

Stress and irradiation effects on solute diffusion to dislocations

Dallas R. Trinkle¹, Zebo Li¹, Thomas Garnier¹, Venkateswara Manga², Maylise Nastar³,
Pascal Bellon¹, Robert Averback¹

¹ Materials Science and Engineering, University of Illinois, Urbana-Champaign; Urbana,
IL

² Materials Science and Engineering, University of Arizona; Tuscon, AZ

³ CEA, DEN, Service de Recherches de Métallurgie Physique, 91 191, Gif-sur-Yvette,
France

Study of creep under irradiation requires a quantitative description of diffusion of point defects such as vacancies, interstitials, and solutes to traps like dislocations. Prediction of dislocation creep rates involves consideration of diffusion under non-uniform, non-hydrostatic stress, the increased point defect density from irradiation, and the interaction of defects. We present calculations of the diffusion of Si in Ni, which has both vacancy- and mixed-dumbbell mediated diffusion under stress at dilute concentrations. First-principles calculations and self-consistent mean field method (SCMF) calculate the fluxes of various species under stress. Stress reduces the symmetry for hops in FCC Ni, and SCMF provides a direct calculation of phenomenological coefficients—including off-diagonal terms—for the lower-symmetry geometry. In particular, stress changes solute drag in particular directions, which affects the diffusion to sinks under irradiation and the resulting microstructure near dislocations. The final results are combined with the dislocation strain field to model these effects.

Inverse Relation between Strain Rate and Yield Strength of Dislocation-Obstacle Interaction in bcc Fe

Yue Fan¹, Akihiro Kushima¹, Sidney Yip^{1,2}, Bilge Yildiz¹

¹Department of Nuclear Science and Engineering, MIT, Cambridge, Massachusetts
02139

²Department of Materials Science and Engineering, MIT, Cambridge, Massachusetts
02139

Irradiation creep is an important long-term macroscopic degradation phenomenon in nuclear structural materials that involves dislocation interactions with irradiation induced obstacles. The yield strength of dislocation-obstacle interactions exhibit complex relations, for example an inverse relation to strain rate, that is decreasing of critical resolved shear stress while increasing strain rate. To quantitatively assess the dislocation-vacancy cluster interaction in bcc Fe at the time scale beyond conventional atomistic simulations, we combined a novel atomistic approach, the Autonomous Basin Climbing (ABC) method, with transition state theory. The directly simulated strain rates at the atomic level span a wide range from 10^8 s^{-1} down to 10^3 s^{-1} , the lower end of which is far beyond reach to traditional molecular dynamics (MD).

We examine the relation between the critical resolved shear stress (CRSS) and the strain rate, and demonstrate the origin of the inverse behavior between CRSS and strain rate below 10^5 s^{-1} . This behavior arises because of the competition of two driving forces: strain rate and thermal activation. At low strain rate, the obstacle has enough time to nucleate to a stable structure and thus has strong interaction with the dislocation. At high strain rate, however, the vacancy cluster is split into parts because of less time available for nucleation. The split vacancy cluster has larger surface area attached to the dislocation and yields a higher CRSS as well. Therefore the interaction leads to a “V” shape relation between the CRSS and strain rate (that is, decreasing at low strain rate and increasing at high strain rate) with the minimum at 10^5 s^{-1} . The interactions at high strain rates are directly benchmarked against MD simulations, and the results are well consistent with each other. This work shows that even a unit process can induce an inverse behavior, which complements the previous macroscopic models.

Interactions between mobile dislocations and radiation induced loops: a multiscale approach

L. Dupuy¹, X. Shi¹, L. Vincent¹, B. Devincere², D. Terentyev³, A. Etcheverry⁴, P. Blanchard⁴, O. Coulaud⁴, E. Ferrie⁵, M. Bletry⁶

¹SRMA, CEA-Saclay, 91191, Gif-sur-Yvette, France,

²Laboratoire d'Etude des Microstructures, CNRS-ONERA, 92322 Châtillon, France

³SCK-CEN, Nuclear Materials Science Institute, B-2400 Mol, Belgium

⁴HiePACS team, Inria Bordeaux Sud-Ouest

⁵Laboratoire SIMAP, CRNS-Grenoble-INP, 38402 St Martin d'Hères, France

⁶Institut de Chimie et des Matériaux Paris-Est, 94320 Thiais, France

The mechanical behavior of reactor pressure vessels steels and internals is affected by neutron irradiation, which induces the presence of defects such as Frenkel pairs, voids or loops. In this study, particular focus is given to interstitial loops. The modelling of this phenomenon requires a multi-scale approach going from the study of individual dislocation-loop interactions at atomic scale to the study of the collective behavior of dislocations at grain scale using dislocation dynamics simulations.

The interactions mechanisms between individual loops and gliding dislocations have been thoroughly studied at atomic scale using molecular dynamics within the Perform 60 project. Building on these results we show how it is possible to introduce these elementary mechanisms in our dislocation dynamics code Numodis [1], and to reproduce both qualitatively and quantitatively most of these hardening mechanisms. Various configurations are considered in both ferritic and stainless steels, with different dislocation characters (screw/edge) and different types of loops.

The good agreement between these two scales proves the validity of this multiscale approach, and opens the door to large scale simulations that are required to feed crystal plasticity models. Such simulations are currently made possible through the development of a new parallel code OptiDis based on a hybrid OpenMP/MPI paradigm. The performance of OptiDis will be demonstrated on a system containing a high density of radiation-induced loops involving about a million of interacting segments.

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[1] Numodis: <http://www.numodis.fr/>

Modeling of Tensile Deformation in Irradiated RPV steel

Pritam Chakraborty, S. Bulent Biner

Idaho National Laboratory, Idaho Falls, Idaho 83401, USA

The fracture behavior of Reactor Pressure Vessel (RPV) steels shows a strong dependence to temperature and irradiation. A transition from ductile (higher fracture toughness) to cleavage mode of fracture (lower fracture toughness) is observed with decreasing temperature. Also, due to the inherent statistical nature of cleavage fracture, large scatter in fracture toughness values is common in the ductile to brittle fracture transition (DBT) regime. Irradiation introduces additional lattice defects and precipitation/segregation of alloying elements, thus reducing the ductility of the material, and increasing the DBT temperature. To capture such variable fracture behavior of RPV steels, a combination of ductile damage and statistically based weakest link models has been successfully used in the past. Though these models provided satisfactory comparison of fracture properties with experiments, their accuracy strongly depends on the temperature and irradiation dependent flow stress (true stress-plastic strain) behavior obtained from tensile experiments. Under low dose irradiation or unirradiated conditions, significant strain hardening prior to onset of necking can be observed in the stress-strain behavior of tensile specimens. Hence the strain hardening behavior in the flow stress evolution can be clearly separated from damage initiation and growth. However with increasing irradiation level, a significant decrease in uniform elongation in conjunction with increase of yield stress are usually observed. The dislocation channeling has been considered to explain the strain softening behavior. Inverse methods using finite element (FE) simulations has been used to obtain the flow stress behavior under such situation [1]. However, ductile damage, which also contributes to strain localization and softening, has been neglected. In the present work, an attempt has been made using the GTN model [2] for ductile damage and, power law hardening and exponential softening for flow stress evolution, to identify their respective contribution on the engineering stress-strain behavior. Both stress and strain based void nucleation criterion are considered in the GTN model to investigate the effect of damage initiation on uniform and total elongation. Correlations between GTN and flow stress model parameters, and irradiation dose and temperature are also developed by simulating engineering stress-strain curves from the tensile tests. These model parameters will be used in a subsequent study to predict DBT in RPV steels under irradiated condition.

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Multiscale simulation of strengthening induced by small dislocation loops

Ghiath Monnet

EDF, MMC

It is widely known that irradiation induces point defect clusters which grow to form Dislocation Loops (DLs) of different natures and sizes in addition to other defects as voids, stacking fault tetrahedrons, precipitates, etc. The evolution of the microstructure under irradiation is accompanied by a significant strengthening and a loss in ductility. The origin of these effects is still under debate and no physically-based quantitative theory is known to explain the basic features of radiation strengthening.

In this work we present a multiscale approach of strengthening induced by dislocation loops. Molecular Dynamics (MD) simulations have shown that dislocation interactions with DLs depend on the temperature, the loop nature and size and the dislocation character. In many cases, MD results revealed that small DLs of sizes less than 4 nm are often absorbed by the moving dislocation, forming super-jogs on edge dislocations and helical turns on screw dislocations. This feature has been implemented in Dislocation Dynamics (DD) simulations in order to compute the strengthening induced by the small DLs. In these simulations, we investigate the effect of the: loop size, dislocation character, friction stress and strain rate. In all simulation conditions, results show a large strengthening, substantially larger than the strengthening induced by impenetrable obstacles of equivalent size and density. Small dislocation loops are dragged by the moving dislocation creating a strong heterogeneity in the DL density and distribution.

Simulation for dislocation core structure of solute atom clusters using generalized stacking fault energy

- Dislocation core structure and shear modulus of ternary iron alloy of FeCuMn, FeSiMn, and FeNiMn -

Toshiharu Ohnuma, Kenichi Nakashima

Central Research Institute of Electric Power Industry
2-11-1, Iweado Kita, Komae-shi, Tokyo, 201-8511 Japan

Solute atom clusters enriched with Cu, Ni, Mn, and Si are formed in the reactor pressure vessel (RPV) steels of light water reactors irradiated by fast neutrons. The clusters become obstacles impeding the movement of dislocations, resulting in the embrittlement of RPV steels. Therefore, understanding the mechanism through which clusters of solute atoms interact with dislocations is important in order to correlate the changes in the microstructures of RPV steels with the mechanical property changes of RPV steels. Generalized stacking fault energy, which represents the total change in energy when a crystal that is partly in the slip plane rigidly shifts, is a key parameter used to determine the structure and mobility of dislocations that run through a given metal crystal. We calculated from first principles the generalized stacking fault energies and shear modulus for the FeCuMn, FeSiMn, and FeNiMn ternary-iron-alloy crystals and used the fractional dislocation model to calculate the dislocation core structures in the crystals.

Defect-induced plasticity in CuNb nanocomposites

Enrique Martínez¹, Alfredo Caro¹, Irene J. Beyerlein²

¹Material Science and Technology Division, MST-8, Los Alamos National Laboratory,
Los Alamos, 87545 NM, USA

²Theoretical Division, T-3, Los Alamos National Laboratory, Los Alamos, 87545 NM,
USA

Nanolaminate composites have been proven stable under light ion irradiation. In this paper we analyze the change in mechanical properties of model CuNb nanocomposites in vacancy supersaturated environments. We have performed compression tests using molecular dynamics for different defect contents. We have added different number of vacancies into the misfit dislocation intersections (where their formation energy is lower), and calculated the yield stress. We observe that for a small number of defects, the yield point hardly varies, while when the number of vacancies is large, the yield point substantially decreases, nucleating twins instead of partial dislocations. We have also tested the effect of heavy ion irradiation including different distributions of stacking fault tetrahedra (SFTs) in the Cu layer and voids in the Nb side. We see that dislocations nucleate at the SFTs at about 1/3 of the stress needed to nucleate dislocations at the interface in the pristine sample. In the Nb layer, vacancy loops nucleate at voids, and glide to be absorbed at the interface modifying considerably the nucleation stress compared to the pristine sample. We have analyzed in detail the dislocation-interface interaction mechanisms under different conditions, showing how dislocations react with the misfit dislocations present at the interface to modify the atomic structure of the boundary, which suggests that the interface could be designed to optimize its defect healing properties. We conclude that interfaces help in recovering materials subjected to heavy-ion irradiation.

Modelling of the effect of slip localization on grain boundary fracture in pre-irradiated austenitic stainless steels. Comparison with experimental data

Maxime Sauzay¹, Mohamed Ould Moussa¹, Boubakar Diawara², François Lebreau²

¹ CEA, SRMA, Bât. 455, 91191 Gif sur Yvette, France;

² Ecole Chimie Paris, 75005 Paris, France

Slip localization is a common feature in post-irradiated metallic poly-crystals undergoing tensile straining. This effect takes place for instance in the form of thin slip bands called channels or clear bands, formed after the local vanishing of irradiation defects induced interactions with gliding dislocations. Channel impingement towards grain boundaries (GBs) should induce local stress concentrations along GBs, in the quasi-elastic surrounding matrix. It has been shown extensively that this trigger GB crack initiation [1].

Since the fifties, the clear band stress fields have been modeled using the dislocation pile-up theory, which leads to stress singularities similar to the LEFM ones [2]. But such theory does not allow fair predictions of GB fracture, neither in inert or PWR environment [3]. In practice, channel thickness is at least 50 nm depending on material, temperature and loading conditions. As a matter of fact, many slip planes are plastically activated through the channel thickness. Numerous crystalline finite element (FE) computations have been carried out using microstructure inputs varying in broad ranges (slip band aspect ratio and spacing). Slip bands (low critical resolved shear stress) are embedded in a matrix or small aggregates (high CRSS). Microstructure inputs as well as plasticity parameters are evaluated based on TEM observations and dislocation dynamics computation results. High local stress fields are highlighted but they are nevertheless considerably lower than the ones deduced from the pile-up theory. Analytical formulae are deduced from the numerous FE results, accounting for channel thickness, grain size, channel density and crystal / GB orientations [6,7].

Grain boundary fracture is simulated using a double criterion based on both critical normal stress and fracture energy as deduced from atomistic computations of GB fracture [4]. The critical stress is deduced from the fracture energy using the universal-binding-energy relationship (UBER). In the case of brittle fracture, the fracture energy is defined as the two fresh free surface energy values minus the GB energy. A close-from expression giving the remote tensile stress to GB fracture is then deduced [6,7].

Finally, GB fracture of pre-irradiated SS (dose > 10 dpa) loaded in either inert or pressurized water reactor (PWR) environment is predicted for comparison with the existing experimental results obtained in similar conditions.

In the case of inert environment, free surface and GB energy values are easily found in literature. The predicted remote tensile stress to GB fracture is then equal to the yield stress in agreement with various experimental data.

In the case of PWR environment, GBs are assumed to be oxidized up to a depth of a few μm due to Cr depletion induced by the strong RIS observed at high irradiation dose [1]. Either literature data have been used (iron oxides [5]) or they have been computed by the DFT method for various GBs and by accounting for hydration / hydroxylation of the fresh free surfaces in PWR water (Cr_2O_3 oxide). Using the lowest fracture energies corresponding to the weakest GBs, the predicted remote tensile stress to oxidized GB fracture is about one-half of the yield stress, once more in fair agreement with many experimental data despite no parameter fitting is required. The influence of irradiation dose, strain rate and irradiation creep is finally quantitatively discussed.

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Multiscale cleavage fracture initiation model accounting for material microstructure and effects of irradiation

Anssi Laukkanen, Tom Andersson, Tapio Planman, Kim Wallin

VTT Materials and Manufacturing, Espoo 02044-VTT, Finland

Fracture initiation models typically contain limited information regarding material behavior at the mesoscale, especially with respect to polycrystalline microstructures. As a result, the methodologies and criteria can be quite phenomenological as far as their description of the micromechanical chain of events is concerned. This limits their use as far as being able to yield any exploitable predictive ability. One proposed solution has been the direct inclusion of microstructural deformation and anisotropic plasticity mechanisms on an aggregate scale in derivation of improved next generation cleavage initiation models, and as such, creating a multiscale cleavage fracture initiation model. This route is adopted also in current work to enrich the treatment of cleavage fracture and better incorporate the effects of irradiation in the fracture toughness predictions.

To that effect, crystal plasticity analyses founded on a dislocation dynamics based constitutive model are carried out for “Eurocurve Material A”. The crystal plasticity model is applied to a lath containing aggregate mesh over three differing states of imposed constraint in order to derive triaxial stress states ranging from those of uniaxial tensile tests to those indicative of near crack-tip plane strain conditions. The aggregate in question is founded on the microstructural morphology present in lower bainitic pressure vessel steels. Effects of irradiation are directly introduced to the crystal plasticity constitutive model via a defect density parameter, and as such influence the anisotropic deformation behavior of the material.

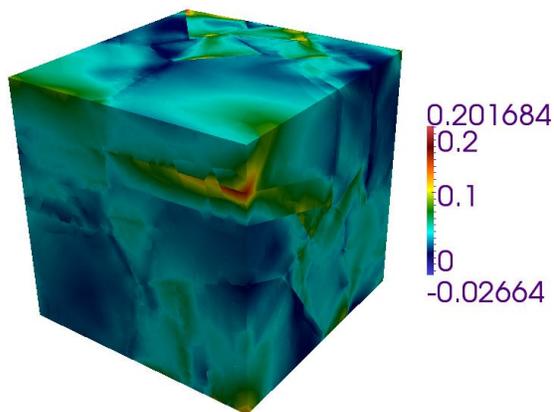


Figure 1: Contours of axial strain in a polycrystalline crystal plasticity aggregate of reactor pressure vessel steel.

The findings demonstrate the effects of temperature and crack-tip constraint on the distribution of stress and strain fields within the polycrystal aggregate, and are utilized further in the hierarchical multiscale modeling chain in development of a cleavage fracture model, a revised implementation of the micromechanically informed WST cleavage initiation model. The hierarchically upscaled crystal plasticity and cleavage fracture model is demonstrated to yield improved fracture toughness predictions within the ductile to brittle transition region.