Atomistically informed discrete dislocation dynamics simulations and the origin of anomalous slip in tungsten

K. Srivastava[1], D. Weygand[1], C. Marichal[2,3] H. Van Swygenhoven[2,3], P. Gumbsch[1,4]

[1]Karlsruhe Institut of Technology KIT, Institute for Applied Materials, Kaiserstr. 12, 76131 Karlsruhe, Germany
[2]Materials Science and Simulation, NUM/ASQ, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland
[3]Neutrons and X-rays for Mechanics of Materials, IMX, École Polytechnique Fédérale de Lausanne, CH-1012 Lausanne, Switzerland
[4]Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

A computational framework for the discrete dislocation dynamics (DDD) simulation of body-centered cubic (bcc) metals which incorporates atomistic simulation results [1] is developed here on the examples of iron and tungsten. Atomistic simulations suggest kink-pair nucleation on {110} planes only. Mobility rules for the screw dislocations in the DDD simulations are based on the kink-pair mechanism which is controlled by a stress-dependent activation enthalpy. This activation enthalpy not only depends on the resolved shear stresses but also incorporates so called non-Schmid stresses. It is demonstrated that this description of the dislocation mobility provides a physical basis to naturally explain many experimentally observed phenomena in bcc metals like the tension–compression asymmetry, the orientation dependence of loading, and the temperature dependence of the yield stress. We demonstrate the power of such atomistically informed DDD techniques by analysis of anomalous slip behaviour in tungsten.

Several bcc metals exhibit significant plastic flow on planes with low stresses, a phenomenon which is not generaly understood and termed anomalous slip. Here and in [2] we report on experimental observations of the occurrence of anomalous slip during compression of tungsten micropillars within an in-situ Laue microdiffraction setup. DDD simulations of the compression of micrometer sized tungsten single crystals in exactly the same geometry as in the in-situ experiments also show the occurrence of a significant amount of anomalous slip. A detailed analysis of the evolving dislocation microstructure reveals the underlying mechanism. Anomalous slip mainly occurs as a consequence of so called cross-kinks, topological configurations generated by prior dislocation interactions.

[1] K. Srivastava, R. Gröger, D. Weygand, P. Gumbsch, Dislocation motion in tungsten: Atomistic Input to Discrete Dislocation Simulations, International Journal of Plasticity 47 (2013) 126–142
[2] H.v.Swygenhoven et al., presented at MMM 2014

Screw Dislocation Cross-slip at Cross-slip Plane Jogs and Screw Dipole Annhilation in FCC Cu, Ni Investigated via Atomistic Simulations

S.I. Rao[1], D.M. Dimiduk[1], J.A. El-Awady[2],
T.A. Parthasarathy[3], M.D. Uchic[3], C. Woodward[3]

[1]Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLM
Wright-Patterson AFB, OH 45433-7817
[2]Johns Hopkins University, Baltimore, MD
[3]UES, Inc., 4401 Dayton-Xenia Rd, Dayton, OH 45432-1894

Using atomistic (molecular statics and molecular dynamics) simulations and embedded-atom-method potentials, cross-slip of screw dislocations at cross-slip plane jogs and screw dipole annihilation at cross-slip plane jogs were examined for FCC Cu, Ni. After conjugate gradient energy minimization, two different core structures were obtained for the screw dislocation having a cross-slip plane jog: a) a configuration where most of the screw dislocation was dissociated on the (111) glide plane, having an extended jog spread on the (11-1) cross-slip plane, and b) most of the screw dislocation was dissociated on the (111) glide plane having a sharp jog on the (11-1) cross-slip plane. The sharp jog configuration had an energy approximately 0.4 eV lower than the extended configuration in FCC Cu. Nudged-elastic-band-method calculations of the energy pathway between the sharp and extended jog configurations showed that the energy hump near the extended configuration is shallow and, that the activation energy required to transform the screw dislocation from the sharp to the extended configuration (activation energy for cross-slip) is close to 0.4 eV in FCC Cu (a factor of 4-5 lower than the activation energy for cross-slip in the absence of a jog). Similar results were obtained for FCC Ni.

Molecular dynamics simulations were used to study the annihilation of a jog-containing screw dipole. The dipole was separated approximately by 14 and 45 nm along the (111) direction in each of two simulations and, under application of Escaig stresses acting to constrict the screw dislocation on the (111) glide plane. The simulations showed that the critical Escaig stress for dipole annihilation significantly drops from the 0K value (~400 MPa) and, dipole annihilation is nearly athermal at room temperature. At 5K, Escaig stresses on the cross-slip plane are a factor of 1.5 less effective than the Escaig stresses on the glide plane and, glide stresses on the cross-slip plane are a factor of 3 less effective for dipole annihilation by cross-slip. However, it was found that if the screw dislocations are initially positioned away from each other by 14nm along the y direction on the (111) glide plane, in addition to their separation perpendicular to the glide plane, the screw dislocations move toward each other with the jog acting as a pinning point and extending an edge dipole due to their movement. This process makes cross-slip at the jog on the screw dislocation almost prohibitive. Application of glide stresses on the (111) glide plane accentuated this effect.

Based on these atomistic simulation results, dislocation dynamics simulations accounting for Shockley partials were also used to investigate the dipole annihilation process in FCC Cu, and Ni. These atomistic simulation results are expected to be useful in physics-based modelling of bulk cross-slip in higher length scale 3-D dislocation dynamics simulations investigating dislocation pattern formation and fatigue structures in FCC crystals.

From atomic to mesoscale diffusion equations for alloys

M. Nastar

CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette, France

Up to now there is no satisfying atomic theory of diffusion. Although diffusion at the atomic scale is strongly involved in aging phenomena of nanoscale devices and bulk materials with nanoscale microstructures. Bulk diffusion experiments are conducted at a micrometric spatial scale which is too large to highlight the atomic scale features of diffusion phenomena. Instead, interdiffusion experiments performed on nanoscale composition-modulated foils are perfect for the characterization of atomic diffusion. Since the 70s, a complex variation of the interdiffusion coefficient D with respect to the wavevector of a sinusoidal concentration modulation has been evidenced: while at small wavevector, a linear variation of D with respect to the square of the wavevector is observed; at wavelengths smaller than a few lattice parameters a deviation from linearity is observed. The implementation of Atomic Kinetic Monte Carlo simulations and new developments of the Self-Consistent Mean Field (SCMF) theory demonstrate that in alloys with short range interactions, a non-linear deviation of D is due to wavevector dependent kinetic correlations produced by the vacancy diffusion mechanism. A measure of this deviation can be used to determine the off-diagonal phenomenological coefficient of the Onsager matrix which is extremely difficult to extract from classical diffusion experiments, although it is an essential parameter for the prediction of microstructures induced by irradiation. To conclude, a new atomic diffusion equation for non-homogeneous alloys has been established. As wavevector gets small, it tends to a general diffusion equation different from the Cahn-Hilliard equation, showing that the latter currently used in phase field methods to describe vacancy diffusion controlled phenomena should include the interface-dependent kinetic correlations in addition to the interface-dependent driving forces.

Thermal properties of point defects and their clusters in bcc Fe

D. Murali[1], M. Posselt[1], M. Schiwarth[1,2], J. Kortus[2]

[1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O.Box 510119, D-01314 Dresden, Germany
[2]TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09596 Freiberg, Germany

Ferritic Fe and Fe-Cr alloys are basic structural materials of present and future nuclear fission and fusion reactors. The formation of the micro- and nanostructure of these alloys and the structural evolution under irradiation is essentially influenced by the interaction between solutes, vacancies and self-interstitials. These processes take place in different alloys such as reactor-pressure-vessel and oxide-dispersion-strengthened steels. The understanding of the nanostructure of those materials and of its radiation-induced evolution is indispensable for nuclear reactor safety. First-principle calculations based on the Density Functional Theory (DFT) are a very useful method to get atomistic insights into the interactions between solutes, vacancies and self-interstitials in bcc Fe. Traditionally, formation and binding energies of these species are investigated at T=0 and these data are further used in calculations on larger length and time scales such as in kinetic Monte Carlo simulations and Rate Theory.

The main objective of present work is the determination of the temperature-dependent free formation and binding energy of selected point defects and their clusters in bcc Fe. For this purpose DFT is used to obtain the corresponding vibrational free energies within the framework of the harmonic approximation. The substitutional solutes Cu, Y and Ti, the interstitial solute atom O, the vacancy as well as small clusters consisting of solute atoms and vacancies are considered. The results are compared with theoretical data obtained by other authors and discussed in relation to experimental solubility data. Fig. 1 (a) shows the temperature dependence of the free formation energy of substitutional Cu in comparison with recent DFT data of Reith et al. [1], whereas Fig. 1 (b) depicts the data for interstitial O. In both cases a significant dependence on temperature is found. This must be taken into account in multiscale simulations that use DFT input data.

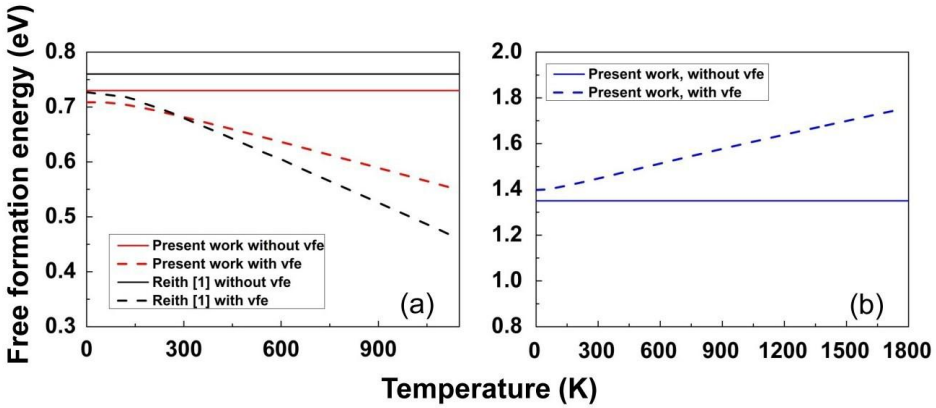

Figure 1: Total free formation energies of Cu (a) and O (b) in bcc Fe determined with and without considering the contribution of the vibrational free energy (vfe).

[1] D. Reith et al., Phys. Rev. B **80**, 054108 (2009).

Theory of Solid Solution Strengthening in High Entropy Alloys

Céline Varvenne[1], Aitor Luque Gomez[1], Satish I. Rao[1,2], William A. Curtin[1]

[1]Laboratory for Multiscale Materials Modeling, EPFL, Lausanne CH-1015, Switzerland
[2]UES Inc., 4401 Dayton-Xenia Road, Dayton, OH 45432 USA

High-entropy alloys represent a new class of advanced materials with unique properties that cannot be achieved by microalloying processes. In particular, mechanical strength and toughness are usually seen to be improved by increasing the number N of alloy components [1]. The origins of strengthening in these alloys remain uncertain, and there have been no theories that predict the observed trends. We present a new theory which generalizes the predictive dilute-solute strengthening model of *Leyson et al.* [2] to the case of N components with high concentration of all elements. The theory predicts that energy barriers for dislocation motion and zero temperature yield stresses do not scale with N, but are mainly driven by the effective misfit volumes of the alloy components. Together, these quantities provide predictions for the finite-T, finite-strain-rate strengthening and show that increasing the number of components N leads to higher strengths, provided that their volume misfits follow some rules. Application of the model to recent experiments shows that the theory predicts the same trends as found in experiments, as well as some deviations from the general trends including that some binary alloys are as strong as ternaries and that some ternaries as strong as quaternaries. Extensions of the model to include the effects of stacking fault energy, solute-solute interactions, and chemical short-range-order are discussed.

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The Evolution Process of Transformation Crystallography in Cu-Cr System
------A Hybrid Monte Carlo and Molecular Statics Method Simulation

Fu-Zhi Dai, Wen-Zheng Zhang

School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

Morphology of precipitates in various alloys is an essential microstructure feature that affects the properties of the alloys. Precise measurements of precipitate morphologies in metallic systems often reveal reproducible habit plane (HP) in irrational orientations together with irrational orientation relationship (OR). It is now clear that the HP of a well-developed precipitate usually contains a singular interfacial structure of a single set of dislocations (O-line criterion), which is possible only in interface(s) of discrete irrational orientations and with irrational ORs. An unsolved problem is why a particular HP is preferred among numerous interfaces that can meet the O-line criterion. While it would be desirable to investigate the process of precipitate evolution from beginning of the growth, the experimental study is extremely difficult with the available techniques. Atomistic simulation serve as an alternatively approach to solve this problem. In this work, a hybrid method which combines Monte Carlo and Molecular Statics is adopted to study the evolution process of crystallographic features. A Cu-Cr alloy is chosen as a model system, since reliable experimental crystallographic data of Cr-rich precipitates in this system is available for testing the simulation results [1, 2].

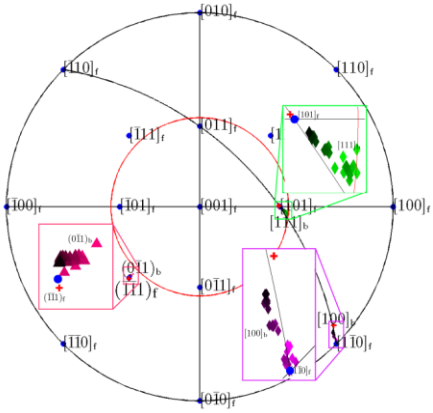

Figure 1. Stereographic projection of the simulated OR evolution. Δ represents the projection of $(0\text{-}11)_b$ plane, while ◊ shows the projection of $[100]_b$ (purple) and $[111]_b$ (green). + is the projection of values corresponding to the ideal O-line criterion. The darkness of the marker indicates the size of the precipitates, i.e., the darker is the marker, the bigger is the size.

The evolution of the OR is demonstrated in Figure 1. At the early stage, the OR between a small coherent precipitate and the matrix is close to the N-W OR ($[100]_b$ near $[1\text{-}10]_f$). The OR changes towards the K-S OR ($[111]_b$ near $[101]_f$) discontinuously with generation of each dislocation loop during the growth of the precipitate. Simultaneously, the long axis of the precipitate changes from $[101]_f$ towards the invariant line direction that lies on $(\text{-}1\text{-}11)_f$ and the HP changes from $(\text{-}1\text{-}11)_f$ towards the orientation which meets the O-line criterion. This result agrees with the observation by Fujii et al. [2], in that the near N-W OR disappears and the near K-S OR prevails as the precipitates grow. In addition, by extrapolating the results with the same dislocation loops to meet the O-line criterion, we found that the simulated crystallographic features agreed consistently with the measurements by Luo et al. [1]. This HP was proved to be the O-line interface with the lowest energy in a recent calculation [3].

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[3] Dai and Zhang *Modelling Simul. Mater. Sci. Eng.* **21** (2013) 075002.

Creep modeling in Olivine by 2.5D dislocation dynamics simulations

Francesca Boioli[1], Benoit Devincre[2], Philippe Carrez[1], Patrick Cordier[1]

[1] UMET, University of Lille1, Villeneuve d'Ascq, France
[2] LEM, CNRS-ONERA, Chatillon, France

Large scale flow in the Earth's mantle involve plastic deformations of rocks and their constitutive minerals. Due to the extremely slow strain rate conditions in the Earth's mantle, it is very challenging to identify the fundamental mechanisms controlling such process. Thus, the development of a multi-scale approach linking the atomic scale properties and the microscopic elementary mechanisms to the macroscopic behavior is needed [1]. Within this framework, we present a model to investigate the creep of olivine, one of the main constituent of the Earth's mantle, at the mesoscopic scale. In the past years, it has been demonstrated that dislocations play an important role in the creep flow of rocks and minerals. However, the influence of the climb mechanism, which is expected to be dominant in high temperature plasticity, and extent of the glide versus climb process have not yet been clarified. To this aim, we performed 2.5D Dislocation Dynamics (DD) simulations coupling the climb with the glide dislocation motion. Within this approach, dislocations are approximated by straight segments and their dynamics is modeled in a reference plane, as sketched in Fig. 1a,b). Moreover, local rules are implemented to reproduce the relevant three-dimensional dislocation mechanisms, as originally proposed to model fcc metal plasticity [2]. Finally, the transport of matter through vacancy diffusion is taken into account and directly related to the climb dislocation velocity, similarly to Ref. [3]. In this work, we discuss the interplay between thermally activated glide and climb motion and we study the effect of climb on the creep strain rate. As shown in Fig. 1c), at high temperature and low applied stress, climb plays a key role in the creep behavior.

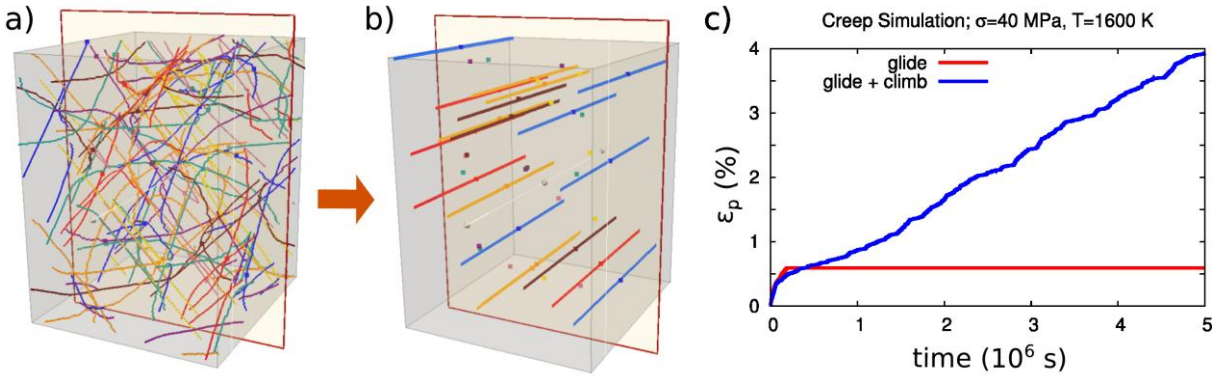

Figure 1: Sketch of full 3D- a) and 2.5D-DD simulation volume. c) Plastic deformation ε_p vs. time, as obtained by 2.5D-DD simulations in creep conditions, assuming glide only (red curve) and glide coupled with climb (blue curve) dislocation motion.

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Deformation and failure of curved nanocrystalline shells

M. Carmen Miguel

Departament de Física Fonamental, Facultat de Física, Universitat de Barcelona Diagonal 645, E-08028 Barcelona, Spain

We study the mechanical response of curved crystalline shells subject to load. These structures, mainly conceived for encapsulation purposes at small scales, show peculiar behavior due to their topological properties, i.e., the minimum energy configuration of any curved crystalline surface contains geometrically necessary topological defects in agreement with its Euler characteristic. The microstructure evolution is therefore influenced by the dynamics of those topological defects on the curved interface and exhibits a rather rich and non-trivial phenomenology. The quasi-static deformation of these structures is characterized by intermittent dynamics with collective particle reorganizations mediated by the proliferation of dislocation pairs and the dynamic delocalization of disclinations in the form of grain boundary scars. At large deformations, depending on bending rigidity, sample size, and geometry, one may observe buckling instabilities and structural failure phenomena such as the cavitation of the crystal shells.