International Workshop on

Ab initio Description of Iron and Steel: Mechanical Properties

Ringberg Castle 3 - 7 October 2016

Ab initio Description of Iron and Steel: Mechanical Properties

ADIS2016, Ringberg Castle, 3-7 October, 2016

Preface

It is our pleasure to welcome you to our workshop on

"Ab initio Description of Iron and Steel: Mechanical Properties"

at Ringberg castle. The series of ADIS workshops is inspired by the impressive variety of competing mechanisms on the microscopic/atomic scale, which determine the performance of engineering materials such as steels. Accordingly, the main scope of the workshops is a thorough and detailed discussion of this behavior, in order to understand the underlying physics and to contribute to a further systematic improvement of the materials. We are convinced that a truly predictive approach to materials modeling needs to be based on a fundamental ab initio level, rooted in the laws of nature rather than empiricism. This is also the driving force for the collaborative research centre SFB761 Steel ab initio, which is devoted to a quantum-mechanically guided design in high- and medium-Mn steels and funding this workshop. We are grateful that the importance of this development is further recognized by the Psi-k Charity, which is financially supporting ADIS2016.

Recent years have seen dramatic progress in ab initio based methods, which now makes the exploration of chemical trends, the determination of parameters for phenomenological models and the identification of new routes for the optimization of steel properties feasible. Having used the previous workshops to get an overview of these methods (ADIS2006) with a focus on thermodynamics and kinetics (ADIS2012), on approaches to magnetic phenomena (ADIS2008 and ADIS2014), we shall use the present workshop (like ADIS2010) to discuss recent progress in the simulation of mechanical properties.

The spectrum of materials properties and microstructure features on its mechanical behaviour is manifold. We want to focus the discussions on those aspects that are also relevant for steel design, while examples are from a wide range of materials including high-entropy alloys. In particular we will have contributions about

- **Plasticity**. Multiscale approaches from atomistics to the macroscopic response for questions like thermally activated slip and crack-microstructure interaction are discussed.
- **Dislocations**. The spectrum of considered aspects ranges from the description of their (core) structure, via the interaction with solutes up to understanding the mechanisms of hardening.
- **Planar defects**. The structure, chemical composition, strain state and mobility of grain boundaries is addressed, since they are important for the strength of materials. Further, the energy of stacking faults is decisive for deformation and twinning mechanisms.
- **Precipitates**. This includes questions like nucleation, thermodynamics stability, the partitioning of elements and elastic properties of these phases.

The workshop will be dominated by ab initio and atomistic simulations. Nevertheless, alternative theoretical methods and experimental techniques will also be addressed.

The workshop is intended to provide a platform to discussion and exchange recent results / scientific developments and therewith initiate future collaborations. As in previous years, a key characteristic of the workshop will be the tutorial-like one hour invited talks. However, the workshop critically depends on all contributions, talks and posters, but most importantly on stimulating discussions of the presented material. Hence, there will be ample time for discussion after each talk, in the poster session, in various breaks, during the excursion or with a glass of wine in the witches room to discuss methods, their physical interpretation and results. You are encouraged to contribute to the exchange of ideas, making the meeting exciting and fruitful for all of us.

The organizers:

Tilmann Hickel   Ralf Drautz   Jörg Neugebauer

Ab initio Description of Iron and Steel: Mechanical Properties

ADIS2016, Ringberg Castle, 3-7 October, 2016

This seminar is supported by Psi-k network and the Collaborative Research Centre (SFB761) "Steel - ab initio":

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Ab initio Description of Iron and Steel: Mechanical Properties

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Programme

Monday, October 03rd

12:00	Opening and Introduction into the topic: **Organizers**
12:30	Lunch

Atomistic simulation of plasticity

Chair: **Jörg Neugebauer**

14:00-15:00	**Erik Bitzek** (Universität Erlangen-Nürnberg, Germany): *Atomistic simulations of fracture and crack-microstructure interactions in BCC metals*
15:15	Coffee
15:45-16:45	**Roman Gröger** (Academy of Sciences of the Czech Republic): *Plasticity of BCC metals from atomic scale to continuum*
17:00-18:00	**Adrian Sutton** (Imperial College London, UK): *Modelling shocks in metals (or real dislocation dynamics)*
18:30	Dinner
20:00	Poster session

Programme

Tuesday, October 04th

Complex alloys: High-entropy alloys and stacking faults

Chair: **Thomas Hammerschmidt**

08:00	Breakfast
08:45-09:45	**Easo P. George** (Ruhr University Bochum, Germany): *High-Entropy alloys and complex solid solutions - fundamental mechanisms of deformation and fracture*
10:00-10:30	**Duc Nguyen-Manh** (Culham Centre for Fusion Energy, Abingdon, UK): *Precipitate phase and local strain in high-entropy alloys: a first-principles assessment*
10:35	Coffee
11:00-11:30	**Blazej Grabowski** (MPI für Eisenforschung, Düsseldorf, Germany): *High accuracy finite temperature stacking fault energies*
11:35-12:05	**Song Lu** (University of Turku, Finland): *Stacking fault energy of C-alloyed steels: the effect of magnetism*
12:30	Lunch

Stability of precipitate phases

Chair: **Jutta Rogal**

14:00-15:00	**Christian Elsässer** (Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany): *Atomic-scale modeling of point defects, phase stability, and the formation of Z phases CrMN (M=V, Nb, Ta) in steel*
15:15-15:45	**Hideaki Sawada** (Nippon Steel & Sumitomo Metal Corporation, Japan): *Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics*
15:50	Coffee

Grain boundaries and interfaces

Chair: **Gabor Csanyi**

16:15-17:15	**Gerhard Wilde** (University of Münster, Germany): *Grain boundaries in severely deformed metallic materials*
17:30-18:00	**Sherri Hadian** (MPI für Eisenforschung, Düsseldorf, Germany): *Grain boundary faceting and its effect on migration kinetics*
18:30	Dinner
20:00-20:30	**Mojmir Šob** (Academy of Sciences of the Czech Republic): *Grain boundary segregation and embrittlement: recent advances and open problems*
20:35-21:05	**Martin Friák** (Academy of Sciences of the Czech Republic): *Anisotropic elastic properties and mechanical stability of $\Sigma 5(210)$ grain-boundary complexions in Ni_3Al from ab initio calculations*
21:10-21:40	**Francesco Maresca** (Ecole Polytechnique Federale de Lausanne, Switzerland): *Structure and mobility of the austenite/martensite interface in steels*

Wednesday, October 05th

Method development

Chair: **Eunan McEniry**

08:00	Breakfast
08:45-09:45	**Alessandro De Vita** (King's College London): *Materials chemomechanics by inference-boosted first principles modelling*
10:00-10:30	**Ralf Drautz** (ICAMS, Ruhr-Universität Bochum, Germany): *From density functional theory to magnetic interatomic potentials and phase transformation kinetics*
10:35	Coffee
11:00-11:30	**Thomas D. Daff** (University of Cambridge, UK): *Atomistic models for hydrogen embrittlement*
11:35-12:05	**Casper D. Versteylen** (Technische Universiteit Delft, the Netherlands): *Modelling self-healing creep damage and healing in Iron*
12:30	Lunch
13:15	Excursion
18:30	Dinner

Complex alloys: Precipitates

Chair: **Martin Friák**

20:00-20:30	**Christian H. Liebscher** (MPI für Eisenforschung, Düsseldorf, Germany): *Hierarchical microstructure of ferritic superalloys*
20:35-21:05	**Sascha B. Maisel** (MPI für Eisenforschung, Düsseldorf, Germany): *Design of Ti-based alloys with austenitic Ni-Ti nanoprecipitates*
21:10-21:40	**Sergiy V. Divinski** (University of Münster, Germany): *High-pressure torsion of Cu/Ta layered system*

Programme

Thursday, October 06th

Dislocations I
Chair: **Ralf Drautz**

08:00	Breakfast
08:45-09:45	**Lorenz Romaner** (Materials Center Forschung GmbH, Leoben, Austria): *Ab-initio simulations of dislocations in BCC transition metals and alloys*
10:00	Coffee
10:30-11:30	**François Willaime** (CEA-DEN, Gif-sur-Yvette, France): *Ab initio modeling of dislocation core properties in bcc metals*
11:45-12:15	**Matous Mrovec** (ICAMS, Ruhr-University, Bochum, Germany): *Atomistic studies of non-screw dislocations in iron using magnetic bond-order potentials*
12:30	Lunch

Dislocations II
Chair: **Tilmann Hickel**

14:00-15:00	**Dallas R. Trinkle** (University Illinois, Urbana-Champaign, USA): *Solute interactions with dislocations in BCC Fe*
15:15	Coffee
15:40-16:10	**Gerard Leyson** (MPI für Eisenforschung, Düsseldorf, Germany): *Multiscale modeling of local phase transitions at dislocations*
16:15-17:15	**William A. Curtin** (Ecole Polytechnique Federale de Lausanne, Switzerland): *Structure, energetics, and transformations of* $\langle a\rangle$ *and* $\langle c+a\rangle$ *dislocations in HCP metals*
17:30	Closing remarks: **n.n.**
18:30	Conference dinner
20:00	Discussion: Results of the workshop and future perspectives

Friday, October 07th

08:00	Breakfast
09:00	Discussions

ABSTRACTS

INVITED AND CONTRIBUTED TALKS

Invited talk	Monday, October 03th, 14:00

Invited talk Monday, October 03th, 14:00

Atomistic simulations of fracture and crack-microstructure interactions in BCC metals

Erik Bitzek[1], Polina Baranova[1], Johannes J. Möller[1,2]

[1] *Department for Materials Science and Engineering, Institute I,*
Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany;
[2] *now at Fraunhofer IWM, Freiburg, Germany;*

The resistance to crack propagation is undoubtedly one of the most important properties of structural materials. Whether a stressed component fractures by brittle cleavage or by ductile rupture is determined by the competition between bond-breaking at the crack tip and plastic deformation in the vicinity of the crack. Which of these processes dominates at a given temperature and strain rate depends on the nature of the chemical bond between the atoms as well as on the microstructure of the material. While meso- and continuum-scale methods can be used to model the elastic loading of the crack tip and the plastic dissipation in the process zone, only atomistic simulation methods can be used to study the direct interactions between cracks and constituents of the microstructure (e.g., dislocations, grain boundaries, particles or voids) or the nucleation of dislocations at the crack front[1]. However, up-to-date most atomistic fracture simulations use idealized setups with perfectly straight crack-fronts in quasi-2D geometries. Only few simulations address the full complexity of 3D crack - microstructure interactions, including curved crack fronts and dislocations on oblique slip systems. Here we present our recent work on large-scale atomistic fracture simulations using EAM-type potentials for α-Iron and other BCC metals, focusing on often neglected 3D aspects.

The first part will be devoted to a tutorial-style overview of different approaches to perform atomistic fracture simulations, explaining the methodological background and challenges as well as providing best practices regarding the selection of interatomic potentials[2], simulation setups and boundary conditions. We then compare the results of straight crack fronts in quasi-2D set-ups with curved crack fronts in 3D set-ups[3]. General aspects relevant for crack-microstructure interactions in BCC metals will be discussed using exemplary simulations of cracks interacting with pre-existing dislocations, voids and precipitates in 3D. Finally, quasi-2D grain boundary fracture simulations[4] will be compared to recent large-scale simulations on penny-shaped grain boundary cracks. All these results demonstrate the importance of 3D models to study crack nuclei and crack-obstacle interactions and the inability of 2D models with straight crack fronts to predict the behavior of curved crack fronts.

[1] E. Bitzek, J.R. Kermode and P. Gumbsch, Int. J. Fract. **191**, 13 (2015).

[2] J.J. Möller, E. Bitzek, Modelling Simul. Mat. Sci. Eng. **22**, 045002 (2014).

[3] J.J. Möller, E. Bitzek, Eng. Fract. Mech. **150**, 197 (2015).

[4] J.J. Möller, E. Bitzek, Acta Mater. **73**, 1 (2014).

Invited talk	Monday, October 03th, 15:45

Invited talk	Monday, October 03th, 15:45

Plasticity of BCC metals from atomic scale to continuum

Roman Gröger[1], Vaclav Vitek[2]

[1] *Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Rep.;*
[2] *Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, USA*

Body-centered cubic (BCC) metals are crystallographically simple materials whose plastic deformation is nevertheless governed by processes that are not common in face-centered cubic (FCC) metals. These differences are rooted at the atomic level, where the cores of $1/2\langle 111\rangle$ screw dislocations in BCC metals are inherently nonplanar[1], which contrasts the plane cores of dissociated $1/2\langle 110\rangle$ dislocations in FCC crystals. Due to the nonplanar spreading of the former dislocations, their motion is not affected only by the shear stress in the $\{110\}$ slip plane acting parallel to the slip direction (i.e., the Schmid stress) but, in principle, by all components of the stress tensor[2]. Under small strains and strain rates relevant for engineering applications, the critical resolved shear stress (CRSS) acting in the maximum resolved shear stress plane (MRSSP) parallel to the slip direction was shown[2,3] to depend on: (i) the angle χ of the MRSSP, and (ii) the magnitude of the shear stress perpendicular to the slip direction. This information was obtained by molecular statics simulations on isolated screw dislocations[4] using Bond Order Potentials (BOP)[5] and predicts the occurrence of anomalous slip in BCC Mo and W that has been observed experimentally in all nonmagnetic BCC metals. We have represented the obtained atomistic data mathematically using a relatively simple yield criterion, $\tau_0 + \sum_{i=1}^{3} a_i\tau_i = \tau^*_{cr}$ that depends linearly on two shear stresses parallel and two perpendicular to the slip direction, both acting in two different $\{110\}$ planes in the zone of the slip direction. The four adjustable parameters (a_1, a_2, a_3, τ^*_{cr}) are obtained by fitting the results of atomistic simulations. We will utilize this criterion to predict the activity of twelve $\{110\}\langle 111\rangle$ systems in BCC Mo and W under tension and compression. It suggests the existence of tension-compression asymmetry, which has been observed in the past five decades in all BCC metals. The parametrization sometimes requires further fine-tuning using experimental data as evidenced by comparing theoretical predictions with recent in situ experiments on compressed micropillars[6].

The link between the atomistic studies of isolated screw dislocations and macroscopic response of the material is established by formulating a thermodynamic model of thermally activated slip that is based on the Arrhenius law $\dot\gamma = \dot\gamma_0 \exp[-\Delta H(\tau)/kT]$. Here, $\Delta H(\tau)$ is the activation enthalpy needed to transform a straight screw dislocation at the applied stress τ into the curved configuration that needs no additional energy to surmount the periodically varying lattice friction and thus to move through the crystal. This stress dependence of the activation enthalpy can be obtained from a model derived using the variational calculus[7]. The most important inputs into this model are the Peierls barrier, its variation with the applied stress, and the curvature of the dislocation pathway, all of which can be obtained using Nudged Elastic Band (NEB) calculations on a straight dislocation[8]. We will highlight the underlying assumptions in these models and propose ways to include further details such as the orientational dependence of the dislocation line energy and interactions between dislocation segments in the activated state. This thermodynamic model will be used to predict the temperature dependence of the flow stress and compare it with experimental measurements[9,10]. This methodology is applicable not only to all nonmagnetic BCC metals but also to ferromagnetic α-Fe whose plastic deformation is simplified by the lack of anomalous slip.

[1] V. Vitek, R. C. Perrin, D. K. Bowen, Philos. Mag. **21**, 1049 (1970). [2] K. Ito, V. Vitek, Philos. Mag. A **81**, 1387 (2001). [3] R. Gröger, Philos. Mag. **94**, 2021 (2014). [4] R. Gröger, A. G. Bailey, V. Vitek, Acta Mater. **56**, 5401 (2008). [5] R. Drautz, T. Hammerschmidt, M. Čák, D. G. Pettifor, Model. Simul. Mater. Sci. Eng. **23**, 074004 (2015). [6] C. Marichal, H. Van Swygenhoven, S. Van Petegem, C. Borca, Sci. Rep. **3**, 254 (2013). [7] J. E. Dorn, S. Rajnak, Trans. AIME **230**, 1052 (1964). [8] R. Gröger, V. Vitek, Mat. Sci. Eng. A **643**, 203 (2015). [9] W. Wasserbäch, Phys. Stat. Sol. A **147**, 417 (1995). [10] A. Seeger, L. Hollang, Mater. Trans. **41**, 141 (2000).

Invited talk	Monday, October 03th, 17:00

Invited talk	Monday, October 03th, 17:00

Modelling shocks in metals
(or *real* dislocation dynamics)

Adrian Sutton[1], Daniel Eakins[1], Beñat Gurrutxaga Lerma[2], Daniel Balint[2], Daniele Dini[2]

[1] *Department of Physics, Imperial College London, UK;*
[2] *Department of Mechanical Engineering, Imperial College London, UK;*

During shocks metals deform at much higher strain rates than those normally encountered in plastic deformation, typically up to 10^{10} s^{-1}. Shock loading occurs during high speed car crashes, birds flying into the compressor blades of aircraft engines, missile strikes on tanks and ships, and more sinister weaponry.

Shocks are studied experimentally by firing projectiles in gas guns at stationary metallic targets at speeds of about 1 km s^{-1}, or pulsing the surfaces of metals with intense lasers. In both cases a shock wave enters the metal at the longitudinal speed of sound. As it travels through the metal, dislocations are generated at the shock front and travel at speeds approaching the shear wave speed. At such high dislocation speeds the finite time it takes for elastic signals to travel through the medium becomes significant. The force on a dislocation per unit length is still the Peach-Koehler force, i.e. the resolved shear stress on the slip plane in the direction of the Burgers vector. But by the time a dislocation experiences the stress wave emitted by another dislocation, that other dislocation is no longer at the position it was when it emitted the wave. This means that the *time-dependent* equations of elasticity have to be solved to describe the interactions between dislocations and their interactions with the shock wave. This is analogous to the distinction between electrostatics and electrodynamics, except that the relevant wave speed in elasticity is the shear wave speed rather than the speed of light.

Describing interactions between large numbers of moving dislocations is the purview of dislocation dynamics. But until our work[1−3] all dislocation dynamics codes were based on a quasistatic description of dislocation interactions: at each time step the instantaneous configuration of dislocations is frozen and their interactions are described in terms of their static, time-independent elastic fields. I will show in this talk how these methods fail spectacularly to model dislocation dynamics during shock loading. It was this discovery that motivated our development of *Dynamic discrete dislocation plasticity (D3P)*[1], the first fully elastodynamic treatment of dislocation dynamics.

In this talk I will show what is involved in an elastodynamic treatment of dislocation dynamics. I will then show its application to solving a long-standing mystery in shock physics, namely why the yield point, which is the stress at which the metal begins to deform plastically, decreases the further a shock wave travels into the metal. Our explanation[2] involves the destructive interference of elastic waves at the shock front - unusual concepts and language to use in the context of dislocations interactions.

This research was carried out in the Centre for Doctoral Training on Theory and Simulation of Materials at Imperial College, funded by EPSRC grant EP/G036888/1.

[1] B Gurrutxaga-Lerma, D S Balint, D Dini, D E Eakins, and A P Sutton, Proc. R. Soc. A 469, 20130141 (2013).
[2] B Gurrutxaga-Lerma, D S Balint, D Dini, D E Eakins and A P Sutton, Phys. Rev. Lett. 114, 174301 (2015)
[3] B Gurrutxaga-Lerma, D S Balint, D Dini, D E Eakins, and A P Sutton, Adv. in Appl. Mechanics 47, 93-224 (2014).

Invited talk	Tuesday, October 04th, 8:45

Invited talk Tuesday, October 04th, 8:45

High-entropy alloys and complex solid solutions - fundamental mechanisms of deformation and fracture

Easo George, Guillaume Laplanche, Aleksander Kostka, Gunther Eggeler

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There is worldwide interest in high-entropy alloys (HEAs), which are generally defined as consisting of five or more elements in nearly equal atomic ratios. Some HEAs exhibit excellent mechanical properties, for example, simultaneous increase of strength, ductility and toughness with decreasing temperature, which breaks the inverse strength-ductility relationship that is typical in most materials. They are scientifically interesting because their local atomic arrangements are difficult to characterize and it is not trivial to relate their local structural and chemical fluctuations to global average properties. It is also difficult to visualize the operative deformation mechanisms in such complex solid solutions. As a result, despite the recent fascination with HEAs, fundamental aspects of their mechanical behavior remain largely unclear.

In this talk I will summarize what we have learned about the behavior of compositionally complex solid solutions with the help of a model, face-centered cubic, high-entropy alloy and its simpler medium-entropy relatives. Various microstructural features contributing to plasticity will be discussed, including grain size, texture, dislocations, stacking faults, and nano-twins. Microstructural features will be quantified (e.g., dislocation density, twin density) and their evolution with strain and temperature will be related to flow stress, work hardening rate, and ductility. To the extent possible, compositional effects on macroscopic mechanical properties will be related to elementary deformation processes and mechanisms. Gaps in our knowledge will be highlighted with suggestions for future work.

Invited talk	Tuesday, October 04th, 10:00

Invited talk Tuesday, October 04th, 10:00

Precipitate phase and local strain in high-entropy alloys: a first-principles assessment

Duc Nguyen-Manh[1], Jan S. Wrobel[1,2], Sergei L. Dudarev[1]

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[2] *Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland;*

Multi-component systems with predominantly simple phase are an area of current focus in alloy development. Termed High Entropy Alloys (HEAs), different empirical rules have been introduced to understand phase formation in these systems, and determine what the dominant phases may be. The mixture of bcc/fcc in Fe-based HEAs materials is expected to possess balanced mechanical properties, e.g., both high strength and good ductility. However, experimental investigation has revealed that the micro-structures of certain "HEAs" can be very complicated since they often undergo the spinodal decomposition, and ordered and disordered phase precipitate at lower temperatures. Our recent studies of phase stability of ternary fcc and bcc Fe-Cr-Ni alloys using a combination of density functional theory (DFT) with both conventional and magnetic cluster expansion methods show that the dependence of local chemical short-range orders as function of temperature and composition can be the origin of precipitate phases present in HEAs[1]. In the first part of this talk, an integrated modelling and experimental approach is proposed for magnetic HEAs systems by taking electronic structure effects into account in prediction of the phase most likely too be found in multi-component alloys. Good agreement is found when the calculations are confronted with data from experiments, including new magnetic HEAs system CoFeNiV where the precipitate σ phase is predicted to be more stable than the fcc one when the valence electron concentration n ≤ 7.6[2].

In the second part of this contribution, a methodology to investigate one of the main contributions to the yield strength from solid solution hardening (SSH) in HEAs is proposed by comparing DFT calculations and atomistic simulations that accurately describe the distortion in the lattice produced by the interaction of the different chemical species. The benchmark HEAs are the equimolar bcc MoNbWTaV and its 5 sub-quaternary systems[3]. The local atomic strains are described by the forces acting between different pairs of atoms. The interatomic spacing distribution is obtained by imposing force equilibrium for all atomic bonds. The effect of short-range order, which deviates the lattice configurations from randomness, can be studies by means of a elastic system, where the first and second nearest neighbours of each atom are the most influential. The atomic coordinates computed by this method can be used as a better starting point for DFT calculations and to quantify the SSH in HEAs.

Finally, we briefly discuss a generalisation of the first-principles assessment for the radiation induced segregation phenomenon in a non-equilibrium system of multi-component alloys[4].

[1] J.S. Wrobel, D. Nguyen-Manh, M.Yu. Lavrentiev, M. Muzyk and S.L. Dudarev, Phys. Rev. B **91**, 094430 (2015).
[2] . Leong, J.S. Wrobel, S.L. Dudarev, R. Goodall, I. Todd, D. Nguyen-Manh, submitted to Scientific Reports, (2016).
[3] I. Toda-Caraballo, J.S. Wrobel, S.L. Dudarev, D. Nguyen-Manh, P.E.J. Rivera-Diaz-del-Castillo, Acta Mater. **97**, 156 (2015).
[4] S.J. Wrobel, D. Nguyen-Manh, K.J. Kurzydlowski, S.L. Dudarev, ArXiv: 1604.03746 (2016).

Contributed talk	Tuesday, October 04th, 11:00

Contributed talk — Tuesday, October 04th, 11:00

High accuracy finite temperature stacking fault energies

Blazej Grabowski[1], Fritz Körmann[1,2], Andrei Ruban[3], Tilmann Hickel[1], Yilun Gong[4],
Roger Reed[1,4], Jörg Neugebauer[1]

[1] *Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany;*
[2] *Delft University of Technology, Delft, Netherlands;*
[3] *KTH Royal Institute of Technology, Sweden;*
[4] *University of Oxford, Oxford, UK;*

Metals and alloys – whilst crystalline – contain defects which largely determine their mechanical properties. Of particular importance is the planar defect known as the stacking fault, which arises when a dislocation dissociates into so-called Shockley partials. The extent of such partial dissociation is influential in determining the kinematics of dislocation flow when a stress field is applied. It is the *energy* of the stacking fault which is of importance in determining the extent of dissociation. When the stacking fault energy (SFE) is low, dislocation dissociation is favoured and *vice-versa*. Critical phenomena such as the kinetics of dislocation motion, work hardening, recrystallisation and crystalline texture – all of which influence the properties of these materials – are strongly dependent on SFE size. An accurate knowledge of the SFE is important, for example, for controlling the thermal stability of Ni based super alloys or for introducing additional strengthening mechanisms into compositionally complex alloys, such as high entropy alloys. Traditionally, the magnitude of the SFE has been inferred by measurements of the extent of dislocation dissociation. However, the data deduced in this way are prone to significant scatter even for 'simple' unary elements. Moreover, it has not proven possible to deduce the temperature dependence of the SFE with any accuracy.

Computational modelling is one way in which this difficulty can be circumvented. In particular, first principles based methods such as density functional theory (DFT) are now contributing a great deal to understanding and controlling materials properties[1,2]. However, an accurate determination of high temperature properties using DFT has been so far a great challenge due to the difficulty of capturing all the relevant entropic contributions. Only very recent methodological developments have for the first time allowed the accurate calculation of finite temperature properties up to the melting point[3−7].

Here, we extend these methods to the study of the SFE. We compute with high precision the temperature dependence of the SFE, placing emphasis on the face-centered cubic (fcc) metals Al, Cu and Ni. An accurate knowledge of the temperature-dependence of these SFEs is of profound importance, since alloys based on these elements form the basis of many structural components used at elevated temperatures. All relevant temperature-dependent contributions are considered in our work including electronic, vibrational, magnetic and explicit anharmonic Gibbs energy contributions as well as various coupling terms. Particular emphasis is put on a careful comparison of different theoretical concepts to derive the stacking fault energy such as the axial next nearest-neighbor Ising (ANNNI) model or the vacuum-slab approach. Our highly accurate results show that for Ni the temperature induced change is in fact so strong that in the temperature interval relevant for superalloy applications the stacking fault energy falls below one-third of the low temperature value. Such changes are in the same order of magnitude as the impact of alloying elements.

[1] T. Hickel, B. Grabowski, F. Körmann and J. Neugebauer, J. Phys.: Condens. Matter 2, 053202 (2012).

[2] C. Freysoldt, B. Grabowski, T. Hickel, J. Neugebauer, G. Kresse, A. Janotti and C. G. Van de Walle, Rev. Mod. Phys. 86, 253 (2014).

[3] B. Grabowski, L. Ismer, T. Hickel and J. Neugebauer, Phys. Rev. B 79, 134106 (2009).

[4] B. Grabowski, P. Söderlind, T. Hickel and J. Neugebauer, Phys. Rev. B 8, 21410 (2011).

[5] A. Glensk, B. Grabowski, T. Hickel and J. Neugebauer, Phys. Rev. Lett. 114, 195901 (2015).

[6] A. I. Duff, T. Davey, D. Korbmacher, A. Glensk, B. Grabowski, J. Neugebauer and M. W. Finnis, Phys. Rev. B 91, 214311 (2015).

[7] F. Körmann, P-W. Ma, S. Dudarev and J. Neugebauer, J. Phys.: Condens. Matter 28, 076002 (2016).

Contributed talk	Tuesday, October 04th, 11:35

Contributed talk	Tuesday, October 04th, 11:35

Stacking fault energy of C-alloyed steels: the effect of magnetism

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First-principles calculations have been performed to study the effect of C on the stacking fault energy (SFE) of paramagnetic γ-Fe and Fe-Cr-Ni austenitic steel. In these systems, the local magnetic structure is very sensitive to the volume in both fcc and hcp structures, which emphasizes the importance of the magnetovolume coupling effect on the SFE. The presence of C atom suppresses the local magnetic moments of Fe atoms in the first coordination shell of C. Compared to the hypothetical nonmagnetic case, paramagnetism significantly reduces the C effect on the SFE. In the scenario of C being depleted from the stacking fault structure or twin boundaries, *e.g.*, due to elevated temperatures, where the chemical effect of C is dissipated, we calculate the C-induced volume expansion effect on the SFE. The volume induced change in the SFE corresponds to more than $\sim$50% of the total C effect on the SFE.

Invited talk	Tuesday, October 04th, 14:00

Invited talk	Tuesday, October 04th, 14:00

Atomic-scale modeling of point defects, phase stability, and the formation of Z phases CrMN (M=V, Nb, Ta) in steel

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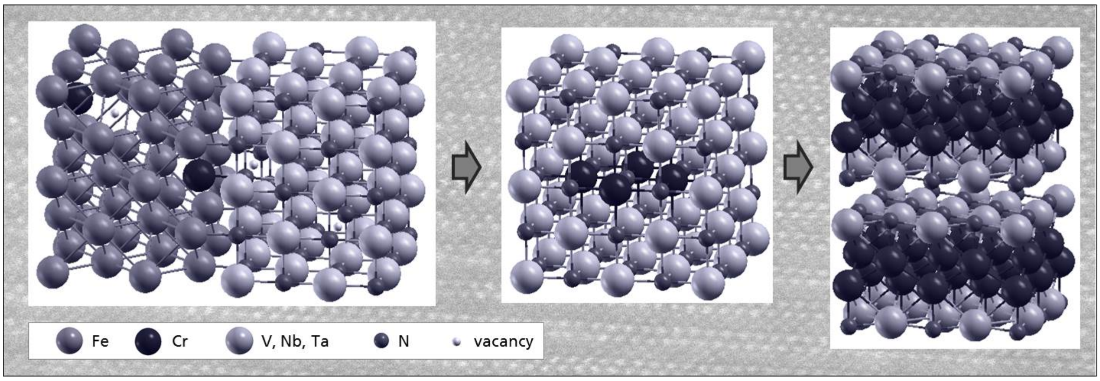
The challenge of raising the steam inlet temperature of fossil-fired power plants calls for creep-resistant steels with a Cr content higher than 9% in order to achieve sufficient corrosion and oxidation resistance. However, it has been observed during long-time power-plant operation that in 11-12% Cr ferritic-martensitic creep-resistant steels strengthened by fine-grained (V,Nb)N particles, precipitation of thermodynamically stable Z-phase particles, CrMN (M=V, Nb, Ta), is unavoidable and detrimental. Usually, Z-phase particles are coarse-grained and brittle, and they grow at the expense of the desired, beneficial (V,Nb)N particles. A promising solution to this problem is provided by the idea to exploit the Z phase as a thermodynamically stable mechanical strengthening agent. Hence the challenge is to control the precipitation of the Z phase such that fine-grained and long-time stable particles are formed.

We present atomistic simulations, based on density function theory calculations, which reveal the essential thermodynamic processes and kinetic mechanisms underlying the formation of ternary Z phases from binary metal-nitride (MN) particles in Cr-containing steel. The scenario that evolves (figure) consists of the diffusion of Cr atoms into MN particles with the rocksalt structure and the subsequent clustering of Cr atoms in a layered arrangement which finally results in the transformation of the MN particles to Z-phase particles with multilayer [Cr/MN] structure. The energetic stability of Z phases with respect to related compounds as well as the thermodynamics and kinetics of atomic defects in MN involved in the Z-phase formation are investigated.



Formation of a Z phase CrMN from MN in Cr-containing steel: Cr atoms diffuse from the Fe matrix into the MN particle (left), they agglomerate to planar Cr clusters (middle), and these grow to extended Cr layers in MN, forming the multilayered [Cr/MN] structure (right) of the Z phase.

This work is part of the research project Z-Ultra (www.z-ultra.eu) funded by the European Commission (FP7-NMP-2012-2.2-3, Grant Agreement No. 309916).

Contributed talk	Tuesday, October 04th, 15:15

Contributed talk — Tuesday, October 04th, 15:15

Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics

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The stability of a significant number of precipitates in steel has not been clarified so far because of difficulties in experimental approaches. One of the methods to predict the stability of such precipitates is to employ first-principles calculations. Recently many studies have been devoted to the calculation of the free energy at finite temperatures from first-principles[1,2,3].

Stability of cementite in steel is known to be very sensitive on impurity additions. For example, Cr stabilizes cementite[4]. On the other hand, the stability has not been clarified for some impurity elements like Si because of its low solubility in cementite[5]. The effect of Si on the solubility of carbon in steel has not been clarified so far, although Si is often used to strengthen steel. Therefore, it is important to know the precise impact of impurity elements on the stability of cementite.

Several first-principles calculations related to the effect of impurity elements on the stability of cementite have been published[6,7,8]. They revealed the partitioning trend of impurity elements to cementite[8]. However, the partitioning enthalpy of Cr indicates that Cr is not partitioned to cementite at 0 K, which seems to be inconsistent with the experimental results. The present investigation is therefore devoted to study the impact of Cr alloying on cementite stability in ferritic steels.

Partitioning of Cr and Si between cementite and ferrite was investigated by first-principles thermodynamics taking into account vibrational, electronic, and magnetic Gibbs energy contributions. At finite temperatures, these contributions lower the partitioning Gibbs energy and compete with the configurational entropy, which favors impurity segregation to ferrite due to its larger volume fraction compared to cementite. Due to the large positive partitioning enthalpy contribution of Si at T=0K, partitioning of Si to cementite is virtually absent in agreement with experiment. The situation is drastically different for Cr impurities. Incorporation of finite-temperature effects resolves the discrepancy between experimental observations and previous T=0K first-principles calculations. Cr strongly segregates to cementite due to the enhanced magnetic entropy of cementite above 400 K, i.e., near the Curie temperature of cementite. The increasing magnetic fluctuations in ferrite cause a strong reduction of the partitioning coefficient in the temperature range from 773 to 973 K in qualitative agreement with experiment. Quantitative agreement with CALPHAD data and experimental data for equilibrium Cr concentrations in a wide range of alloy compositions is achieved by renormalizing the theoretical magnetic partitioning Gibbs energy by a constant scaling factor.

[1] P. Souvatzis and O. Eriksson. Phys. Rev. B, 77:024110, 2008.
[2] A. Siegel, K. Parlinski, and U.D. Wdowik. Phys. Rev. B, 74:104116, 2006.
[3] B. Grabowski, T. Hickel, and J. Neugebauer. Phys. Rev. B, 76:024309, 2007.
[4] M. Ko, T. Sakuma, and T. Nishizawa. J. Jpn. Inst. Met., 40:593, 1976.
[5] H. Saitoh, K. Ushioda, N. Yoshinaga, and W. Yamada. Scripta Mater., 65:887, 2011.
[6] I. R. Shein, N. I. Medvedeva, and A. L. Ivanovskii. Phys. Stat. Sol. (b), 244:1971, 2007.
[7] J. H. Jang, I. G. Kim, and H. K. F. H. Bhadeshia. Comp. Mat. Sci., 44:1319, 2009.
[8] C. K. Ande and M. H. F. Sluiter. Acta Mater., 58:6276, 2010.

Invited talk	Tuesday, October 04th, 16:15

Invited talk	Tuesday, October 04th, 16:15

Grain boundaries in severely deformed metallic materials

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Severe plastic deformation (SPD) has often been applied for refining the microstructure of polycrystalline materials down to the ultrafine grained - or even the nanocrystalline range, yielding bulk materials that are mostly free from porosity or contaminations of the internal interfaces. Materials that were processed by SPD have been shown to possess properties that are modified from their coarse-grained counterparts beyond the expectations given by mere scaling laws. Models for describing the property modifications after SPD processing, mostly with respect to the mechanical properties, are based on assuming modifications of the local atomic grain boundary structures in addition to the drastic increase of the volume fraction of grain boundaries. Yet, along with the enhancement of mechanical properties, several important questions arise e.g. concerning the accommodation of external stresses if dislocation-based processes are not longer dominant at small grain sizes. One question, which has raised continued discussions, concerns the extent of structural modifications of grain boundaries during SPD, since the formation of a specific deformation-induced "state" of high excess free energy density has been postulated. Such "deformation-modified" grain boundaries should possess enhanced excess free energy densities, enhanced residual microstrain and enhanced atomic mobility along the boundary plane and are supposed to present the microstructure element that underlies the property enhancement.

As described above, grain boundaries and particularly grain boundaries with structures that are modified by the interaction with large number densities of lattice dislocations as well as triple junctions of several grain boundaries are important elements of fine-scaled microstructures. Their presence, their structure and particularly their strain state is of importance for the stability, the mechanical performance and also the grain-boundary diffusion and grain-boundary-diffusion-related properties of ultrafine grained or nanocrystalline materials obtained through severe deformation processing. Thus, this contribution focuses on the experimental determination of both, grain boundary diffusion rates and local strain fields with high spatial resolution in severely deformed metallic materials and on their relationship with macroscopic properties. As an outlook, the possible importance of rotational defects for the stability of fine-grained microstructures will also be discussed.

Contributed talk	Tuesday, October 04th, 17:30

Contributed talk Tuesday, October 04th, 17:30

Grain boundary faceting and its effect on migration kinetics

Sherri Hadian[1], Blazej Grabowski[1], Chris Race[2], Jörg Neugebauer[1]

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[2] *School of materials, University of Manchester, United Kingdom;*

We have studied the migration behavior of mixed tilt and twist grain boundaries in the vicinity of a symmetric tilt $\langle 111 \rangle$ $\Sigma 7$ grain boundary in aluminum. We show that these grain boundaries nano-facet[1,2] onto the symmetric tilt plane and have differing kinetics than the atomically flat symmetric tilt boundary. Based on their geometric structure and atomistic mechanisms they fall into two main categories of stepped and kinked boundaries in close correlation to surface growth mechanisms. We use the knowledge of their mesoscopic migration mechanisms to derive analytical kinetic models that explain the dependence of the migration barrier on the driving force. We are then able to extract energy barrier data for the experimentally relevant case of vanishing driving forces that are not accessible from direct molecular dynamics simulations. Further investigation shows that even though the facet length of the mixed boundaries increase with the annealing time, their migration kinetics remains unchanged.

[1] R. Hadian, B. Grabowski, C.P. Race, J. Neugebauer, Phys. Rev. B *accepted* (2016).
[2] C.P. Race, R. Hadian,B. Grabowski, J. Neugebauer Phys. Rev. B **92**, 174115 (2015).

Contributed talk	Tuesday, October 04$^{\text{th}}$, 20:00

Contributed talk Tuesday, October 04th, 20:00

Grain boundary segregation and embrittlement: recent advances and open problems

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Intergranular brittle fracture is closely related to the chemistry of grain boundaries and to the difference of the segregation energies of the grain boundaries and the free surfaces (Rice-Wang model). To elucidate the effect of individual solutes on embrittlement of various base materials such as steels and nickel-base superalloys, grain boundary and surface segregation was extensively studied in many laboratories. As a result, numerous data on surface and grain boundary segregation have been gathered in literature. They were obtained in two main ways, by computer simulations and from experiments. These results are frequently applied to quantify the embrittling potency of individual solutes. Unfortunately, the values of the segregation energy of a solute at grain boundaries as well as at the surfaces obtained by various authors sometimes differ by more than one order of magnitude: such a difference is unacceptable as it cannot provide us with representative view on the problem of material temper embrittlement. In some cases it seems that these values do not reflect physical reality or are incorrectly interpreted. Here we summarize the available data on interfacial segregation and embrittlement of various solutes in nickel and bcc iron and critically discuss their reliability, assessing also limitations of individual approaches employed to determine the values of segregation and strengthening/embrittling energies. We demonstrate that theoretical approaches are limited by the size of the computational repeat cell used for the calculations of the segregation energy. On the other hand, even when using repeat cells that are not sufficient for reliable evaluation of the segregation energy, the change in the grain boundary cohesion (strengthening/embrittling energy) may be obtained with a reasonable accuracy. For many impurities, there is lack of experimental segregation data. Therefore, many calculated results are theoretical predictions which may motivate future experimental work.

Contributed talk	Tuesday, October 04th, 20:35

Contributed talk	Tuesday, October 04th, 20:35

Anisotropic elastic properties and mechanical stability of $\Sigma 5(210)$ grain-boundary complexions in Ni_3Al from ab initio calculations

Martin Friák[1,2], Monika Všianská[2,1], David Holec[3], Mojmír Šob[2,1,4]

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[2] *Central European Institute of Technology, CEITEC MU, Masaryk University, Kamenice 5, CZ-625 00 Brno, Czech Republic;*
[3] *Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, A-8700 Leoben, Austria;*
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We employ quantum-mechanical calculations within the density functional theory to study elastic properties of $\Sigma 5(210)$ grain boundaries (GB) in Ni_3Al with and without segregated Si atoms substituting Al atoms. Anisotropic elastic properties of 64-atom computational supercells (as periodic approximants of GBs) are determined using the stress-strain method. We compare elastic properties of two chemical compositions of the $\Sigma 5(210)$ GB in Ni_3Al with those with Si atoms at different Al positions at this GB. The elastic properties of the $\Sigma 5(210)$ GB Ni_3Al grain boundaries are found to be very different from the bulk (they possess orthorhombic symmetry and are softer) and exhibit high sensitivity to the chemistry of the grain-boundary interface and its surrounding atomic neighborhood. This sensitivity is, nevertheless, limited to only a few atomic layers away from the grain boundary. Comparing our quantum-mechanical results with predictions obtained by linear-elasticity approach we demonstrate deficiencies of the latter and thus a clear need to use *ab initio* methods in this field.

Contributed talk	Tuesday, October 04th, 21:10

Contributed talk	Tuesday, October 04th, 21:10

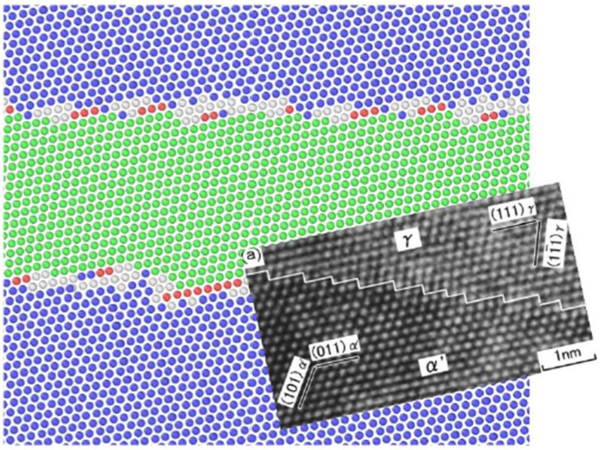
Structure and mobility of the austenite/martensite interface in steels

Francesco Maresca, W. A. Curtin

Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland;

The austenite/martensite interface is prevalent across many new classes of high-strength steels (e.g. Quenched and Partitioned, TRIP, bainitic and nanobainitic). The fundamental structure and mechanism of motion of this specific interface, which plays a key role in the mechanical properties of these steels, is not clear in spite of decades of research.

We have created an atomistic fcc-bcc iron interface having a structure that completely matches experiments (figure)[1]. The interface shows $[\bar{1}01]_{\mathrm{fcc}}$ steps with adjacent screw dislocations having $a_{\mathrm{fcc}}/2[\bar{1}01]$ Burgers vector and gliding on $(111)_{\mathrm{fcc}}$. We also find edge dislocation segments with $a_{\mathrm{bcc}}/2[1\bar{1}\bar{1}]$ Burgers vector that glide on $(\bar{1}01)_{\mathrm{bcc}}$, which were never envisioned by any previous theory assumptions. With these two sets of dislocations, the interface is glissile, moving as an integral unit, under a less-stringent interpretation of the long-established conditions for glissile interfaces[3].



Comparison between atomistic interface and HRTEM micrograph from [2].

Based on the atomistically-observed interface defect structure, we have proposed a revisited, parameter-free crystallographic theory of lath martensite, that provides predictions in good agreement with simulations and experiments. Theory shows that the dominant factor controlling the transformation strain and hence toughening is the fcc/bcc lattice parameter ratio. Predictions for Fe-Mn-Ni alloys yield a transformation strain of $\sim$ 50%, while even larger strains can be achieved in Fe-C alloys. These are well above the previous common belief of a maximum $\sim$ 30% strain based on low resolution experiments[4]. There is therefore potential for developing materials with even higher ductilities than previously expected. The knowledge of the interface defect structure can guide further control of TRIP as well as properties influenced by the interaction with solutes (e.g. Mn, C, but also H). Therefore, the new understanding of this interface provides guidelines for the design of new high strength steels.

[1] F. Maresca, and W.A. Curtin, *Under review.*

[2] T. Moritani, N. Miyajima, T. Furuhara, and T. Maki, Scripta Mater. **47**, 193-199 (2002).

[3] J.W. Christian, and A.G. Crocker, In: F.R.N. Nabarro (Ed.) Dislocations in Solids, vol. 3, Ch. 11, 165-252 (North Holland, Amsterdam, 1980).

[4] K. Wakasa, and C.M. Wayman, Acta Metall. **29**, 1013-1028 (1981).

Invited talk	Wednesday, October 05th, 8:45

Invited talk — Wednesday, October 05th, 8:45

Materials chemomechanics by inference-boosted first principles modelling

Alessandro De Vita[1,2,3]

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[2] *Thomas Young Centre for Theory and Simulation of Materials, London UK*
[3] *Department of Engineering and Architecture, University of Trieste, Italy*

Many technologically important phenomena coupling complex chemistry with high-gradient elastic fields such as thermally activated fracture[1], or stress corrosion[2] of brittle materials are beyond the reach of First-Principles Molecular Dynamics (FPMD)-techniques, whether based on standard or O(N) implementations. This is ultimately because the required model system sizes are too large, and/or the required simulation times are too long, for these high-accuracy traditional approaches. In most (but not all) situations, using classical MD is not a viable alternative, as suitably general and accurate reactive force fields are not available, nor are fitting databases a priori guaranteed to contain the information necessary to describe all the chemical processes encountered along the dynamics. The problem, widespread in covalent/brittle systems, can arise in ductile metallic systems too[3]. Finally, QM/MM techniques combining quantum and classical zones in a single calculation also pose significant difficulties, especially when the target processes involving sustained mass transport into and out of the (e.g., fast moving) QM zone.

This situation strongly calls for the use of big-data based MD techniques, capable of locating and using QM-accurate information pre-stored in massive databases, or generating it if no such information is available. In practical realisations, these could be configuration databases dynamical coupled with specially-tuned Machine Learning force fields which minimise the computational workload of MD runs by allowing QM subroutine calls only when chemically novel configurations are encountered along the systems trajectory. I will present one such Learn On the Fly technique, effectively unifying First-Principles Molecular Dynamics and Machine Learning into a single, information efficient simulation scheme capable of learning/predicting atomic forces through Bayesian inference[4]. Recently developed covariant kernels specifically designed for direct force learning by Gaussian Process regression are at the core of this technique[5]. Interestingly, QM-zone partitioning approaches followed by execution via any of the existing O(N^3) QM engines is predicted to be a better option than using O(N) QM methods when dealing with large QM zones in QM/MM calculations running on high-end parallel platforms[6−7].

[1] J.R.Kermode et al., PRL 115, 135501 (2015).

[2] A. Gleizer et al., PRL 112, 115501 (2014).

[3] F.Bianchini et al., Mod. and Simul. in Mat. Science and Engineering 24, 045012 (2016).

[4] Z. Li, J. R. Kermode and A. De Vita, Phys. Rev. Lett., 114, 096405 (2015).

[5] A.Glielmo and A. De Vita, in preparation.

[6] Cf., e.g., the US-DOE INCITE on SiO2 ML-Fracture Project https://www.alcf.anl.gov/projects/sio2-fracture-chemomechanics-machine-learning-hybrid-qmmm-scheme

[7] M. Caccin et al., Int. J. of Quantum Chemistry 2015, DOI: 10.1002/qua.24952

Contributed talk	Wednesday, October 05th, 10:00

Contributed talk Wednesday, October 05th, 10:00

From density functional theory to magnetic interatomic potentials and phase transformation kinetics

Martin Staadt, Ning Wang, Thomas Hammerschmidt, Jutta Rogal, Ralf Drautz

ICAMS, Ruhr-Universität Bochum, Germany

Density Functional Theory (DFT) enables the accurate prediction of many properties of high-temperature materials, but it is often difficult to reach experimental length and time scales or to represent the chemical complexity of materials directly from DFT. In these cases simplified representations of the interatomic interaction are required that enable simulations on relevant length and time scales. In this talk I will discuss the derivation and application of simplified models of the interatomic interaction. Examples will be given for the the modeling of phase stability in TCP phases, finite temperature properties of iron and the atomistic simulation of phase transformation kinetics.

Contributed talk	Wednesday, October 05th, 11:00

Contributed talk Wednesday, October 05th, 11:00

Atomistic models for hydrogen embrittlement

Thomas D. Daff, Gábor Csányi

Department of Engineering, University of Cambridge, UK

Hydrogen is known to cause catastrophic failure in high strength steels, however the exact mechanism by which failure occurs is a topic of debate[1]. The HEmS (Hydrogen in metals — from fundamentals to the design of new steels) project[2] aims to provide a better understanding of hydrogen embrittlement of iron and steel across a wide range of length scales from experimental testing down to modelling of processes at the atomistic scale. It is a collaboration between Universities of Oxford, Cambridge, Sheffield and Imperial and King's Colleges in London.

As part of this project, we have generated database of ab-initio, atomistic iron simulation data that are being used to better understand the embrittlement process. Total energies, forces and stresses from thousands of atomic environments, calculated at the DFT (PBE) level, including bulk, surface, point defect and gamma surfaces, have been used to train interatomic potentials based on the Gaussian process. These Gaussian Approximation Potentials[3] (GAPs) are able to correctly reproduce the mechanical properties of bulk iron with DFT accuracy (< 0.1 meV per atom) but orders of magnitude faster, with linear scaling. The best of these potentials is also tested to correctly model point defects, surfaces and is currently being tuned to accurately model dislocation motion.

To complement the iron potential, a database of iron-hydrogen configurations have been used to develop a potential that is able to accurately describe hydrogen within bulk iron. Our potential is fast and accurate, and is also independent of the iron potential that it is paired with. Again, this potential is being tested and improved by including more atomistic environments with the end target of being able to accurately simulate systems that are relevant to hydrogen embrittlement, such as dislocations and grain boundaries, but are to large to simulate purely with DFT.

Finally we have used DFT to investigate some mechanisms that have been proposed for hydrogen embrittlement. Can hydrogen enhanced decohesion be described by increasing solubility of hydrogen at less coherent grain boundaries, causing embrittlement? Is there any evidence that would support hydrogen induced phase transition as a mechanism for embrittlement, for example hydride formation? The accuracy of the DFT model used must also be considered in all these calculations.

[1] Robertson, I.M., Sofronis, P., Nagao, A. et al.

Metall and Materi Trans B (2015) 46: 1085. doi:10.1007/s11663-015-0325-y.

[2] http://www.hems.ox.ac.uk.

[3] Bartók, A.P., Payne, M.C., Kondor, R., Csányi G.

Phys Rev Lett (2010) 104: 136403. doi:10.1103/PhysRevLett.104.136403.

Contributed talk	Wednesday, October 05th, 11:35

Contributed talk Wednesday, October 05th, 11:35

Modelling self-healing creep damage and healing in iron

Casper D. Versteylen, M.H.F. Sluiter

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Time-dependent damage, in the form of the formation and growth of voids on grain boundaries of metals, eventually leads to the formation of a crack and to fracture. This process relies on the diffusional flux of vacancies towards a void, which determines both the growth rate of the void and in many diffusional creep cases also directly the strain rate. A mechanism of solute based self-healing of those voids has been found experimentally to prolong the life-time of iron based alloys[1]. The mechanism relies on the selective precipitation of supersaturated solute on damage sites.

This mechanism is studied by means of a finite element model, which is used to determine the relevant parameters involved in the healing of the voids. The diffusivities in the grain boundary and in the bulk, solubility of the solute and possible supersaturation and the geometries of the problem have been varied in order to discern the relative contributions of each of these parameters. A critical ratio between grain boundary and bulk diffusivity contributions is found to control the relative importance of grain boundary and bulk diffusion.

In many cases, the strain-rate of a steady-state diffusional creeping sample is dependent on the self-diffusivity of in the bulk[2]. The healing rate is found to be directly connected to the strain-rate in the samples, which makes a full analysis of diffusivities of all substitutional elements vital for the determination of the optimal self-healing solute in steel.

Advancement of computational techniques make the determination of diffusivities of a large spread of different impurities in bcc-iron feasible. Ab-initio calculations have been performed, determining the diffusivities of impurity elements in bcc-iron. Two different exchange-correlation functionals, PW91 and PBEsol, were used to determine the vacancy formation and binding energies and migration barriers. Excess entropies and the attempt frequency for a jump were determined by calculating phonon frequencies in the harmonic approximation. The Le Claire 9-frequency model and transition state theory are used to determine the effective jump frequencies of each diffusing element. It is found that elements with low migration barriers, have a low correlation factor and this correlation is temperature dependent, which acts as an effective activation barrier for diffusion.

The self-healing concept has been applied in ceramics, polymers, composite materials and in very successfully in concrete and asphalt. The concept is relatively new to metals, but the promise of prolonging creep life could be interesting from both an academic and industrial perspective.

[1] S. Zhang, C. Kwakernaak, W. G. Sloof, E. Brck, S. van der Zwaag, N.H. van Dijk, Adv. Eng. Mater. **17**, 598 (2015).
[2] O. D. Sherby and J. Weertman, Act. Met. **27**, 401-403 (1979).

Contributed talk	Wednesday, October 05th, 20:00

Contributed talk	Wednesday, October 05th, 20:00

Hierarchical microstructure of ferritic superalloys

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[2] *National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA;*
[3] *Nanotechnology and Functional Materials Center, Faculty of Technology and Metallurgy, University of Belgrade and Serbian Academy of Sciences and Arts, 11120, Belgrade, Serbia;*
[4] *Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA;*
[5] *Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA;*

A new class of ferritic alloys[1] with hierarchical microstructure are presented, were the bcc-Fe matrix is strengthened by coherent, two-phase $L2_1$-Ni_2TiAl/B2-NiAl precipitates. Electron diffraction, diffraction contrast imaging and aberration corrected scanning transmission electron microscopy (STEM) are applied to study the underlying phase transformation pathways leading to the hierarchical microstructure. The experimental observations are complemented by cluster-expansion based Monte-Carlo simulations.

In an alloy with 2 wt.% Ti, spherical B2-NiAl precipitates are forming in the bcc-Fe matrix during rapid solidification. In the course of the aging heat treatment at 700 °C for 10 h the $L2_1$-ordered Ni_2TiAl phase is exclusively nucleating within the B2-NiAl primary precipitates, representing a hierarchical microstructure in terms of chemical ordering and dimension of the phases. The $L2_1$-precipitate substructure adopts a plate shaped geometry with a dimension of 15-20 nm. Aberration corrected STEM reveals a diffuse interface profile between the B2- and $L2_1$-phases and the experimental observations are in good agreement with an observed interfacial broadening from Monte-Carlo simulations[2].

By increasing the overall Ti content to 4 wt.%, $L2_1$-Ni_2TiAl precipitates are forming in the bcc-Fe matrix after the quench. An internal network of $1/2<100>$ antiphase domain boundaries (APB) is revealed within the Ni_2TiAl-precipitates. After solid-state aging for 3 h at 700 °C wetting of initial APBs by the B2-NiAl phase is confirmed by aberration corrected STEM. The B2 wetting layer is growing in width to ~7 nm after aging for 10 h at 700 °C[3]. The experimentally observed wetting transition is verified by Monte-Carlo simulations.

[1] Sun Z, Liebscher CH, Huang S, Teng Z, Song G, Wang G, Asta M, Rawlings M, Fine ME, Liaw PK. Scr Mater 68 (2013).

[2] Liebscher CH, Radmilovic VR, Dahmen U, Vo NQ, Dunand DC, Asta M, Ghosh G. Acta Mater 92 (2015).

[3] Liebscher CH, Radmilovic V, Dahmen U, Asta M, Ghosh G. J Mater Sci 48 (2012).

Contributed talk Wednesday, October 05th, 20:35

Contributed talk	Wednesday, October 05th, 20:35

Design of Ti-based alloys with austenitic Ni-Ti nanoprecipitates

Sascha B. Maisel[1], J. Zhang[1,2], W.-S. Ko[3], E. Povoden-Karadeniz[4], B. Grabowski[1], J. Neugebauer[1]

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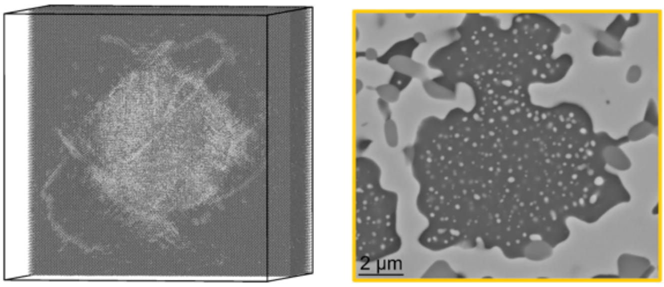
The properties of Ni-Ti nanoparticles differ significantly from the properties of bulk Ni-Ti, yet they retain their characteristic phase transition and the resulting shape memory effect. Austenitic Ni-Ti nanoprecipitates can be dispersed in intermetallic matrices of appropriate lattice spacing and it has been speculated that this will lead to a phase-transition-based strengthening effect due to its intrinsic shape-memory property. Therefore, this is considered a promising approach to confer so-called "self-healing" features to intermetallic alloys. Here, we present a combined experimental and theoretical investigation of such nanoprecipitates embedded coherently in Ti-V and Ti-Nb matrices.

We study the properties of the compound using three-dimensional atomistic simulations based on the modified embedded atom method (MEAM). Suitable potentials for our simulations have been developed in house[1,2] and were found to be computationally feasible even for large supercells ($> 10^7$ atoms). From these simulations, we are able to determine the conditions under which the martensitic phase transition of such a nanoparticle is triggered, which in general may depend on the size of the particle, the composition of the surrounding matrix, temperature and strain state of the system.

We propose synthesizing such alloys using prior knowledge of the Ni-Ti-V phase diagram based on a combination of density-functional theory and CALPHAD methods. Preliminary TEM investigations on our first samples suggest that such nanoparticles with sizes of around $200 - 300\,\mathrm{nm}$ can form in Ni-V matrices with $\approx 45\,\mathrm{at.\,\%}$ V.



Spherical Ni-Ti nanoparticles as observed in MEAM simulations (left) and SEM experiments (right).

[1] W.-S. Ko, B. Grabowski, J. Neugebauer: Phys. Rev. B **92**, 134107 (2015).

[2] W.-S. Ko, S. B. Maisel, B. Grabowski, J. B. Jeon, J. Neugebauer: submitted to Acta Mater.

Contributed talk	Wednesday, October 05th, 21:10

Contributed talk Wednesday, October 05th, 21:10

High-pressure torsion of Cu/Ta layered system

Nazar Ibrahim, Martin Peterlechner, Friederike Emeis, Matthias Wegner, Sergiy V. Divinski,
Gerhard Wilde

Institute of Materials Physics, University of Münster, Germany

Mechanical alloying via high pressure torsion (HPT) is investigated for the immiscible Cu-Ta system. Stacks of alternating Cu/Ta sheets as well as pure Cu and pure Ta stacks were subjected to HPT processing at a pressure of 4 GPa for 10, 30, 50, 100 and 150 revolutions. The effect of subsequent heat treatment on the phase composition and microstructure evolution of Cu/Ta and pure Cu or pure Ta foil stacks is examined by X-ray diffraction, scanning and transmission electron microscopy, differential scanning calorimetry and microhardnes measurements. The HPT processing of the Cu/Ta assembly by 150 revolutions is shown to produce a mixture of ultrafine grains corresponding to a Cu-16% Ta solid solution with embedded nano-scaled Ta-rich particles and almost pure Ta grains. The ultrafine microstructure is characterized by extremely high microhardness and reveals a superior thermal stability remaining fine-grained even after annealing at 1000°C for 1 hour.

Invited talk Thursday, October 06th, 8:45

Invited talk	Thursday, October 06th, 8:45

Ab-initio simulations of dislocations in BCC transition metals and alloys

Lorenz Romaner[1,2], Hong Li[2], Vsevolod Razumovskiy[1], Claudia Ambrosch-Draxl[2], Reinhard Pippan[3]

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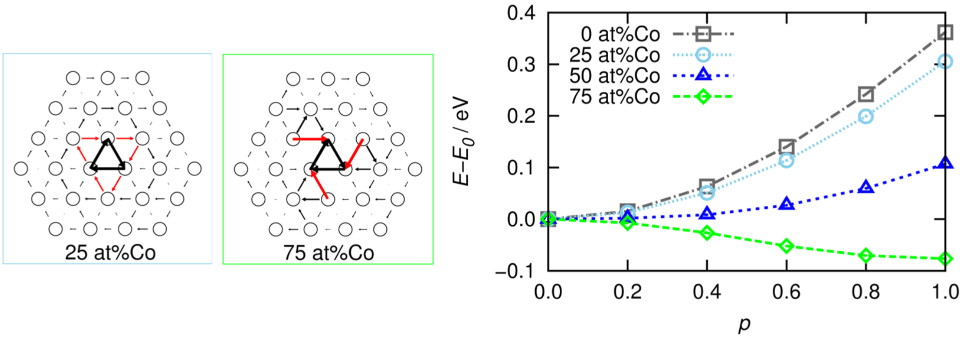
Understanding and predicting plastic deformation of bcc transition metals is a topic of intensive research. In comparison to fcc metals, bcc metals exhibit several unusual features of plastic deformation[1] including the presence several possible glide planes, i.e. the {110}, {112} and {123} plane, a pronounced temperature-dependence of the flow stress, solid solution softening, break-down of the Schmid law of the critical resolved shear stress, anomalous slip and a ductile-to-brittle transition. These features are all related to the properties and behavior of dislocations where a prominent role is assigned to the $1/2 < 111 >$ screw dislocation (in the following just referred to as screw dislocation). Due to its nonplanar core structure, this dislocation is relatively sessile and is regarded as a key limiting factor for plastic deformation. Recently, however, also the importance of other dislocations with a planar core structure, in particular the M111 dislocation, has been highlighted.[2]

In this talk we will present atomistic ab-initio simulations of screw dislocations and M111 dislocations in bcc transition metals. A special focus is laid on tungsten which is the metal with the highest melting point and a high ductile-to-brittle transition temperature. Furthermore, we also focus on Fe due to its obvious relevance as a structural material. The simulation techniques based on the periodic dipole approach and the Peierls-Nabarro model will be introduced. The fundamental properties of the screw dislocations and M111 dislocations in pure bcc metals will be discussed and their research history shortly outlined. On this basis, the impact of alloying on the core structure of screw dislocation at 0K within the framework of the virtual crystal approximation will be discussed.[1,2,3] It will be shown how the d-band filling induces a change in core structure in both W-Re and Fe-Co alloys (see Figure) but not, for instance, in W-Ta alloys.



Differential displacement map of the screw dislocation in $Fe_{75}Co_{25}$ (left) and $Fe_{25}Co_{75}$ (middle) illustrating a change in core polarity p from 0 to 1. To the right, the energy per burgers vector of one dislocation as a function of core polarity is shown for several FeCo alloys.

Furthermore, the evolution of the Peierls stress with d-band filling of the screw dislocation for W-based alloys will be shown. A discussion on how these changes are related to other fundamental properties such as elastic constants, gamma surfaces or interstring potential and how they compare with available experiments from the literature will be presented.

As the next step we will discuss temperature-induced changes in the core structure of the screw dislocation. Such changes have been observed in some molecular dynamics simulations[6,7] but their occurrence is still unclear. For nonmagnetic materials the transition is rooted in the lattice vibrations and the arising lattice expansion. For Fe the situation is more complex as also a transition from the ferromagnetic to the paramagnetic state arises. We will present preliminary results where the spin-wave[8] method is used to model a screw dislocation in the paramagnetic state. After a short outline of the essential elements of the spin-wave method, we will show what the impact of the paramagnetic state on the core structure is.

After concluding the main topics and challenges for future ab-initio modeling of dislocations in bcc metals will be highlighted.

[1] J. W. Christian Metall. Mater. Trans. A **14A**, 1237 (1983).
[2] K. Kang, V. V. Bulatov, W. Cai Proc. Nat. Acad. Soc. **109**, 15174 (2012).
[3] L. Romaner, C. Ambrosch-Draxl and R. Pippan, Phys. Rev. Lett. **104**, 195503 (2010).
[4] H. Li, S. Wurster, C. Motz, L. Romaner, C. Ambrosch-Draxl, R. Pippan, Acta Mat. **60**, 748, (2012).
[5] L. Romaner, V.I. Razumovskiy, R. Pippan, Phil. Mag. Lett. **94**, 334 (2014).
[6] J. Chaussidon, M. Fivel, D. Rodney, Acta Mater. **54**, 3407, (2006).
[7] D. Cereceda, A. Stukowski, M. R. Gilbert, S. Queyreau, L. Ventelon, M-C. Marinica, J. M. Perlado and J. Marian J. Phys.: Condens. Matter **25**, 85702, (2013).
[8] A. V. Ruban and V. I. Razumovskiy Phys. Rev. B **85**, 174407 (2012).

Invited talk	Thursday, October 06th, 10:30

Ab initio modeling of dislocation core properties in BCC metals

François Willaime[1], Lisa Ventelon[2], Lucile Dézerald[3], Bérengère Luthi[2], David Rodney[4], Emmanuel Clouet[2]

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[2] *CEA-DEN, Service de Recherches de Métallurgie Physique, Gif-sur-Yvette, France;*
[3] *Institut Jean Lamour, Université de Lorraine, Nancy, France;*
[4] *Institut Lumière Matière, Université Lyon 1, Villeurbanne, France;*

The modeling of dislocations and their mobility using ab initio density functional theory (DFT) calculations has made tremendous progress these past few years, in part thanks to an increase in computing power, but also because of methodological developments, including methods to correct the energy for elastic interactions between periodic images. In this talk, we will review recent advances in dislocation plasticity based on ab initio calculations, mainly in body centered cubic (BCC)transition metals. We will discuss our new understanding of the screw dislocation two-dimensional Peierls potential and its close connection to the well-known deviations from the Schmid law[1]. Alloying effects on the dislocation core structure and mobility will be addressed; highlighting in particular how interstitial atoms can restructure the screw dislocation core[2].

[1] L. Dezerald, D. Rodney, E. Clouet, L. Ventelon, F. Willaime, Nat. Commun. **7**, 11695 (2016).

[2] L. Ventelon, B. Luthi, E. Clouet, L. Proville, B. Legrand, D. Rodney, F. Willaime, Phys. Rev. B **91**, 220102 (2015).

Contributed talk	Thursday, October 06th, 11:45

Contributed talk	Thursday, October 06th, 11:45

Atomistic studies of non-screw dislocations in iron using magnetic bond-order potential

Matous Mrovec[1,2,3], Peter Gumbsch[2,3]

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Glide of dislocations and their mutual interactions govern the intrinsic plastic behavior of most metals. In the case of bcc metals like alpha-Fe, dislocations exhibit large differences in their mobilities. While pure screw dislocations experience high lattice resistance due to their non-planar cores, all non-screw dislocations are expected to glide easily at low applied stresses. However, details about their core structures and glide mechanisms are largely unknown.

In this work, we carried out atomistic simulations for a number of non-screw dislocations in alpha-Fe using the magnetic bond-order potential (BOP), which is able to provide a correct description of both directional covalent bonds and magnetic interactions in iron. We will present an analysis of both static (structural, magnetic) and dynamic (behavior under applied stress) properties of these dislocations and discuss the implications on the plastic behavior.

Invited talk Thursday, October 06th, 14:00

Invited talk Thursday, October 06th, 14:00

Solute interactions with dislocations in BCC Fe

Dallas R. Trinkle[1], Anne Marie Z. Tan[1], Michael R. Fellinger[1], Louis G. Hector, Jr.[2]

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[2] *General Motors R&D Center, Warren, MI, USA.*

Integrated computational materials engineering of third-generation steels requires a multiscale approach that passes first principles data to mesoscale (e.g. microstructural) models. In particular, we are interested in the effects of solutes on mechanical behavior—both elastic and plastic. The challenge of lattice constants can be computed efficiently using density-functional theory from the elastic dipole tensor that quantifies how solutes induce stress in the host crystal. The changes in elastic constants can be similarly computed from changes in the elastic response of the unstrained cells combined with higher order elastic constant data. To model solid solution strengthening, however, we require not just misfit data that captures the long-range interaction, but the quantification of solute interaction with the dislocation core.

Modeling isolated dislocations is challenging due to their long-ranged strain fields. While there are a variety of possible coupling or "multiscale" techniques available, I will focus on flexible boundary conditions, which use the lattice Green's function to couple electronic structure to an infinite harmonic bulk; this approach greatly simplifies many "hand-shaking" problems, and generally provides a computationally efficient approach. This methodology has explained solid-solution softening in molybdenum (explaining a 50-year-old mystery of metallurgy), dislocation cores in aluminum and titanium, and provided a wide range of mechanical behavior predictions for magnesium alloys. I will discuss our recent work improving the accuracy and efficiency of flexible boundary condition methods specifically for a dislocation geometry, and the application to dislocations cores in BCC Fe.

These results provide the starting point for direct calculation of solute-dislocation interactions in BCC Fe. We start with relaxed dislocation core geometries, introduce solutes at different locations in and around the core, and relax to map out the interaction energy landscape. I will conclude with our results for Al, B, Cu, Mn, Si substitutional solutes and C and N interstitial solutes in BCC Fe, their interactions with dislocations, and comparisons with experimental data.

Contributed talk	Thursday, October 06th, 15:40

Contributed talk Thursday, October 06th, 15:40

Multiscale modeling of local phase transitions at dislocations

Gerard Leyson, B. Grabowski, J. Neugebauer

Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany;

Atom probe tomography experiments have revealed that chemical and structural states can exist at dislocations in Fe-Mn alloys[1]. These one dimensional complexion states are fcc in a bcc matrix, characterized by high Mn content. This phenomenon is studied using a multiscale model that describes locally stable equilibrium states near dislocations. The model use atomistic calculations to inform a continuum model based on Eshelby's inclusion. The local elastic field around the dislocation is determined using a semi-empirical embedded atom (EAM) method, and the change in formation energy due to the phase transformation is estimated using CALPHAD and ab-initio calculations. The stability of a local fcc inclusion around an edge dislocation is examined as a function of of inclusion size. The results show that, under certain conditions, local phase transformation can occur around the dislocation due to its stress field. This quasi-one-dimensional defect has an equilibrium size and is stable against coarsening.

[1] Kuzima M, Herbig M, Ponge D, Sandlöbes S, and Raabe D, Science **349**, 1080-1083 (2015).

Invited talk	Thursday, October 06th, 16:15

Invited talk Thursday, October 06th, 16:15

Structure, energetics, and transformations of $\langle \mathbf{a} \rangle$ and $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations in HCP metals

William A. Curtin[1], Z. X. Wu [1,2], B. L. Yi[1]

[1] *Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland;*
[2] *Institute for High Performance Computing, Singapore;*

HCP metals such as Ti, Mg, and Zr are of high technological importance, but the mechanisms of deformation are complex due to the HCP crystal structure. Fundamental understanding of the dislocations in HCP metals is thus lacking, particularly for the $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations. The $\langle \mathbf{c}+\mathbf{a} \rangle$ slip is the only mode capable of providing slip in the crystallographic $\langle \mathbf{c} \rangle$ direction, and is therefore essential to enabling generalized plastic flow in polycrystalline HCP metals. Here, we present a systematic study of slip modes, and the competition and transformation between different possible dissociated dislocation structures having the same Burgers vector. We first present careful DFT results on the stacking fault energies for the basal, prism, and pyramidal I and II systems, which is a first step toward rationalizing operative slip systems in each individual HCP metal. Results show that the $\langle \mathbf{c}+\mathbf{a} \rangle$ stacking fault involves significant multi-plane relaxations, such that standard methods to compute the γ surface are inadequate. We then use anisotropic elasticity to analyze competing dissociation paths for full $\langle \mathbf{a} \rangle$ and $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations. We show that both Pyr. I mixed and Pyr. II edge dislocations should undergo a transformation from dissociation on the Pyramidal plane to dissociation along the basal plane separated by a basal stacking fault, with the resulting dislocation being immobile. This prediction explains experimental observations in Mg, Ti, Ti-Al, and Zr. Direct MD studies using a validated interatomic potential for Mg show the thermally activated transition directly, with a relatively small energy barrier, thus rationalizing the proliferation of such dislocations in Mg and the consequential rapid strain hardening and low ductility in Mg. The analysis also shows the energy difference between Pyr. I and II screw dislocations, which determines the ability of $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations to cross-slip. The analysis further shows that the Pyramidal screw dislocations dissociate into pure or nearly-pure screw partials. An NEB analysis in Mg then shows that $\langle \mathbf{c}+\mathbf{a} \rangle$ cross-slip occurs by a mechanism entirely different than that in fcc metals (which also have dissociated partials). In Mg, cross-slip barriers are also found to depend on non-Schmid/non-Escaig stresses, thus affecting the relative prevalence of Pyr. I vs. Pyr. II slip in Mg, and explaining tension/compression asymmetry in the Pyramidal slip deformation of Ti. All of these results point toward directions for alloy design to prevent unfavorable phenomena and encourage favorable phenomena, so as to achieve desired strength and ductility in HCP alloys. Overall, our studies demonstrate how the combination of density functional theory, anisotropic elasticity, and targeted molecular simulations can provide in-depth insight into competing slip modes in complex metals.

[1] J.A. Yasi and D.R. Trinkle, Phys. Rev. E **85**, 066706 (2012).

[2] L. Ventelon, B. Luthi, E. Clouet, L. Proville, B. Legrand, D. Rodney, and F. Willaime, Phys. Rev. B **91**, 220102 (2015).

[3] Z. Wu and W. A. Curtin, Nature **526**, 62 (2015).

ABSTRACTS

POSTERS

.

Interstitial solution enthalpies derived from first-principles: knowledge discovery using high-throughput databases

Ugur Aydin, Tilmann Hickel, Jörg Neugebauer

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Interstitial elements play a decisive role for the performance of transition metals. Carbon, for example, is important for microstructure formation; hydrogen is known to yield embrittlement phenomena; boron can support the stabilization of grain boundaries, while oxygen yields their internal oxidation. Furthermore, the strain imposed by interstitial elements is often used to trigger magnetic or structural properties of compounds. The computational design of innovative materials therefore requires the reliable prediction of interstitial concentrations.

We have extended and applied our python-based high-throughput workbench in order to reveal the underlying physical mechanisms that determine interstitial solution enthalpies in transition metals. A careful first principle analysis has started with hydrogen to identify possible chemical and mechanical descriptors that determine the solubility. The study was in a second step extended to first-principles calculations of hundreds of solute-solvent combinations along with the determination of the physical properties of the host materials. In order to analyse the data, complex simulation protocols based on Pearson correlation coefficients, factor analysis, and singular value decomposition have been implemented into our workbench. As a result we have discovered a previously unknown formula containing only a few descriptors, which captures the solution process for all solute-solvent combinations with high accuracy. It allows one to predict interstitial concentrations solely from the knowledge of a couple of host-material properties such as bulk modulus and bandstructure parameters. The formula is used to reveal and design the solubility of interstitials in (multi-component) materials that were not incorporated in the high-throughput study.

Prediction of the mechanical properties of carbide-steel interfaces from first-principles

Elric Barbé[1,2], Chu-Chun Fu[1], Maxime Sauzay[2]

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[2] *CEA, DEN, Service de Recherches Métallurgiques Appliquées, F-91191, UPSay, Gif-sur-Yvette Cedex, France;*

Fracture of interfaces between some carbides and metallic lattices is often observed during creep. It may be responsible for the intergranular creep cavitation and ductile damage initiation. Understanding the mechanisms of fracture allows us to predict further the creep and ductile damage evolution. This study focuses on interfaces between a metallic matrix (Fe, Cr, Ni) and a representative carbide: $\mathrm{Cr_{23}C_6}$.

Surface, interface and fracture energies are calculated via density functional theory (DFT) based on chemical potential analysis. Then, interfacial fractures stresses are estimated by the UBER (Universal Bonding Energy Relation) model[1,2] and compared with the results of DFT simulations of tensile tests. We consider metallic lattices with different chemical composition, and magnetic ordering, in order to investigate the dependence of the interfacial mechanical behavior on these properties. It is found that the magnetic effect on the critical stress is mainly due to the dependence on magnetic ordering of the elastic constants. Also, in general, the coherent interfaces show rather high fracture stresses and energies, which is consistent with experimental observations showing that the interfacial fracture occurs much more often at incoherent interfaces[3]. The deduced interface fracture properties will be used as input data for cohesive-zone modeling in crystalline finite element computations, in order to predict the nucleation rate of cavities at the interfaces, observed experimentally.

[1] J. H. Rose, J. Ferrante, and J. R. Smith, Phys. Lett. **47**, 675 (1981)
[2] J. R. Rice and J. S. Wang, Materials Science and Engineering: A **107**, 23 (1989)
[3] Y. Cui et al, Engineering Failure Analysis, **58**(2), 452 (2015)

Poster session 3

A density-functional theory investigation of Fe_4N and $Fe_{16}N_2$ precipitates in an Fe-N solid solution

Sam De Waele[1,2], Kurt Lejaeghere[1], Lode Duprez[3], Roger Hubert[3], Elke Leunis[3], Stefaan Cottenier[1,2]

[1] *Center for Molecular Modeling, Ghent University, Belgium;*
[2] *Department of Materials Science and Engineering, Ghent University, Belgium;*
[3] *OCAS NV, Ghent, Belgium;*

For steels, knowledge of the thermodynamic stability and nucleation rate of precipitates is often essential to fully understand their thermal and mechanical properties. The Fe-C system is relatively well studied with respect to these aspects, but such information is not generally available for the Fe-N system. We therefore aim to investigate the formation of Fe_4N and $Fe_{16}N_2$ precipitates in an Fe-N solid solution. The free energies of the bulk phases are obtained from Density-Functional Theory (DFT) calculations with the GGA-PBE approximation and electronic and vibrational temperature contributions are calculated within the quasiharmonic approximation. The magnetic entropy is obtained by imposing a localized model, using a Heisenberg Hamiltonian. The magnetic exchange coefficients and spin quantum numbers are calculated from DFT, while the Heisenberg model itself is solved with a classical Monte Carlo (cMC) approach. Thus spin quantization is neglected, but the cMC result is corrected per the scheme proposed by Körmann *et al.*[1], to approach the correct solution. Also of importance are the interface energies for the phases concerned: Fe/Fe_4N and $Fe/Fe_{16}N_2$. High resolution scanning transmission electron microscopy (HR-STEM) is used to identify the orientation relationship (OR) between the precipitated phases and the matrix, and the strain on both phases. This guides the DFT calculations from which the interface energies can be derived.

This is a work in progress, and we will report about its present status.

[1] F. Körmann, A. Dick, T. Hickel, and J. Neugebauer, Physical Review B **81**, no. 13 (April 19, 2010):

Poster session	4

Error estimates for density-functional theory predictions of surface energy and work function

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[3] *OCAS NV, Ghent, Belgium;*

Density-functional theory (DFT) predictions of materials properties are becoming ever more widespread. With increased use comes the demand for estimates of the accuracy of DFT results. In view of the importance of reliable surface properties, this work calculates surface energies and work functions for a large and diverse test set of crystalline solids. They are compared to experimental values by performing linear regression, which results in a measure of the predictable and materialspecific error of the theoretical result. Two of the most prevalent functionals, the local density approximation (LDA) and the Perdew-Burke-Ernzerhof parametrization of the generalized gradient approximation (PBE-GGA), are evaluated and compared. Both LDA and PBE-GGA are found to yield accurate work functions with error bars below 0.3 eV, rivaling the experimental precision. LDA also provides satisfactory estimates for the surface energy with error bars smaller than 10 %, but GGA-PBE significantly underestimates the surface energy for materials with a large correlation energy.

Poster session 5

Off-stoichiometric composition of κ carbide in Fe-Mn-Al-C steels: An ab-initio study combined with experiment

Poulumi Dey[1], Roman Nazarov[2], Biswanath Dutta[1], Mengji Yao[1], Emanuel Welsch[1], Michael Herbig[1], Martin Friák[3,4], Marta Lipińska-Chwałek[5,6],Tilmann Hickel[1], Christina Scheu[1], Dierk Raabe[1] and Jörg Neugebauer[1]

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[2] *Lawrance Livermore National Laboratory, Livermore, CA 94550, USA;*
[3] *Institute of Physics of Materials, v.v.i., Academy of Sciences of the Czech Republic, 61662 Brno, Czech Republic;*
[4] *Central European Institute of Technology, Masaryk University, 62500 Brno, Czech Republic;*
[5] *RWTH Aachen, 52074 Aachen, Germany;*
[6] *Forschungszentrum Jülich GmbH, 52425 Jülich, Germany;*

Regularly arranged nano-sized κ carbides (Fe,Mn)$_3$AlC play a crucial role in upgrading the mechanical properties of quaternary Fe-Mn-Al-C alloys, which exhibit an exceptional combination of high strength and ductility along with low density and high corrosion resistance. These beneficial effects are strongly connected to the thermodynamic stability and chemical composition of these precipitates. We have therefore investigated the underlying reason behind the off-stoichiometry of these particles by the means of density functional theory (DFT) calculations. We thoroughly investigated the partitioning of the constituent elements mainly C between the precipitate and the γ matrix with an aim to understand the interplay between elastic and chemical contributions. Our analysis is substantiated by advanced experimental techniques, as e.g., atom probe tomography (APT) and high-resolution scanning transmission electron microscopy (HRSTEM).

Within the DFT calculations, the carbides are considered to be coherent, based on the observations made by HRSTEM. The latter confirm the absence of misfit dislocations at the interface or within the surrounding γ matrix. Based on this assumption, our investigations predict a deviation from stoichiometry for both Al and C in these κ carbides. The C off-stoichiometry is an outcome of the compromise between the elastic and chemical energies of the system. While the inherent elastic strain in the coherent microstructure drives C away from κ into the surrounding γ matrix, the chemical energy gain by the retention of C in the precipitate prevents such a C outflow. Furthermore, our study clearly shows that the off-stoichiometry of C is coupled to the reduced Al content, since the latter can be explained by a combination of strain effect and Mn antisites in the vicinity of C vacancies. Our ab-initio based prediction has been confirmed by APT, which provides a high spatial and chemical resolution for the atomic distribution across the $\kappa - \gamma$ interface. The underlying methodology can be extended to determine the composition of other kinds of coherent microstructures.

[1] M. J. Yao, P. Dey, J. -B. Seol, P. -P. Choi, M. Herbig, R. K. W. Marceau, T. Hickel, J. Neugebauer and D. Raabe, Acta Mater. **106**, 229 (2016).

[2] P. Dey, R. Nazarov, B. Dutta, M. Yao, M. Herbig, M. Friák, T. Hickel, D. Raabe and J. Neugebauer, under review in Phys. Rev. B.

Poster session 6

Towards a microscopic understanding of lattice vibrations in disordered systems: implications for high entropy alloys

Biswanath Dutta[1], Tilmann Hickel[1], Raina J. Olsen[2], Bennet C. Larson[2], Malcolm Stocks[2], German D. Samolyuk[2], Jörg Neugebauer[1]

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The thermodynamics of random alloys is an area of extreme importance in materials science. The lattice dynamics driven by different disorder-induced phenomena often plays a pivotal role in determining the thermodynamic properties of these materials. For instance the phase stability of the high entropy alloys (HEAs), which have received a lot of attention in the last few years due to their excellent mechanical properties, can be dictated by the vibrational entropy contributions. Phonon contributions to the thermal conductivity can also be decisive for determining their transport properties and hence for the usage of HEAs as radiation resistant materials.

The main challange to study phonons in these random alloys lies in an appropriate treatment of the mass and force-constant fluctuations present in the system. The most common approach to treat such disorder is the coherent potential approximation (CPA), which, being a single-site theory is unable to handle non-local fluctuations and therefore, usually fails for phonons. A recent progress in this direction is the itinerant CPA (ICPA), which is a Greens function based formalism and can address various fluctuations in chemically disordered systems. In the present work, we use this method to study phonons in several binary alloys which are subsystems of the HEA $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$ also known as Cantor alloy. To simulate the chemical randomness, we employ special quasi-random structures (SQS), which can closely mimic the fluctuations in the inter-atomic force constants in a random alloy. These force constants are calculated using density functional theory and are fed into the ICPA to perform the necessary configuration averaging.

Our calculations for the NiCo alloy provide good quantitative comparison with experimental results for both the phonon dispersion spectra and the line-widths, which highlights the reliability of the coupled SQS+ICPA approach. Another interesting observation is the poor agreement between theory and experiment for the transversal phonon line-widths in the NiFe alloy. A thorough comparison of the local bond distances in the two investigated systems reveals significantly larger local lattice distortions in the NiFe alloy, which are not addressed within ICPA. This provides an indication that in addition to mass and force-constant fluctuations, such distortions can also influence the vibrational properties of HEAs and hence need to be addressed in an appropriate manner.

[1] S. Ghosh, P. L. Leath and M. H. Cohen, Phys. Rev. B **66**, 214206 (2002).
[2] B. Dutta, K. Bisht and S. Ghosh, Phys. Rev. B **82**, 134207 (2010).
[3] O. Granäs, B. Dutta, S. Ghosh and B. Sanyal, J. Phys.: Condens. Matter **24**, 015402 (2012).
[4] D. Ma, B. Grabowski, F. Körmann, J. Neugebauer and D. Raabe, Acta Mater. **100**, 90 (2015).

Chemo-mechanical coupling from first principles: on the strain dependence of oxygen adsorption on Pd(111) and Ir(111)

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Mechanical deformation can affect the adsorption and reaction processes of reactants on surfaces. Thus, by straining catalytically active surfaces their reactivity as well as selectivity can be influenced, which is of high importance, for example, in the field of heterogeneous catalysis.[1,2]

Here, Pd(111) and Ir(111) surfaces interacting with atomic oxygen are used as model systems. At first, the adsorption characteristics, e.g. the energetics, are investigated within the framework of density functional theory (DFT). Furthermore, the incorporation of oxygen below the Pd surface, which is considered to be the first step of an oxide formation, is studied. The most favourable adsorption configurations are identified via the cluster expansion approach using DFT input data. Secondly, for various favourable oxygen configurations at the Pd and the Ir surfaces biaxial strain is applied in the surface plane to obtain the response of the adsorption energetics. Particularly, the coupling parameter between strain and adsorption energies is of interest to allow for a comparison with experiments. The coupling parameter is affected by the oxygen coverage as well as the occurrence of oxygen incorporation.

[1] Gsell et al., Science **280** (1998) 717 .
[2] Mavrikakis et al., Physical Review Letters **81** (1998) 2819.

Poster session 8

Ab initio based insights into the thermodynamics and kinetics of precipitate formation in Al-Sc alloys

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Al-based light-weight alloys are promising for structural applications. A critical strengthening mechanism in these alloys is precipitate formation. The inherent evolution of these precipitates over time plays a key role in governing the mechanical behaviour of these alloys. On the one hand, in order to fine tune the mechanical properties, an in-depth understanding of the precipitation kinetics is crucial. On the other hand, a thorough thermodynamic investigation is necessary to explain the stability of these phases. In this work, we study these two aspects for the example of Al-Sc alloys.

Firstly, we study the precipitation kinetics in a model binary system employing kinetic Monte-Carlo (kMC) simulations. A linear bond-cutting model has been used to describe the underlying energetics. The kinetics has been analysed in terms of size distribution of the precipitates and their temporal evolution. The final results have been plotted as time-temperature-transformation (TTT) diagrams. The critical factors controlling the key features of the fully atomistically derived TTT diagrams such as asymptotic and nose temperature are discussed. Since the key observations are independent of the specific material system, they can be applied to tailor the precipitation kinetics in many applications.

Secondly, we investigate the thermodynamic properties of the Al_3Sc precipitate phase employing first-principles based density functional theory (DFT) calculations. Going beyond the routine quasi-harmonic approximation, the effect of finite-temperature excitations viz. electronic and anharmonic contributions on the heat capacity and the thermal expansion has been investigated. In particular, we highlight the importance of electronic contribution in explaining the low temperature phenomenon observed in the heat capacity measurements of Al_3Sc.

Poster session 9

Tracking defect migration in molecular dynamics-finite element method multiscale calculations

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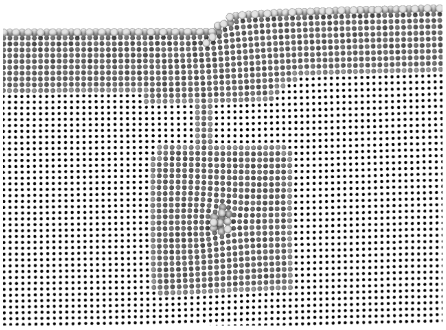
Atomistic simulations are a powerful tool for understanding underlying mechanisms which control material behaviour and are a critical component of knowledge-based design for new alloys. However, even with modern computational power and highly efficient algorithms, molecular dynamics (MD) simulations still have trouble reaching experimental time- and length-scales. For the problem of length-scales one approach is to couple MD to a less expensive continuum model, often represented using the finite element method (FEM).

Since the seminal work of Kohlhoff *et al.* in 1991[1], coupled MD-FEM methods have been an active area of research and there are now many flavours of coupling[2]. We focus our attention on the exceptionally elegant variety originally proposed by Kohlhoff, a force-based approach in which MD and FEM domains are coupled through the displacement of atoms/nodes at their interface. The most recent advances for this particular technique demonstrate its usefulness even for treating complex systems and dynamic events at finite temperatures[3].

We improve on this method by making it fully adaptive with respect to which parts of the system are treated atomistically and which are treated by the continuum model. This allows the MD-domain to track the migration of planar and line defects while maintaining the cost-advantage of the coupled method. This is accomplished by on-the-fly reconstruction of the ideal lattice sites for the "bulk-like" atoms which lie in the FEM domain. Discontinuities in this ideal lattice are accommodated by a thin MD domain, as can be seen in the figure, where a dislocation surrounded by a small MD domain has glided through the system. Dynamic domain partitioning has been performed behind the dislocation and a thin trail of MD atoms shows the approximate path it traveled. In principle, the FEM mesh can be coarsened far from the MD domain, but in the current implementation we maintain a one-to-one atom-to-node correspondence everywhere.



Portion of a quasi-2D system under indentation. The largest atoms are those identified by structural analysis as interesting, medium atoms provide the balance of the MD domain, and the smallest atoms belong to the FEM domain.

[1] S. Kohlhoff, P. Gumbsch, and H.F. Fischmeister, Phil. Mag. A **64**, 851 (1991).
[2] R.E. Miller and E.B. Tadmor, Model. Simul. Mater. Sci Eng. **17**, 053001 (2009).
[3] F. Pavia and W.A. Curtin, Model. Simul. Mater. Sci Eng. **23**, 055002 (2015).

Poster session 10

Phonon dispersion relations of disordered alloys using the band-unfolding method

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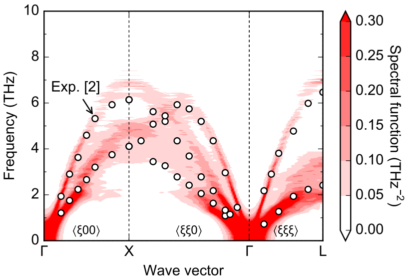
Many steels are disordered alloys. Atomic sites in such disordered alloys are randomly occupied by different chemical elements, and hence the alloys lose the symmetry of their underlying crystal structures in microscopic viewpoint. In experiments such chemical disorder is "averaged" when measuring the phonon dispersion relations, while in first-principles calculations using supercell models, the calculated phonon dispersion relations do not show the symmetry of the underlying crystal structures. This makes it difficult to directly compare the computational results with experimental data. In this study, we develop the band-unfolding method[1] to obtain the "effective" phonon band structures of the disordered alloys that have the symmetry of the underlying crystal structures. This approach is applied to disordered face-centered cubic (fcc) $\mathrm{Cu}_{0.75}\mathrm{Au}_{0.25}$ and $\mathrm{Ni}_{0.50}\mathrm{Pt}_{0.50}$, and characteristic behavior found in their phonon dispersion relations are discussed.

The plane-wave basis PAW method was employed in the framework of density-functional theory within the GGA of the PBE form as implemented in the VASP code. The disordered alloys are approximated using the supercell models including 108 atoms based on the special quasirandom structures. In the band-unfolding method, mode-eigenvectors obtained from the supercell models are projected onto the space that contribute to the wave vector $\mathbf{q}$ with the translation symmetry of the underlying crystal structures. The norms of the projected vectors are regarded as the weights on $\mathbf{q}$, and the spectral function at $\mathbf{q}$ is calculated from the sum of the weights of the mode-eigenvectors. The effective phonon dispersion relations are obtained from the spectral function.

The figure shows the effective phonon dispersion relation of fcc $\mathrm{Cu}_{0.75}\mathrm{Au}_{0.25}$ calculated using the band-unfolding method. The phonon dispersion relation shows linewidths of the phonon modes caused by the chemical disorder. The peak positions of the spectral functions are mostly in good agreement with experimental data. We also find some characteristic behavior that cannot be seen for pure fcc materials. For example, the spectral function of the lowest-frequency phonon branch along the $\langle 110 \rangle$ direction changes discontinuously. From the detailed analysis of the spectral function, we find that the discontinuous branch arises because Cu and Au contribute to different regions of frequency for this phonon mode. This phenomenon occurs due to the large fluctuations of atomic masses and force constants in the disordered alloys.



Phonon dispersion relation of fcc $\mathrm{Cu}_{0.75}\mathrm{Au}_{0.25}$ calculated using the band-unfolding method.

[1] P. B. Allen, T. Berlijn, D. A. Casavant, and J. M. Soler, Phys. Rev. B **87**, 085322 (2013).
[2] S. Katano, M. Iizumi, and Y. Noda, J. Phys. F **18**, 2195 (1988).

Poster session 11

Automatized convergence and error analyses for the ab initio calculation of mechanical properties

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Over the last years methodological and computational progress in atomistic simulations has substantially improved the predictive power in the ab initio description of iron based alloys. This includes elastic parameters, finite temperature phase stabilities of precipitates as well as the formation energies of point and extended defects. To compare the simulation results with experimental data, however, it is necessary to quantify the various sources of uncertainty. In particular, for parameters derived from a complete set of ab initio calculations, such an analysis is highly non-trivial.

We therefore leverage the capabilities of our recently developed Python based workbench PyIron, to implement an automatized stochastic sensitivity analyses with the aim to determine and differentiate model errors, statistical errors and systematic errors contributing to mechanical properties. For each error type the convergence gradient based on our sensitivity analyses is determined and combined with the individual cost function of the parameters. Based on this function we derive an algorithm for automated convergence, which allows to quantify the precision of derived quantities such as elastic constants. The efficiency of the approach will be demonstrated for the bulk modulus of iron.

Poster session 12

Hydrogen behaviour at structural defects in high-strength steels

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The behaviour of hydrogen in high-strength steels is well-known to play a very significant role in the long-term stability and mechanical properties of such materials. Experimental and theoretical work has indicated that structural defects, such as grain boundaries, dislocations, nanovoids and phase boundaries between the matrix and precipitates present in the material, play the most significant role in the phenomenon of hydrogen embrittlement.

Due to the large system sizes required to simulate, for example, low-symmetry grain boundaries or misfit dislocations between the matrix and non-metallic inclusions such as TiN, conventional *ab initio* simulations are no longer feasible. In this direction, we have developed scale-bridging atomistic potentials based on the tight-binding approximation, which still allow for a fully quantum-mechanical treatment of the system. Using the developed potentials, we have performed extensive atomistic simulations to understand the energetics and diffusion behaviour of hydrogen in the vicinity of such extended defects, as well as simulated mechanical testing and dynamical simulations to examine the competition between possible embrittlement mechanisms.

Electro-mechanical response of metal surfaces from first principles

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Coupling between mechanical stress or strain of a surface and its electronic properties is relevant for diverse applications from sensors and actuators to heterogeneous catalysis. The surface stress f of metallic surfaces reacts sensitively to excess charge q. Due to their high surface-to-volume ratio, nanoporous metals thus respond with a macroscopic deformation to electric charging in electrolyte. Therefore, such materials are interesting alternatives to conventional actuators. The key quantity for characterizing the performance of such actuators is the electrocapillary coupling parameter $\varsigma = \mathrm{d}f/\mathrm{d}q$. Owing to Maxwell relations, ς can be determined using apparently unrelated quantities, which are, however, considerably easier to calculate with high accuracy. For clean metal surfaces, it is possible to evaluate the charge-induced surface stress change in terms of the response of the work function to in-plane strain in an ab-initio framework.

Using this approach, we have determined ς for several metal surfaces, focusing mainly on the response of sp-bonded metals. It is found that aluminum surfaces exhibit positive coupling coefficients, whereas the other sp-bonded metals show the usual negative sign known from previous experimental and theoretical studies of clean transition metal surfaces.

In addition, we investigate the impact of excess charge on surface structure and bonding via ab-initio simulation of metal surfaces in an external electric field in order to gain further insight into the underlying mechanisms. Both the direct effect on the surface stress via charging of the bonds and the indirect effect resulting from the charge-induced relaxation will be analyzed and discussed in relation to the trends of the determined coupling coefficients.

Atomic-scale mechanisms of dislocation transmission across a twin boundary in Cu bi-crystals

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Despite an intense interest in coherent twin boundaries, the details of the interaction between dislocations and coherent twin boundaries, such as dislocation transmission, remain unclear[1−3]. In the present study, a combination of molecular dynamics simulations, *in situ* Laue micro-diffraction, and scanning electron microscopy is used to investigate the impact of the direction of applied strain on the slip transmission in a Cu bi-crystal with a coherent $\Sigma3\{111\}$ twin boundary. To this end, compression of Cu nano-pillars in different crystallographic directions is performed on samples including the twin boundary parallel to the compression axis and additionally on single-crystalline reference samples, both in the simulations and experiments.

Laue micro-diffraction and postmortem scanning electron microscopy results reveal multiple transmission events through the twin boundary. In some cases a limited number of dislocations is observed to pile up in front of the twin boundary[4]. The analysis of the simulated trajectories and forces on atoms in the grain boundary close to the transmission area and on the transmitted dislocation reveals the details of the atomistic mechanism of the transmission event as a function of applied strain. Further, the simulations show that break-through stresses of dislocations for the transmission across the $\Sigma3\{111\}$ twin boundary vary between 10-800 MPa. This range is in good agreement with the observed experimental values (20-500 MPa). The break-through stress is shown to depend on the local defect structure of the boundary.

[1] Q. Liu, L. Deng, X. Wang, Mater. Sci. Eng., A, **676**, 182-190, (2016).
[2] Z. Shen, R.H. Wagoner, W.A.T. Clark, Acta. Mater., **36**, 3231-3242, (1988).
[3] K. Lu, L. Lu, S. Suresh, Science **324**, 349-352 (2009).
[4] N. V. Malyar, J.S. Micha, G. Dehm, C. Kirchlechner, In progress.

Poster session 15

Simultaneous sampling of atomic and magnetic degrees of freedom in iron using bond-order potentials

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Magnetism plays a key role in the description of iron at all temperatures. The body-centered cubic (bcc) phase of iron at room temperature is stabilized by magnetism. With increasing temperature, iron undergoes a transition from a ferromagnetic to a paramagnetic state, a structural transition from bcc to face-centered cubic (fcc) and another structural transition back to bcc before it finally melts. It is known from experiments that magnon-phonon coupling is important for both structural and magnetic transitions in iron. Up to now, simulations of iron often lag a proper treatment of paramagnetism and of the interplay between atomic and magnetic degrees of freedom which are often described by separate models. We use bond-order potentials to sample atomic and magnetic degrees of freedom simultaneously using a unified description. This includes a non-collinear description of the spins. With a Metropolis Monte Carlo sampling algorithm, we sample atomic displacements and electronic degrees of freedom including spin directions and magnitudes to obtain reliable ensemble averages. The fast and efficient algorithm allows us to sample large systems that are necessary to accurately model paramagnetism and includes an explicit treatment of the electronic structure.

With our approach, we sample the bcc and the fcc phase of iron in the isothermal-isobaric ensemble in a temperature range from 100K to 2000K. Monitoring the spin ordering, we correctly observe the transition from the ferromagnetic state at low temperatures to the paramagnetic state at high temperatures in bcc and extract the Curie temperature.

Additionally, we investigate the influence of a single vacancy on the magnetization of the bcc phase.

Effects of Manganese on the hydrogen embrittlement of a carbon segregated grain boundary in α-Fe

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The cohesion of grain boundaries (GBs) is dependent on their chemical composition and structure and greatly influences the mechanical properties of the material. It is well known that H prefers segregating to the GBs (and other defects). Hydrogen enchanced decohesion is one important mechanism of Hydrogen embrittlement. Therefore it is necessary to understand the effects of the impurities and alloying additions that segregate to the GB on the cohesion of GBs. Mn and C being important additions in iron alloys, were chosen for the study.

The embrittling effects of H in the presence of alloying elements Mn and C at the $\Sigma5(310)[001]36.9^\circ$ symmetrical tilt grain boundary (STGB) in body centered cubic Fe was investigated by performing spin polarized DFT calculations. The calculations were carried out with respect to the effect of a varying number of Mn, C and H atoms at different segregation sites of the GB. The impact of segregation of Mn, C and H on the GB energy, work of separation and theoretical strength has been studied. Uni-axial tensile tests were performed perpendicular to the GB and theoretical strength was determined from the energy-displacement data fitted using the universal binding energy relationship. The work of separation was split into mechanical and chemical contributions. The thermodynamic model of Rice and Wang[1] was used to determine the (cohesion enhancing or weakening) nature of the segregated elements. Mn was found to be a cohesion enhancer at the considered GB. C exhibited an enhancement of the GB cohesion. H does not strongly change the strength of pure Fe STGB. However there is a pronounced reduction of cohesion and strength in the three component Fe-C-H system, when H replaces the cohesion enhancing C[2]. In contrast, in the presence of Mn, H itself shows a detrimental effect on cohesive properties of the GB. Co-segregation of H and C in the presence of Mn was also studied. The segregation energies show that Mn attracts H to the GB but repels C, making the alloys with high Mn content more vulnerable to H embrittlement. With this work we could demonstrate that ab-initio calculations are an important tool to understand the influence of chemical composition on H embrittlement.

[1] James R. Rice, Jian-Sheng Wang, Materials Science and Engineering: A, Volume 107, 1989.

[2] A.M. Tahir, R. Janisch, A. Hartmaier, Materials Science and Engineering: A, Volume 612, 2014.

Spin dynamics with magnetic bond-order potentials

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Dynamic simulations of many microscopic processes in magnetic materials require to account for magnetic excitations. We apply spin dynamics in order to simulate the trajectories of the atomic subsystem and the spin subsystem simultaneously. The simulations are based on magnetic bond-order potentials that provide total energies, atomic forces and magnetic torques in systems with non-collinear magnetism. In order to generate trajectories in micro-canonical ensembles, we apply Newton's equation of motion (EOM) for the atomic degrees of freedom and a semi-classical EOM for spin precession. For simulations in the canonical ensemble we use the Langevin EOM for both, the atomic and the spin subsystem.

The role of interfacial planar defects for structural transformations in Fe-C alloys

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Structural transformations play a central role for the development of a large variety of microstructures in steels, which ultimately impact their mechanical performance. Despite the fact that steels have been extensively investigated by both theoretical and experimental techniques, it is still not fully clear how these structural transformations occur on the atomistic level. In particular, the realistic structural transformations are not a spontaneous rearrangement of the lattices, but are often realized by a moving interface scenario. A comprehensive exploration of the interface structure and how it triggers the microstructure evolution would allow us to better tune or improve the mechanical properties of steels.

Focusing on the major ingredients of steels, the Fe-C system, we have shown that interfaces play a decisive role for the formation of typical microstructures in steels, such as pearlite[1] and martensite[2]. Unlike the normal consideration of a direct interface between two phases, we have identified a metastable intermediate structure (MIS), which serves as an ordered short-range interface structure similar to the concept of complexions[3]. The MIS itself consists of a periodic arrangement of planar defects – $\Sigma3$ twin boundaries in bcc Fe. Due to its structural characteristics, the MIS has the flexibility to evolve to fcc austenite, bcc ferrite, orthorhombic cementite (Fe_3C) as well as bct (body centered tetragonal) martensite depending on the respective local conditions (magnetism, strain and C concentration). Distinguished by the different behavior of C atoms (diffusional or diffusionless redistributions) and their interplay with the transformation of the host Fe lattices, the pearlitic or martensitic microstructures are understood within a unified framework.

[1] X. Zhang, T. Hickel, J. Rogal, S. Fähler, R. Drautz, and J. Neugebauer, Acta Mater. **99**, 281 (2015).

[2] X. Zhang, T. Hickel, J. Rogal, and J. Neugebauer, Phys. Rev. B **94**, 104109 (2016).

[3] S. J. Dillon, M. Tang, W. C. Carter, and M. P. Harmer, Acta Mater. **55**, 6208 (2007).

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