Void Dynamics in Phase Field Modeling

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Void growth in Mo and Cu is studied in the phase-field framework. The void-metal diffuse interface is customarily modeled by a Ginzburg-type gradient energy term with a parameterized coefficient. Following the previously obtained results, the latter is treated as a constant independent of void size. Realistic vacancy supersaturations, as well as the real time and real length scales are used in the simulations. This allows us to make a direct comparison between the results obtained in the phase-field model and those derived from the sharp boundary approach. It is found that the developed phase-field model reproduces reasonably well the dynamical behavior of an individual void, well-known from the rate-theory treatment of void evolution. The ultrafine characteristic spatial scales of the void-metal diffuse interface present a challenge to numerically efficient modeling of the evolution of a void ensemble under irradiation.

Key words: Phase-field modeling, sharp boundary approach, rate theory, void evolution

Vacancy assisted diffusion and clustering of interstitial solutes in α-Fe from first principles

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Under irradiation, a large amount of vacancies (V) are produced. They strongly interact with interstitial solutes (X) such as carbon (C), nitrogen (N) and oxygen (O) atoms, which are always present in steels, either as alloying elements or as impurities. The V-X attraction influences the mobility of both the solutes and the vacancies. On one hand, a decrease of the vacancy mobility has been revealed experimentally in the presence of carbon and nitrogen, most likely due to the trapping of vacancies at small vacancy-solute complexes [1, 2]. On the other hand, however, it is not clear whether vacancies always reduce the mobility of the interstitial elements.

Density Functional Theory (DFT) calculations have been performed to study the energetic and kinetic properties of V_nX_m clusters. Low-energy configurations of small V_nX_m have been determined. It has been revealed that vacancies enhance the clustering of solutes. Moreover, a systematic comparison of C, N and O - neighbors in the Periodic Table – shows different behaviors of the solutes in the neighborhood of vacancies as a function of the electronic band filling. For instance C atoms tend to decorate the surface of V clusters whereas O atoms will preferentially gather inside the V clusters.

The mobility of the V_nX_m clusters has been carefully studied. We especially focused on the V_nX clusters as it has been shown that V_2 and V_3 are even more mobile than a monovacancy in α-Fe [3]. As a result, all the V_3X have been found to be very mobile. In particular, some clusters can be as mobile as the isolated solutes. Therefore, vacancies may be efficient to drag the interstitial solutes towards sinks such as grain boundaries, dislocations and free surfaces. Also, the result found on the mobility of small V_nN clusters may explain the apparent discrepancy between the resistivity recovery experiments and the DFT data [2].

The interpretation of such experiments may be worth revisiting in the light of the present DFT prediction.
The obtained DFT data have been used to parameterize a Cluster Dynamics model, based on the Rate Theory, which allows to predict the time evolution of the clusters concentration. The consequences of small highly mobile clusters on the kinetic properties of vacancies and solutes under various irradiation conditions have been explored using this model.

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Study of hydrogen behavior on beryllium surfaces from the first principles

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Presently beryllium and its alloys are considered as a material for fusion reactor blanket and plasma facing first wall. The interaction of hydrogen and its isotopes with beryllium surfaces leads to a significant change of the surface properties of the material. However, this phenomenon is not yet well investigated in the literature.

Static *ab-initio* calculations of surface energies were performed for five various close-packed beryllium planes: basal, prismatic (types I and II), pyramidal (types I and II). In order to achieve the convergence of the results, different sizes of the simulation cell were used (72–128 atoms). The free surfaces were separated by a 17-23Å thick vacuum region. The volume and the shape of the simulation cell were rigidly fixed during relaxation. No restrictions on the motion of atoms were imposed.

The calculations have shown that the basal plane is the most energetically favorable. The energy of prismatic (type I) and pyramidal (type I) planes are almost equal and they are found to be the second energetically favorable planes in beryllium. The other planes have noticeably higher surface energies. Usually up to 5 outmost atomic layers are involved in surface relaxation. The largest change from the interlayer spacing occurs near the free surfaces (up to 25% with respect to ideal hcp lattice).

A behavior of a single hydrogen atom on the different beryllium surfaces was studied. Hydrogen atom was placed in all nonequivalent positions within each considered plane. Stable positions of the hydrogen were found. Almost in all possible configurations the presence of hydrogen atom leads to a noticeable reduction of the surface energy.

Increase of hydrogen coverage of the beryllium surfaces results in reduction and thereafter to an increase of the surface energy while coverage proceeds. At high coverage the basal plane is not the most energetically favorable anymore. Stable positions of the hydrogen are somewhat different in contrast to the case of a single hydrogen atom. Interplanar relaxation at higher hydrogen coverage was analyzed as well.

Molecular dynamics study on interaction between an edge dislocation and a Frank loop in Fe-10%Ni-20%Cr alloy

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Inhibition of dislocations motion by irradiation-induced defects, such as dislocation loops, is one of the main mechanisms of irradiation hardening of austenitic stainless steels. In this work, Molecular Dynamics (MD) simulations of interaction between an edge dislocation and Frank loops in Fe-10%Ni-20%Cr ternary alloy mimicking austenitic stainless steels are carried out to investigate and model dislocation behavior. An empirical interatomic potential developed recently for a ternary FeNiCr system is used for the MD calculations. The interactions are calculated at different temperatures, loop orientations, loop size and solute atom configurations. The results show that the loop strength and the interaction processes depend on the solute atom configuration, the geometrical configurations between the dislocation and the loop and temperature. It is also demonstrated that a small Frank loop is not so weak obstacle in the alloy. The interaction leads microstructural change such as loop shearing, loop unfaulting and loop absorption in the dislocation. In the former two cases, the loop remains after the interaction, however in some cases absorption of the remaining loop by subsequent interactions with successive dislocations is observed.

Stability of SIA clusters in Fe: the role of substitutional atoms – ab initio study

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The ageing and the evolution of mechanical properties of pressure vessel steels under radiation has been correlated with the formation of more or less dilute solute clusters. Point defect produced under irradiation can form clusters and these clusters interact with solute atoms.
We have used DFT calculations to investigate the impact of substitutional atoms representative of the alloying elements of pressure vessel steels (e.g. Cu, Ni, Mn, Si, P, Cr) on the stability of Self Interstitial Atom (SIA) clusters. All the solute atoms studied were found to interact with isolated SIAs as well as SIA clusters. Different small SIA clusters can be formed with non parallel ⟨110⟩ SIAs which are found to be the most stable configurations, compared to small ⟨111⟩ loops. The solute interactions with small SIA clusters (consisting of several non parallel ⟨110⟩ SIAs) is most often at least 0.4 eV. The most attractive configuration depends on the solute size, chemistry and magnetism. The same trends were found for C15 Lave phase based SIA clusters and small ⟨111⟩ loops. In that later case, the most attractive sites are found at the periphery of the loop. These fine scale calculations are important to assess the validity of coarse grained approaches (Kinetic Monte Carlo or Molecular Dynamics) which rely on more empirical cohesive models.

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Nucleation of point defect clusters in displacement cascades near edge and screw dislocations in fcc metals subjected to fast particle irradiation

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Along with grain boundaries, free surfaces, secondary phase interfaces and other structural defects, dislocation network constitutes an essential part of the microstructure of advanced structural materials for demanding engineering applications. Being a key factor that determines the yield strength, fracture toughness, plasticity, creep and fatigue resistance and other materials' service properties, dislocations can also contribute to elemental partitioning, facilitate segregation of impurities and alloying elements or change the balance of residual point defects in materials exposed to fast particle irradiation. Existing phenomenological models implement thermodynamic or kinetic approaches to describe the interaction of dislocations with radiation defects. In the undertaken study we have considered athermal coupling of collision cascades with screw and edge dislocations in aluminium and nickel at the timescale of the order of cascade lifetime.

The velocity-Verlet molecular dynamics simulations have been applied to study the radiation damage created in collision cascades in aluminium and nickel crystals harbouring an isolated screw or edge dislocation with 1/2[110] Burgers vector and in the two defect-free metals for comparison. The total of more than 2000 displacement cascades formed by the recoil of primary knock-on atoms (PKA) with energy, E_{PKA}, ranging from 5 to 20 keV in crystals at temperatures $100K < T < 600K$ (aluminium) or $100K < T < 1200K$ (nickel) were simulated to get statistical reliability of the results.

We evaluated the number of residual vacancies and self-interstitial atoms created in displacement cascades as a function of (E_{PKA}, T) and compared the obtained data with the number of Frenkel pairs formed in collision cascades in the pristine materials under the same conditions. The conditions that control dislocation climb by absorbing point defects from the displacement cascade region were revealed and a few visualisations were prepared in order to illustrate point defect redistribution in the two considered materials. Special attention was paid to studying governing factors that determine formation of point defect clusters in collision cascades near edge and screw dislocations in aluminium and nickel exposed to fast particle irradiation. Preliminary results of the undertaken research were published in [1, 2].

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Mesoscale simulation of phonon mediated thermal transport in UO_2: Perturbation theory based Monte Carlo solution of Boltzmann Transport Equation

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Safety of nuclear reactors depends on the reliability of materials under harsh radioactive conditions inside the core of the reactor. The worst part originates from radiation induced damaging effects that lead to microstructural and compositional changes and ultimately can cause material failure. To design materials with enhanced radiation resistant properties, the behavior of materials under irradiation need to be well understood and reliable predictive theoretical models need to be established along with experimental verification techniques. As it is the most widely used nuclear fuel, the advancement of the nuclear technology passes necessarily through a complete understanding of uranium dioxide's properties on every aspect. The revival of vigorous research in the nuclear energy field had instigated a wide interest in UO_2 in an attempt to study its mechanical, thermal and electronic properties, among others. Fuel thermal conductivity controls the fuel operating temperature, and hence affecting nuclear fuel performance and many important processes. There are several factors that can contribute to the change of thermal conductivity under irradiation, most significantly are the change of oxygen-to-metal ratio and defects concentrations. Studying phonon transport represents an adequate paradigm to understand heat transfer phenomena in crystalline semiconductor and insulator materials at the nanoscale level. Unlike phenomenological heat diffusion models, which can not be applied at this length scale, phonon transport theory can capture the microstructure and nanostructure effects on the thermal conductivity. Boltzmann Transport Equation (BTE) provides the capability of tracking phonon evolution in phase space, however solving BTE exactly is not possible in most of the realistic cases. We present a Monte Carlo solution of BTE for phonons in uranium dioxide with various levels of defects. BTE is linearized by introducing the Relaxation Time Approximation (RTA). Individual phonon relaxation times, timescale measure of the scattering strength of each phonon interaction processes (causing transition between phonon states), are calculated by Fermi's Golden Rule under time dependent perturbation theory approximation. Total relaxation time, for each phonon, is calculated by adding individual phonon relaxation times (by all possible mechanisms) together using Matthiessen's rule. The simulation scheme accounts for all acoustic and optical branches of the dispersion relationships and considers the 3D representation of the actual shape of the UO_2 Brillouin zone (truncated octahedron). Experimental dispersion data of UO_2 in high symmetry directions were employed to model phonon anisotropic dispersions. Unlike most other works on solving this equation by Monte Carlo method, the momentum and energy conservation laws for phonon-phonon interactions in uranium dioxide are treated exactly by considering only the interactions that obey the pertinent conservation laws. Using periodic boundary conditions, our results illustrate the diffusion limit of phonon transport in uranium dioxide, and make possible the prediction of thermal conductivity. A simple kinetic theory model is also implemented in which conductivity is calculated using phonon heat capacity, velocities, and scattering time-scales. The effect of temperature and defect concentration on conductivity is predicted with both models and the results are compared with experimental data available in the literature.

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Examination of multiscale concept for swelling description of metals and alloys

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The multiscale concept for material under irradiation has the long history and started from the description of point defects and small clusters by the atomistic simulations and finished at macroscopic description for a long time of irradiation. For the moment there are a lot of atomistic simulations of materials behavior under irradiation in literature, a lot of theoretical models of defects evolution (growth, nucleation). The time and spatial bridges between atomistic simulation and rate theory are covered by kinetic Monte-Carlo (KMC) and cluster dynamics (CD). So it seems that the multiscale concept is filled to methods and materials parameters. The main goal of our work is to examine the today's possibility of quantitative description by the multiscale concept of materials under irradiation. The examination is carried out in order to emphasize present-day problems: large uncertainties in constants, unreasonable physical models, insufficient computational methods, codes and resources.

The multiscale concept consists of atomistic simulations, KMC, CD based on KMC solver and rate theory. Two different tests are considered: irradiation of thin foils by ion beams [1,2,3], irradiation of bulk sample by neutron beam in reactor. The conditions of irradiation in these two experiments differ from each other by dose rate (about three orders of magnitude), production bias (average PKA energy under neutron beam is smaller than ion beam energy), sink strength (the influence of the surface for thin foil experiments is very sufficient). We consider pure Fe and Mo, FeCr alloy, and alloys based on Mo and FeCr. These metals are better investigated than others and have the real application today. At low doses we compare the calculated dislocation loop or cluster concentrations and radius distribution with experimental results. At high doses the swelling rate is compared. Based on the comparison the conclusions of sufficiency of material constants and models are made.

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Assessment of the influence of elastic anisotropies on dislocation loops sink strength: a phase-field approach

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Long term prediction of irradiated materials ageing relies on proper comprehension of microstructural defect behaviour. Evolution of those irradiation defects (dislocation loops, voids) is responsible for dimensional instabilities and embrittlement of metals. Particle irradiation of a metallic crystal leads to the production of vast amounts of point defects (PDs) – vacancies and self-interstitial atoms (SIAs) – which diffuse in the material and are absorbed by various sinks, such as dislocations, grain boundaries, voids, surfaces, etc. The sink efficiencies depend on the migrating mechanism, the sink geometry (cylinder, spherical, toroidal) and the intensity of the long range elastic interactions between defects and the sink. These quantities are crucial parameters in long time scale rate-theory predictions.

Most of analytical models rely on simplifying assumptions to calculate those sink efficiency: (i) the sink is generally isolated in a defect-free region with arbitrary geometry, (ii) a concentration is fixed on the outer boundary of the sink-free region instead of uniformly produced PDs, (iii) the point defects are considered as pure dilatation centres in an isotropic crystal when elasticity is accounted for.

As a consequence, more accurate models must be developed to rigorously calculate sink efficiencies in complex microstructures. For this purpose, a 3D phase-field (PF) model is proposed to include the anisotropic microelasticity theory coupled to the diffusion of PDs in any dislocation network.

Numerical results on benchmark cases have been compared with analytical solutions, when available. This preliminary step allowed to validate the method. Nevertheless, calculations show that for dislocation loops, capture efficiencies have been significantly underestimated by existing models, even in the simplest cases.

As an application, we computed the anisotropic properties of PDs in zirconium by atomic scale *ab initio* method, and used them as input data in the PF model, to calculate the sink efficiencies of dislocation loops with different Burgers vectors and habit planes. Results show a preferential absorption of SIAs by prismatic loops due to the strong deformation of SIAs in the basal plane. This effect tends to promote the growth of experimentally observed basal vacancy loops.

Towards a quantitative modeling of radiation induced segregation in alloys

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Recent developments of the Self-Consistent Mean Field (SCMF) kinetic theory provide the exact phenomenological coefficients Lij of dilute alloys, starting from vacancy and split interstitial jump frequencies calculated ab initio [1]. Binding energies between solute atom and point defect at distances beyond the first nearest neighbor site distance are considered. The effect of a strain field on the migration energies and the resulting transport coefficients Lij can be considered as well [2]. Kinetic correlations are accounted for through a set of time-dependent effective interactions within a non-equilibrium distribution function. In the case of strong binding energies between vacancy and solute atom, the kinetic correlations may lead to a solute drag by the vacancies from the bulk towards grain-boundaries. Starting from a Master Equation written at the atomic scale, generalized diffusion equations for alloys under irradiation are derived. They are applied to the modeling of radiation-induced segregation at grain boundaries in dilute Fe-based model alloys and radiation-enhanced spinodal decomposition in Fe-Cr alloys.

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Point defect modeling in materials : coupling *ab initio* and elasticity approaches

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Point defects in crystalline solids play a crucial role in controlling material properties and their kinetic evolution. This is true for both intrinsic defects such as vacancies, self-interstitials, and their small clusters, and extrinsic defects such as impurities and dopants. As a consequence, a proper understanding and modeling of material properties require a precise knowledge of point defect characteristics, in particular their formation and migration energies. To this end, *ab initio* calculations based on density functional theory and performed with periodic boundary conditions have become a valuable tool. But they are technically limited to a few hundred atoms, so the long-range elastic fields of the defect induce a spurious interaction energy with the periodic images. Convergence of point defect properties can therefore be out of reach, especially for clusters.

Here, we propose to couple *ab initio* calculations and linear elasticity to get rid of this limitation [1]. We use elasticity theory to model the interaction of the defect with its periodic images so as to withdraw it from the *ab initio* results. Properties of the isolated defect are then accessible with reduced supercell size. The reliability and benefit of our approach are demonstrated for three problematic cases: the self-interstitial in hcp zirconium, clusters of self-interstitials in bcc iron and and the neutral vacancy in diamond silicon. In all cases, our coupled approach allows a more accurate description of point defects than what could be achieved with a simple *ab initio* calculation. The extension of our corrective scheme to the case of charged point defects will be discussed.

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Multiscale modeling of dislocation-precipitate interactions: implementing precipitate pinning in Discrete Dislocation Dynamics

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Plasticity in crystalline materials is due to motion of crystal defects known as dislocations. Dislocations create an anisotropic stress field around themselves which can be quite complex giving rise to rich variety of possible interactions. Discrete Dislocation Dynamics (DDD) is method where the dislocation segments are modeled as straight lines connected by discretization points. The stress field is obtained from linear elasticity theory. The reactions related to the dislocation core, such as junction formation and pinning to defects, are beyond the reach of linear elasticity theory and thus require input from more microscopic approaches.

When dislocation encounters an impenetrable precipitate it will become pinned. If the external stress is high enough the dislocation moves past the precipitate and leaves a loop around it. This is called the Orowan process and the loop Orowan loop [1]. New dislocations need more stress to move past the obstacle because they must overcome the old loop in addition to the precipitate. This leads to work hardening of the metal which is important phenomena to understand in the context of building structural parts for nuclear reactors.

Here we combine atomistic simulations to DDD in order to model carbide precipitates interactions with dislocations in BCC-iron. We implement spherical precipitates into ParaDis [2] simulation code by adding a normal force to the segments which come into contact with it. This results in the formation of the aforementioned Orowan loops. The shearing strength of the precipitate is obtained from a molecular dynamics simulations.

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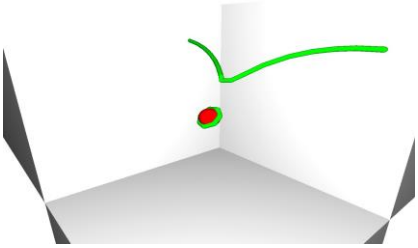

Figure 1: A mixed dislocation has unpinned and left an Orowan loop around a carbide precipitate

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Multiscale modeling of helium-induced nano-fuzz formation on tungsten surfaces

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Although tungsten is a promising candidate for the surface material of the divertor in a Tokamak type fusion reactor, fuzz-like structure growth on the tungsten surface is reported at high temperature under low-energy (60 eV) He ion irradiation. The detailed mechanism of this surface reaction is still not well understood on an atomistic level. Molecular dynamics (MD) simulation has revealed several basic atomistic events, such as migration of interstitial He and bubble formation resulting in W interstitial creation. However, due to the restriction of the time scale, surface topography changes simulated by MD alone are quantitatively far from the experimental conditions (Fig. 1, left).

In order to take into account the effects from events much rarer than those at ns intervals, we have developed a direct combination model of MD and lattice kinetic Monte Carlo simulations, in which the two techniques alternate continuously (Fig. 1, right). For the atomic interactions the Juslin-Wirth EAM potential was used, supplemented by the ZBL potential for small distances. The He concentration, stress from He bubbles, and mobility of W surface adatoms are evaluated, and the surface structure evolution is found to agree closely with the experimentally observed evolution speed under the same condition. The details of atomistic events and the novel multi-timescale simulation model are discussed.

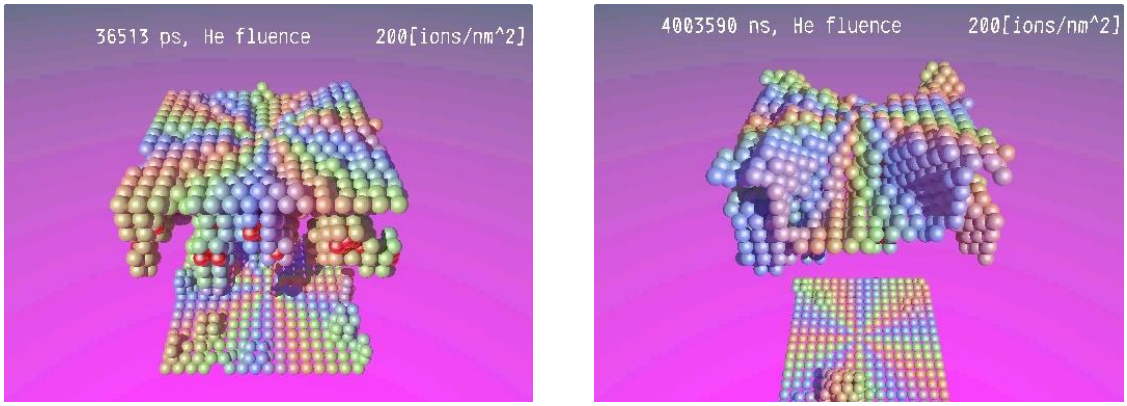

Figure 1: Geometry of a W (100) surface after bombardment by 60 eV He ions with a fluence of 200 ions/nm^2. Left: MD simulation. Right: Alternating MD and lattice kinetic MC simulation. Note the difference in time allowed by these two simulation methods for the evolution of the surface topography and the resulting difference of roughness ('fuzz').

Only W atoms with fewer than 8 neighbors are shown. Bright red atoms are He. Pale colors are used only to differentiate between sectors in the horizontal planes.

Molecular dynamical investigation of the interaction of edge dislocations with carbides in BCC Fe; Parametrization for DDD-simulations

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Steels are not only a homogeneous alloy of Fe and alloying elements but they also, in almost all cases of practical interest, have a complex micro- and nanostructure of grains, different phases, dislocations and inclusions. One of the most common classes of phases is carbide precipitates. These have a strong effect on the mechanical properties of steels. Since the mechanical properties of metals are dominated by dislocations, it is hence important to understand the interactions of dislocations with carbide precipitates. In particular, the effect of carbides is important for structural parts in nuclear reactors, where controllable elongation is crucial.

In this work, we use molecular dynamical simulations to investigate the interaction between edge dislocations and carbide precipitates. This nanoscale phenomenon, simulated by molecular dynamics, can be parametrized to be able to simulate similar properties on a larger scale with discrete dislocation dynamic, DDD, simulations.

A simulation technique proposed by Osetsky and Bacon[1] was utilized on a simulation cell of BCC Fe. In earlier studies either impenetrable infinitely hard obstacles, like fixed atoms, or penetrable obstacles, like voids or loops, were considered. In this study impenetrable obstacles with a finite strength, which is more close to real systems, were investigated. The obstacles were of M_3C-, cementite, and $M_{23}C_6$-type. The effect of size
and temperature on the unpinning stress was studied. Identification of different unpinning mechanisms like Orowan loop formation and climb was done. This knowledge is important for the understanding of how realistic impenetrable obstacles interact with edge dislocations.

How the critical stress depends on the temperature and on the size of the precipitate can be parametrized to calibrate the strength of obstacles in DDD simulations. In this modeling method we can get the atomically correct interaction from molecular dynamics to be used in a simulation method, capable of simulating millisecond and micrometer scales.

This research was funded by the Academy of Finland project SIRDAME (grant no. 259886). We thank the IT Center for Science, CSC, for granted computational resources.

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Mesoscopic Investigation of Homogeneous to Heterogeneous Deformation Transitions in Irradiated BCC Crystals

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Low temperature irradiation of crystalline materials is known to result in strengthening and loss of ductility, which limits the usefulness of candidate materials in harsh nuclear environments. In bcc metals, this mechanical property degradation is caused by the interaction of in-grown dislocations with irradiation defects, particularly small prismatic dislocation loops resulting from the microstructural evolution of displacement cascades. In this work, we present a multi-length scale investigation including dislocation dynamics (DD) simulations, and finite element simulations using a novel set of continuum constitutive equations for the response of irradiated bcc single crystals based on the dislocation dynamics simulation results. Simulations of the response of the material with varying concentrations of prismatic loops are conducted to investigate changes in the mesoscopic and macroscopic flow behavior. The study is motivated by experimental observations of plastic flow localization and softening in a variety of structural materials for nuclear applications. At the mesoscopic scale, the simulations reveal a transition from homogenous to highly localized deformation as the prismatic loop density increases. In the heterogeneous deformation regime defect-depleted channels are created as a principal signature of softening. The mechanism of defect depletion observed in the simulations is the translation and clustering of loops defects into larger structures that no longer act as effective obstacles to glissile dislocation motion. The results of the dislocations dynamics simulations are used to construct and augment a single crystal plasticity constitutive law with a tensorial irradiation damage state variable and evolution equations capable of reproducing the flow behavior observed in the dislocation dynamics simulation and of reaching strains in excess of 10% for linkage with the engineering scale. The calibrated crystal plasticity model is used as the constitutive relation in FE simulations of polycrystalline irradiated Fe systems, and the results compared to experiments for different levels of irradiation damage.

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