Modelling of Precipitation

THURSDAY PM ROOM: ALPINE D-E
SESSION CHAIR: JESPER FRIIS, SINTEF

14:15 Invited

The Use of Density Functional Theory to Explore Precipitation-hardened Alloy Systems: *Chris Wolverton*[1]; [1]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 precipitate phases as well as be able to provide predictions 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, we 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 U-Nb System: *Thien Duong*[1]; Robert Hackenberg[2]; Alexander Landa[3]; Sean Gibbons[1]; Saurabh Bajaj[4]; Andrei Ruban[5]; Levente Vitos[5]; Patrice Turchi[3]; Raymundo Arroyave[1]; [1]Texas A&M University; [2]Los Alamos National Laboratory; [3]Lawrence Livermore National Laboratory; [4]California Institute of Technology; [5]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 factors underlying these specific transformation characteristics and reaction paths, vis-a-vis the monotectoid 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 representations. Good agreements with experiments on different physical/length scales were achieved, which validates 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: *Minsu Jung*[1]; Sai Ramudu Meka[1]; Bastian Rheingans[2]; Eric Jan Mittemeijer[1]; [1]Max Planck Institute for Intelligent Systems (formerly Max Planck Institute for Metals Research); [2]Institute for Materials Science, University of Stuttgart

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 accurately. 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_yI_z, with M as alloying element initially dissolved in the substrate. The model was applied to the gaseous nitriding of iron-based alloys, incorporating the role of excess nitrogen and the ammonia-dissociation 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 Micro-alloyed Steel: Heinrich Buken[1]; Pavel Sherstnev[2]; *Ernst Kozeschnik*[1]; [1]Vienna University of Technology; [2]Leichtmetallkompetenzzentrum Ranshofen

Recrystallization is a phenomenon where the polycrystalline microstructure of metallic materials is entirely rebuild after plastic deformation and subsequent thermal treatment. Nowadays, the kinetics of recrystallization can be well described computationally in many alloy systems. In contrast, physical models describing the influence of recrystallization on precipitation and, 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 modelling approach that describes this phenomenon of recrystallization stop by precipitation and continuation of recrystallization due to precipitate coarsening in the framework of 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

THURSDAY PM ROOM: CALLAGHAN
SESSION CHAIR: CYRIL CAYRON, EPFL IMX LMTM

14:15 Invited

Effect of Free Surface on Martensitic Transformation in Individual Retained Austenite Grains: *Mingxin Huang*[1]; [1]The University of Hong Kong

The stability of retained austenite depends on the chemical composition, morphology, grain size and hardness of the surrounding matrix. Different to these aspects, the present work explores the effect of free surface on the stability of retained austenite. The first part is to employ FIB milling to create free surface around individual retained austenite grains. It was found that martensitic transformation took place automatically in the retained austenite grain when a free surface was introduced, without applying external stress. This is due to the fact that the martensite nucleation energy barrier can be lowered as the strain energy induced by martensitic transformation is largely lowered when the matrix constraints were removed. The second part investigates martensitic transformation in micron-sized pillars which were fabricated by FIB from individual retained austenite grains. It was found that that α'-martensite formed in micron-sized pillars was nearly dislocation free due to the free surface effect.

14:45

3-dimensional Microstructural Observation of Butterfly-type Martensite in Fe-Ni-Cr-C Alloy by Serial Sectioning Method: *Hisashi Sato*[1]; Kousuke Fujimoto[1]; Tomoyuki Tanaka[1]; Yoshimi Watanabe[1]; [1]Nagoya Institute of Technology

Butterfly-type martensite is formed at formation temperature between lath-type and lenticular-type martensites. Although the butterfly-type martensite has more complicate shape comparing with other types, 3-dimensitional shape and its crystal orientation distribution are not clear. In this study, microstructure of butterfly-type martensite in Fe-18mass%Ni-0.7mass%Cr-0.5mass%C alloy is 3-dimensionally 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.

15:00

Excellent Mechanical Properties of Fine 0.1C-2Si-5Mn Fresh Martensite: *Shiro Torizuka*[1]; Toshihiro Hanamura[2]; [1]University of Hyogo ; [2]National Institute for Materials Science

0.1%C-5% Mn steels have a high tensile strength of more than 1400MPa and a high total elongation of 17% and are considered to be very attractive in industrial application. However, the phase transformation behavior in middle Mn steels, e.g. 5.0%Mn steel, has not fully been investigated. In this study, the effect of Mn content in the range of 1.5 - 6.0% in 0.1%C-2.0%Si steels on their transformation behavior has been examined from the points of CCT and TTT. The effect of Mn and prior austenite grain size on tensile properties and work hardening behavior are investigated.

15:15

Effect of Pre-existing Martensite on the Isothermal Transformation Kinetics below the Ms Temperature in a Low-C High-Si Steel: *Alfonso Navarro-Lopez*[1]; Jilt Sietsma[1]; Maria J. Santofimia[1]; [1]Delft University of Technology

Thermomechanical processing of Advanced Multiphase High Strength Steels often includes isothermal treatments around the martensite start temperature (Ms). Investigations show that the presence of martensite prior to these isothermal treatments accelerates the kinetics of the subsequent transformation. This kinetic effect may 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 martensite affects the nucleation kinetics of the subsequent transformation as well as to qualitatively and quantitatively determine this contribution. For this purpose, dilatometry experiments were performed at different temperatures above and below Ms in a low-carbon high-silicon steel. The combination of experimental and theoretical analysis of the nucleation processes led to the identification of the isothermal product as bainite and the proposition of a possible mechanism by which pre-existing martensite affects subsequent transformations below the Ms temperature.

15:30

Grain Refinement by Cyclic Displacive Forward/Reverse Transformations: *Tadachika Chiba*[1]; Goro Miyamoto[1]; Tadashi Furuhara[1]; [1]Tohoku University

Cyclic transformation has been applied to refine microstructure of low-alloyed steels, where diffusional austenite reversion takes place during heating, followed by martensite transformation during cooling. It was reported that finer austenite grain after a few cycles leads to the refinement of final microstructure. On the other hand, we focus on cyclic transformation of displacive reverse and forward transformations by lowering transformation temperature, e.g. high Ni alloys. It is expected that a high density of dislocations is introduced in each transformation and large strain is accumulated without applying explicit deformation and thus, final martensite structure can be refined effectively. Therefore, in this study, we investigated microstructure change in Fe-18Ni and Fe-18Ni-0.1C(mass%) alloys with cyclic transformations. It was found that austenite grain size does not change by cyclic transformations due to austenite memory phenomena while martensite structure got finer, in particular the small amount of carbon markedly enhances refinement of martensite.

15:45 Break