agrees well with DFT, which predicts a minimum in the formation enthalpy when about 25% of the Zn is substituted with Cu. DFT calculations also show that the dense Zn-columns are energetically favoured to substitute, followed by the Zn atoms at the interface.

10:15 Microstructure Evolution during the Homogenization Heat Treatment of Aluminium Alloys: Modeling and Experimental Results: Qiurong Dai1; Chenglu Liu2; Hamid Azizi Nazarnia3; Warren Poole3; 1SINTF, ‘University of British Columbia

A model has been developed recently to track the microstructure evolution during homogenization heat treatment of aluminium alloys. It features full coupling with CALPHAD software (i.e. chemistry dependent) and explicit treatment of diffusion at the scales of the dendrite arm spacing and inter-dispersed spacing. With very few tuning parameters the model is able to predict the precipitation kinetics of intra-granular dispersoids, the transformation between inter-granular constituent particles and the evolution of Dispersoid Free Zones (DFZ). In this contribution, the homogenization model is introduced and its predictive power is demonstrated by successfully reproducing experimentally measured microstructure features for various industrial alloys. As such, the model represents a valuable tool for optimizing the design of industrial aluminium alloy homogenization heat treatment parameters and compositions.
The pressure to transition (~15 GPa) imposes to consider transformation of iron is challenging for numerous reasons. The modeling of pressure induced martensitic plates about 200 nm in width. During deformation, deformed in the austenite phase field. Widmanstätten ferrite of increasing carbon contents, in which specimens are strain-free ferrite. Critical strains of about 0.10-0.14 are ferrite slowly retransforms into austenite by means of non-constant elasticity tensor to reproduce the equation of state (EoS). Cycling forward transformation (from BCC to HCP) and reversion (HCP to BCC) may split the model microstructures. Detailed characterization, reported previously, revealed that the model microstructures represented a wide range of phase fraction and lattice strain provided a measure of the RA transformation behavior as a function of cycle number and local crystalline orientation. This study, effects of alloying elements on TRIP and TWIP behaviors in LDSSs are described in association with microstructural evolution.

Deformation Induced Martensitic Transformation in Iron at 15 GPa: Modeling and Experiment: Christophe Denoux¹; Aurelien Vatine¹; ²CEA

The modeling of pressure induced martensitic transformation of iron is challenging for numerous reasons. The pressure to transition (~15 GPa) imposes to consider non-constant elasticity tensor to reproduce the equation of state (EoS). Cycling forward transformation from BCC to HCP and reversion (HCP to BCC) may split the original alpha BCC crystal into an increasing number of alpha plates. The resulting partition includes relaxations, which enables the use of large strain formalism. The variant multiplication imposes to consider an potential which entails the use of large strain formalism. The non-linear elasticity (and therefore EoS), and plasticity in the automotive industry, in order to properly tailor the manufacturing. The presented work contributes to this understanding by means of nonindentation, which has been instrumented as a micro/nano-probe to induce deformation at sub-nanovol using monotonic and cyclic tests. Analysis of the nonindentation curves including the reloading behaviour allowed conclusions about material properties as a function of cycle number and local crystalline orientation. Remarkably, stepwise hardness drops occurred during increasing indentation cycles, resulting in an enlarged hysteresis. The involved deformation mechanisms were studied by electron microscopy (TEM) and diffraction. It was found that with increasing cycle numbers the phase transformation induced by nonindentation propagates until the grain boundary, and can extend to neighbour grains.

Pressure Induced Alpha to Epsilon Transformation in Iron: Shared Challenges and Diverse Solutions: Takuro Masumura; Nobuo Nakada 1; Toshihiro Tsuchiyama1; Setsuo Takaki 1; Umichiro Ashitaka; 1University of Tsukuba; 2Nippon Steel & Sumitomo Metal Co.

In order to evaluate the effects of carbon and nitrogen additions on the stability of austenite, thermodynamic and deformation-induced α’-martensite transformation behaviors were investigated in type 304 metastable austenitic steels containing 0.1 mass% carbon or nitrogen. Since carbon-added steel has a lower stacking-fault energy (SFE) than nitrogen-added steel, deformation twin and α’-martensite were preferentially formed in carbon-added steel, whereas a dislocation cell structure developed in nitrogen-added steel. Crystallographic analysis using electron backscatter diffraction method revealed that the difference in the deformation microstructure have significant influence on the growth behavior of deformation-induced α’-martensite. The interface of the deformation twin and α’-martensite completely suppresses the growth of α’-martensite, whereas dislocation cell boundaries have little influence on that. As a result, the mechanical stability of carbon-added steel is much higher than that of nitrogen-added steel, although the thermal stabilization effect of carbon is much lower than that of nitrogen.

Dynamic Transformation Behavior of Austenitic Stainless Steels: Takuo Masumura; Nobuo Nakada 1; Toshihiro Tsuchiyama1; Setsuo Takaki 1; Umichiro Ashitaka; 1University of Tsukuba; 2Nippon Steel & Sumitomo Metal Co.

In order to evaluate the effects of carbon and nitrogen additions on the stability of austenite, thermodynamic and deformation-induced α’-martensite transformation behaviors were investigated in type 304 metastable austenitic steels containing 0.1 mass% carbon or nitrogen. Since carbon-added steel has a lower stacking-fault energy (SFE) than nitrogen-added steel, deformation twin and α’-martensite were preferentially formed in carbon-added steel, whereas a dislocation cell structure developed in nitrogen-added steel. Crystallographic analysis using electron backscatter diffraction method revealed that the difference in the deformation microstructure have significant influence on the growth behavior of deformation-induced α’-martensite. The interface of the deformation twin and α’-martensite completely suppresses the growth of α’-martensite, whereas dislocation cell boundaries have little influence on that. As a result, the mechanical stability of carbon-added steel is much higher than that of nitrogen-added steel, although the thermal stabilization effect of carbon is much lower than that of nitrogen.
10:30 Functionally Graded Iron Based Alloys Showing Twining and Martensitic Transformation; Processing, Microstructure and Properties: Thomas Niendorf1; Florian Brenne2; Christian Rüsing3; Matthias Droste1; 1TU Bergakademie Freiberg; 2University of Paderborn; 3Benteler Automotive

In order to provide materials suited for advanced light-weight design, steels showing twinning induced plasticity (TWIP) and transformation induced plasticity (TRIP) have been developed in the last decades. Through alloying, e.g. by manganese, aluminum and carbon, the stacking fault energy (SFE) is set to a value leading to activation of TWIP/TRIP upon deformation. The actual deformation mechanism is additionally influenced by parameters such as texture, grain size and deformation temperature. In order to further improve the properties of these high-performance materials, functional gradation, i.e. setting of local mechanical properties, can be used. The current work introduces concepts suitable for functional gradation of high-manganese iron-based alloys. Thermo-mechanical treatments as well as additive manufacturing were employed to create microstructure manipulation and, thus, property optimization. Based on mechanical testing including local strain analyses employing digital image correlation and thorough microstructure analyses using electron tomography techniques solid process-microstructure-property relationships are deduced.

10:45 Invited In Situ Evaluation of Metallurgical Phenomena Using Laser Generated Ultrasonic Waves: Thomas Garcon1; Matthias Militzer2; 1University of British Columbia

Over the past decade, laser ultrasonics has gained tremendous maturity in in-situ characterize microstructure evolution during thermo-mechanical processing of metals and alloys. In this technique, pulse lasers are used for the generation and detection of ultrasound in materials. The ultrasonic waves are coupled with microstructure parameters such as grain size and phase fractions transformed or recrystallized. Meanwhile the new Laser Ultrasonics for Metalurgy (LUMe) system has been developed such that this technology can be used as a user-friendly tool in the laboratory. Attached to a Gleeble thermomechanical simulator, it allows (dynamic and post-dynamic) recrystallization to form again during cooling. The applied forging conditions allow (dynamic and post-dynamic) recrystallization to occur and precipitation to evolve simultaneously. While many studies are dedicated either to recrystallization in γ matrix or γ precipitation phenomena, the focus is placed here on the coupling of both phenomena: recrystallization influencing γ precipitation, and γ particles influencing recrystallization mechanisms. Nucleation and growth of γ into γ′ has been found to occur with diffusional and transformations. Scenarios are proposed to account for the observed evolutions, based on consideration of stored energy, chemical composition of grains and precipitates, boundary energies and migration.

Phase Transformations in Superalloys
FRIDAY AM ROOM: ALPINE A-B-C
SESSION CHAIR: WALTRAUD KRIVEN, UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

11:45 Invited Evolution of γ′ Microstructure in Ternary Co-Al-W Alloys: Eric Lass1; Yaaow Idel1; 1NiST

The discovery of a two-phase γ (FCC)-γ′ (L12) field in the ternary Co-Al-W phase diagram has sparked significant research interest into possible Co-based alloys to traditional Ni-based superalloys used in turbine engine applications. This work experimentally investigates microstructural evolution ternary Co-AI-W alloys. Nucleation of ordered γ′ precipitates 2 nm to 10 nm in diameter cannot be observed even under rapid solidification conditions. Upon subsequent annealing, growth of these nuclei into irregular, non-cube shaped precipitates is very rapid, resulting in a volume fraction γ′ roughly equal to that in metastable equilibrium with the γ phase after only a few minutes. The microstructure then slowly coarsens to reveal the familiar cubic β (BCC) microstructure similar to that found in the Ni-Al-Cr based γ/γ′ systems. The phase microstructure is ultimately destroyed by the nucleation and growth of the additional phases Co3W (D019) indicating γ′ is metastable in ternary Co-Al-W.

12:15 Simulations of Early Stage Phase Separation in Al-Cr-Ni Superalloys: Stefan Poulsen1; Peter Voorhees2; 1Northwestern University; 2Northwestern University

Nickel-based alloys are the most desirable of their desirable properties to gamma prime (ordered FCC) precipitates in the gamma (disordered FCC) matrix, thus understanding the phase separation process, i.e. nucleation and growth of gamma precipitates is of great technological interest. We have examined the early stages of phase separation in Al-Cr-Ni alloys with a phase-field model, that employs CALPHAD free energies and CALPHAD-style assessed interdiffusion mobilities to make quantitative predictions about the phase separation process. The approach takes into account that 1) The microstructure consists of an ordered and a disordered phase, 2) The diffusivities depend on the local composition, and vary between the phases, and 3) Departures from the equilibrium SAXS pattern is as a result of the diffusional process. The evolution of the phase compositions as a function of time and radius are determined and compared to results from experimental investigations using atom probe tomography.

12:30 Coupling of Precipitation and Recrystallization Phenomena in a γ' Ni-based Superalloy: Marie-Agathe Chapagnac1; Nathalie Bozzolo1; Thomas Bilil1; Jean-Michel Franchet2; 1Mines ParisTech; 2Sneema-Safraan Group, 3Safraan SA

Recrystallization and second phase precipitate evolution during hot working has been investigated in a Ni-Al-Ti based superalloy. The alloy under study contains γ matrix and γ′ matrix phases (Ni3Al,Al3Ti): large primary particles aiming at grain boundary pinning, and fine-hardness ones which are dissolved at the forging temperatures but form again during cooling. The applied forging conditions allow (dynamic and post-dynamic) recrystallization to occur and precipitation to evolve simultaneously. While many studies are dedicated either to recrystallization in γ matrix or γ′ precipitation phenomena, the focus is placed here on the coupling of both phenomena: recrystallization influencing γ′ precipitation, and γ′ particles influencing recrystallization mechanisms. Nucleation and growth of γ′ into γ has been found to occur with diffusional and transformations. Scenarios are proposed to account for the observed evolutions, based on consideration of stored energy, chemical composition of grains and precipitates, boundary energies and migration.

12:45 Coexisting γ/γ′ Nanoscale Precipitation in a Fe-Cr-Al-Ti Alloy: Carlos Capdevila-Montes1; J. Chao1; Gemma Pimentel2; María Martín-Andarad1; Esteban Urones-Garrote3; Mike K. Miller4; 1CENIM-CSIC; 2University of Oxford, 3Centro Nacional de Microscopía Electrónica (CNMEE), Universidad Complutense de Madrid; 4Oak Ridge National Laboratory

The strengthening mechanisms observed in the oxide dispersion strengthened Fe-Cr-Al-Ti system have been investigated during ageing between 435 and 475 °C. The alloy underwent simultaneous nanoscale phase separation into TiAl-rich α′ phase, Fe-rich (α′) phase and Cr-rich (α′) phases that were responsible for the anomalous hardening increase observed. Atom probe tomography indicated that the composition of the intermetallic α′ phase was Fe4Al3Ti1. High-resolution transmission electron microscopy determined that the β′ precipitates were a cubic phase with the Hesler-type Fe2Al5 (L12) structure with lattice parameter a=0.5879 nm and a Fm-3m space group. The β′ particles were oriented along the 110α′ zone axis. The α′ phase could be explained by a number of processes: high anchoring of α′-phase separation, and the interaction of the coherent β′ particles with dislocations. Atom probe tomography was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.
12:15 The Effect of Alloying Element Partitioning on the Interface Velocity during the Isothermal Bainite Formation: Hussein Farahani; Wei Xu; Sybrand van der Zwaag; Detlev University of Technology

Following the previous study on the effect of alloying elements on the isothermal bainitic ferrite formation in quaternary steels with the mean field approximation, the Gibbs Energy Balance (GEB) model is further developed to incorporate the effect of partitioning of alloying elements in both austenite and ferrite domains. In the new model, distributions of alloying elements are updated according to their initial values, progress of the interface and corresponding local equilibrium condition at each time step. The dissipation of carbon (interstitial) diffusion inside and boundaries in austenite and ferrite is calculated as a driving force of the three phases.

12:30 Ab Initio Based Displacive-diffusional Theory for Structural Transformations among Austenite, Ferrite and Cementite in Fe-C Alloys: Xie Zhang; Tilman Hickel; Jutta Rogal; Raphael Dratz; Jong Moonbaeke

Structural transformations in Fe-C alloys are decisive for the mechanical properties of steels, but their modeling remains a theoretical challenge due to the coupling between the displacive rearrangement of Fe matrix and the diffusion of C. Within ab initio approach we have successfully decoupled the two aspects in the displacive-diffusional transformation. For the displacive part, a proper combination of atomistic crystallographic relationships and austenite, ferrite and cementite is decisive. We identify an intermediate structure, which consists of 33 twin boundaries in both the austenite and ferrite. The interfacial atomistic mechanisms during the transformation and the corresponding local equilibrium condition at each time step are described. The results are compared to previous simulations and the metallurgical insights are discussed.

12:45 Computational Materials Design: From Atoms to Applications: Ilya Efremov; Hao Jin; Joerg Rottler; Chad Sinclair; Benqiang Zhu; Matthias Mittelheier; University of British Columbia

Phase transformations assume a crucial role to tailor material properties during materials processing, e.g. the austenite-ferrite transformations are a key metallurgical tool for advancing the so-called high-strength low-alloy steels with improved mechanical properties. Computational materials science offers now tremendous opportunities to formulate transformation models containing fundamental information on the basic atomicistic mechanisms that can be implemented across different length and time scales. The kinetics of phase transformations depends critically on interface migration rates that are frequently significantly affected by the presence of alloying elements, e.g. Mn, Mo and Nb in iron and steel. Here, an approach is illustrated that links atomistic scale models for the solid-state interaction with phase field modelling to describe the formation of microstructures with complex morphologies. The overall status and challenges of multi-scale phase transformation modelling will be analyzed for continuous cooling and intercritical annealing of low-carbon steels.

11:45 Electric Field Induced Microstructure Formation in Polymers: Application in Polymer Blends and Diblock Copolymers: Amr Mubarak; Kumar Amrit; Rajesh Mubarak; Britta Nestler; Karlsruhe University of Applied Sciences; Kartlsruhe Institute of Technology; Indian Institute of Technology

There has been a long-standing interest on the application of external fields to control the morphology of polymer mixtures. Electric field is appealing because of the ease with which it can be applied, its ability to modulate morphologies and scales linearly with sample geometry, leading to a wide range of application in nano-devices. Experimental evidences show that external electric field leads to stretching and orientation of the phase separated domains along the direction of field leading to stripe or column formation. Motivated by experimental findings, in this presentation, we study the effect of electric field on the microstructure evolution of polymer mixture using phase-field method. In addition, coarsening and alignment of the microstructures are studied for critical and off-critical mixtures. A close agreement with the existing experiments and theory is established.

12:00 Spinodal Decomposition of Fe-Ni-C Martensite by Room Temperature Redistribution of Carbon Investigated by Corellative ECCI/TEM/APT: Michael Herbig; Ross Marceau; Lutz Monztorf; Pierk Rabe; Max-Planck-Institut für Eisenforschung GmbH; Deakin University

Carbon in martensite is mobile enough to form nm-scale substructures within hours/days via spinodal decomposition. We investigate this process in Fe-15Ni-1C (wt. %). After homogenization followed by water quench the alloy consists of 100% austenite. Quenching in liquid nitrogen results in the transformation into martensite and when brought back to room temperature the carbon in the martensitic phase undergoes spinodal decomposition. This process has already been investigated by atom probe tomography (APT) and transmission electron microscopy (TEM), but not at the exact same location in the microstructure. Therefore, it is still unclear which part of the complex lenticular martensite microstructure has been measured by APT and how this corresponds to TEM measurements. We illuminate this topic by correlating microstructure characterization using electron channeling contrast imaging (ECCI) and targeted preparation of needle-like APT samples at selected regions of interest, followed by TEM investigation of these needle samples and then subsequent APT investigation.

12:15 Spinodal Decomposition and the Carbon Solubility in BCC Fe-C: By-Na Kim; Ji-Ri Seo; Maria J. Santinovis; T.U. Delft

Recent findings have indicated that (i) carbon solubility in ferrite is larger than that predicted by the conventional Fe-C phase diagram, where a non-cubic structure of ferrite has been proposed, and (ii) local variations in carbon concentration consistently form within the matrix, thought to be the product of spinodal decomposition. These observations give rise to the scientific question of how carbon is distributed within ferrite, which remains under discussion in literature. The current study aims at establishing a thermodynamic explanation for the carbon solubility and partitioning within ferrite. Topics on carbon-competing processes such as spinodal decomposition in the Fe-C system and carbon segregation to defects have been revisited. Particular emphasis is put on the atom probe tomography (APT), a recurrent technique in the literature in the study of carbon redistribution in ferrite, and on its ambiguity in interpreting carbon profiles.

12:30 Phase Separation during Long Term Aged of a Complex Stainless Steel: Laurent Couturier; Frederic de Geuser; Alexis Deschamps; Université Grenoble Alpes, SIMAP, F-38000 Grenoble, France; CNRS, SIMAP, F-38000 Grenoble, France

The 15-5PH is a martensitic Fe-15%C Cr based stainless steel used for aerospace applications, which can be strengthened up to 1200MPa by copper precipitation. This material may be subjected to high temperature at moderate temperatures (250°C-400°C), which results in microstructural changes leading to modifications of its mechanical properties. Those changes include spinodal decomposition and formation of the G phase. In this presentation, we focus on the quantification of the Chromium spinodal decomposition kinetics. We use a combination of small-angle scattering experiments (SAS) and atom probe tomography (APT) to quantitatively describe the kinetics of this transformation both in terms of amplitude and length scale of the composition fluctuations.

12:45 Phase Transformations, Spinodal Decomposition, Precipitation Reaction, and Eutectoid Reaction, of a Fe-12.5 Mn-3 Al-1.28 C (wt%) Austenitic Steel: Wei Chun Cheng; Chih-Yao Cheng; Chia-Wei Hsu; National Taiwan University of Science and Technology

Phase transformations of an Fe-12.5 Mn-6.53 Al-1.28 C (wt%) austenitic steel, that include spinodal decomposition, precipitation transformation, and eutectoid reaction, have been studied after quenching from 1100°C and annealing at low temperatures. Spinodal decomposition takes place in the as-quenched steel. Fine coherent gamma’ particles precipitate homogeneously in the austenite. After annealing at temperature below 875°C, precipitation transformation occurs and kappa-carbide appears in the austenite as either a precipitation, a boundary precipitate or a second phase. The cellular precipitates are composed of lamellar austenite and a carbide. The lamellar kappa-carbide grains are always accompanied with martensite twins in the lamellar austenite grains. The presence of FCC twin layers adhered to the carbide plate may contribute to the lower activation energy for the precipitation of carbide plates. At temperatures below 700°C, the eutectoid reaction takes place and the supersaturated austenite decomposes into lamellar ferrite and kappa-carbide called kappa-pearlite.

13:00 The Co-PT Nanochessboard: Pseudospinodal Decomposition and the Resultant Ferromagnetic Properties: Priya Ghatwai; Eric Vetter; William Sofia; Jerome Fleury; University of Virginia

Eutectoid decomposition of A1 Co-PT alloys near 60% Pt can result in the nanochessboard structure – a 2+1D quasi-periodic tiling of L10 and L12 phases with a period of 15-35 nm. Fundamentally, the transformation can be analyzed as pseudo-spinodal decomposition, where the alloy composition must be slightly hyper-stoichiometric with respect to the composition where the free energy curves for the A1 and L12 phases cross. We find that the chessboard is obtained when a slow-cooling regimen through the eutectoid isotherm is used, followed by isothermal annealing. We are investigating the magnetic properties since the length scales and coherent interfaces should be conducive to exchange-coupling between the hard, uniaxial L12 and the softer, more isotropic L11. This talk will discuss how the chessboard microstructure depends on the thermal processing parameters, and how the aging process affects the coercivity, remanent and magnetic recoil properties. The mechanisms for magnetization reversal will also be discussed.
11:45 Invited 
Surface Precipitation on Engineering Alloys: 
Christopher Hutchinson\(^1\); Yu Chen\(^2\); Xiya Fang\(^1\); Yves Bréchet\(^1\); \(^1\)Monash University; \(^2\)Grenoble Institute of Technology

The nucleation and growth of solid state precipitates is used extensively to tailor the bulk mechanical properties of many engineering alloys. It is less well appreciated that precipitation can also be induced to occur on the surfaces of engineering alloys using simple heat treatments raising the possibility of using precipitation as a form of surface treatment. Surface precipitation occurs through a nucleation and growth process with kinetics that suggest mass transfer by surface (or interface) diffusion plays the dominant role. In this presentation, surface precipitation in a number of Al based alloys is presented, the physical principles underlying the phenomena are discussed and some interesting possibilities for 'surface physical metallurgy' are highlighted. Questions of the competition in phase formation on the surface, the compositions inherited by the growing surface precipitates and the coupling of bulk and surface diffusion are discussed.

12:15 
Precipitation Processes in Nanostructured 7475 
Aluminium Alloy: Małgorzata Lewandowska\(^2\); Agnieszka Kraczyńska\(^2\); Ajit Panigrahi\(^1\); Erhard Schaffler\(^3\); Michael Zöchling\(^2\); \(^1\)Warsaw University of Technology; \(^2\)University of Vienna

In ultrafine and/or nanograin materials, precipitation phenomena are significantly affected by the high surface area of grain boundaries. Therefore, this work tried to evaluate the influence of grain boundaries on precipitation processes in detail. Samples of 7475 aluminium alloy were solution annealed, water quenched and processed at RT by hydrostatic extrusion (HE) and high pressure torsion (HPT). While both processing procedures yield significant reductions in grain size there are differences in the resulting grain shape (fibre-like for HE, pancake-like for HPT) and in the grain boundary type. Extensive grain boundary precipitation occurs in both samples, more pronounced and faster in HPT ones, which can be attributed to the different characters of grain boundaries involved. Inside the grains, precipitates are significantly smaller than in micrograined materials, which has been discussed in terms of HE / HPT induced vacancy concentrations in micro- and nanostructured samples.

12:30 
Metallurgy in High Magnetic Field: From Phase Equilibria to Enhanced Soft Magnetic Properties of Fe-Co Alloys: Sophie Rivard\(^1\); Bianca Frincu\(^1\); Rajasekhar Madugundo\(^2\); Olivier Geoffroy\(^2\); Thierry Wackernagel\(^1\); CNRS/CRETA; \(^2\)GPM Laboratory, Université de Rouen; \(^1\)Monash University

Reducing the energy consumption is one of the driving forces for the development of improved materials. In this respect, both new metallurgical processes and improved magnetic materials can provide future solutions for a sustainable development. Thermo-magnetic processing is presented as a new technology which can lead to improved soft magnetic properties in Fe-Co alloys unattainable through conventional processing. In this work, the effect of a high magnetic field on the $\alpha$-$\gamma$ phase transformation in Fe-Co alloys was quantitatively measured by dilatation measurements up to 16 T. A linear shift of about 2°C/T in Fe-Co alloys was quantitatively measured by dilatation in the presence of a high field. We use Atom Probe Tomography (APT) and Transmission Electron Microscopy (TEM) to determine atomic scale structural and composition information.

12:45 
Enhanced Recovery and Recrystallization of Pure Copper Due to an Applied Current: Damien Fabrigue\(^2\); Xavier Boulnat\(^1\); Bassem Mouawad\(^1\); Christopher Hutchinson\(^3\); \(^1\)MATEIS, INSA Lyon; \(^2\)Monash University

Applying a high current to metals can have drastic effects on their microstructure. But usually the applied currents are very high. However, some recent studies has shown that reasonable currents during straining can permit, for example, to increase the ductility of aluminium alloys. Thus we have investigated the influence of an applied current on the recovery and recrystallization using a SPS machine on a cold drawn pure copper. By comparing samples heated by the Joule effect with those heated in a salt bath, it is shown than recovery and recrystallization are greatly accelerated by the current. At low temperatures, where only recovery occurs during conventional thermal treatments, fully recrystallized microstructures are obtained when the heating is applied through the Joule effect. The influence of the time and of the density of current for a given temperature is also studied.

13:00 
Kinetics of Precipitation in New Generation of Cobalt-based Superalloy: Ahmad Azzam\(^1\); Thomas Philipp\(^2\); Frédéric Danoix\(^2\); Annie Hauet\(^2\); Didier Blavette\(^2\); \(^1\)GPM Laboratory, Université de Rouen; \(^2\)GPM Laboratory, Université de Rouen

Nickel superalloys are widely used in aerospace industry and especially for advanced turbine engines. These materials derive their excellent mechanical properties at high temperature (creep) from the presence of a high volume fraction of ordered L12 $\gamma'$ precipitates embedded in a disordered face centered cubic (FCC) $\gamma$ matrix. New Co-based superalloys hardened by Co$_3$(Al,W) $\gamma'$ precipitates were recently investigated [1,2]. In this work, we study the kinetics of precipitation (nucleation, growth and coarsening) in model Co-Al-W ternary superalloys after heat treatment at 900°C. We use Atom Probe Tomography (APT) and Transmission Electron Microscopy (TEM) to determine atomic scale structural and composition information.

3D atomic maps will be confronted to kinetic Monte Carlo simulations (rigid lattice, residence time algorithm).[1]

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