MM 30: Structural Materials I

Time: Wednesday 10:15–11:30 Location: H52

MM 30.1 Wed 10:15 H52

Thermodynamic properties of ultra-high temperature ceramics: ab initio accuracy up to the melting point — •Andrew Duff[1], Dominique Korbmacher[2], Albert Glensk[2], Blazej Grabowski[2], Joerg Neugebauer[2], and Michael Finnis[1] — [1]Department of Materials, Thomas Young Centre, Imperial College London, Exhibition Road, London SW7 2AZ, UK — [2]Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, Düsseldorf 40237, Germany

A new method for calculating ab initio thermodynamic properties of materials is presented. The new approach, termed TU-TILD (two-stage upsampled thermodynamic integration using Langevin dynamics) captures the full anharmonicity of the lattice vibrations and provides at least an order of magnitude improvement in efficiency compared to the UP-TILD approach on which it is based. Using TU-TILD, free energies can be calculated up to the melting point at the full accuracy of the underlying ab initio theory– in the present case, density functional theory –overcoming limitations of the widely used quasiharmonic approximation, whilst significantly closing the gap in computational efficiency between fully anharmonic and quasiharmonic methodologies. The new approach is used to calculate thermodynamic properties of the ultra-high temperature ceramics: zirconium carbide; zirconium diboride and hafnium carbide. The results show a distinct improvement over quasiharmonic calculations, with heat capacities and thermal expansion data brought more closely in line with experimental results and, where available, the results of CALPHAD assessments.

MM 30.2 Wed 10:30 H52

Atomic-scale modeling of point defects, phase stability, and the formation mechanism of Z phases CrMN (M=V, Nb, Ta) — •Daniel F. Urban, Matous Mrovec, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

The challenge of raising the steam inlet temperature of fossil-fired power plants calls for creep-resistant steels with a Cr content higher than 9% in order to achieve sufficient corrosion and oxidation resistance. However, it has been found that in 11-12% Cr ferritic-martensitic creep resistant steels strengthened by fine (V,Nb)N particles, precipitation of thermodynamically stable Z-phase particles, CrMN (M=V,Nb,Ta), in long-term service is unavoidable and detrimental. Usually, Z-phase particles are coarse and brittle and grow at the expense of the desired fine (V,Nb)N particles.

We present atomistic simulations, using density function theory, which reveal the essential mechanisms underlying the formation of Z-phases. We study the thermodynamic stability of Z-phase, related structures and predecessors as well as the basic phase formation mechanisms. The picture that evolves consists of the diffusion of Cr atoms into MN particles and their subsequent clustering in a layered arrangement which finally yields the transformation of the nitride particles to Z-phase particles. Our results support experimental efforts to control the precipitation of the Z-phase through appropriate microstructural engineering.

MM 30.3 Wed 10:45 H52

Solubility of boron, carbon, and nitrogen in transition metals: getting insight into trends from first-principles calculations — Xiaohui Hu[1,2], Torbjörn Björkman[2], Litao Sun[1], and •Arkady Krasheninnikov[2,3] — [1]FEI Nano-Pico Center, Southeast U., China — [2]Dep. of Appl.Phys., Aalto U., Finland — [3]Helmholtz Zentrum Dresden-Rossendorf, Inst. of Ion Beam Phys. and Mat. Res., Germany

Efficient chemical vapor deposition synthesis of 2D materials such as graphene, boron nitride, and mixed BCN systems requires precise knowledge of the solubility and mobility of B/C/N atoms in the transition metals (TMs) used as substrates for the growth. Yet, surprisingly little is known about these quantities either from experiments or simulations. Using first-principles calculations, we systematically study [1] the behavior of B/C/N impurity atoms in a wide range of TMs. We compute formation energies of B/C/N interstitials and demonstrate that they exhibit a peculiar but common behavior for TMs in different rows of the periodic table, as experimentally observed for C. Our simulations indicate that this behavior originates from an interplay between the unit cell volume and filling of the d- shell electronic states of the metals. We further assess the vibrational and electronic entropic contributions to the solubility, as well as the role of anharmonic effects. Finally, we calculate the migration barriers, an important parameter in the growth kinetics. Our results not only unravel the fundamental behavior of interstitials in TMs but also provide a large body of reference data, which can be used for optimizing the growth of 2D BCN materials. [1] X. Hu, et al., JPC Lett., 6 (2015) 3263.

MM 30.4 Wed 11:00 H52

Modelling yttrium diffusion in ODS steels — •Markus Mock and Karsten Albe — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt, Germany

Oxide dispersion strengthened (ODS) steels are promising structure materials for future fission and advanced fusion materials. They contain yttrium oxide nanoparticles that enable outstanding high-temperature properties and unique irradiation tolerance. The size, shape and distribution of the particles is of utmost importance for the properties of the material and understanding the precipitation process will allow tailoring the material properties for specific applications. Precipitation of yttrium oxide particles requires diffusion of yttrium through the iron lattice even though there is a high binding energy between substitutional yttrium atoms and vacancies. To investigate the mechanism of yttrium diffusion we created an atomic bond order potential for the iron-yttrium interaction and calculated activation barriers of relevant diffusion events. We present a model for the diffusion mechanism of yttrium through iron that helps understanding the precipitation process in ODS steels.

15 min. coffee break