Transactions, SMiRT-22
San Francisco, California, USA - August 18-23, 2013
Division I

DISLOCATION DYNAMICS STUDIES ON REACTOR STRUCTURAL MATERIAL DAMAGE DUE TO IRRADIATION

P.V. Durgaprasad and B.K. Dutta

Reactor Safety Division, Bhabha Atomic Research Centre, Mumbai, India (pvdp@barc.gov.in)

ABSTRACT

Understanding of material degradation due to irradiation in structural materials of future reactors is of prime importance for current research as these materials are expected to operate at severe conditions – high temperature and high irradiation doses. Experimental studies in obtaining mechanical behavior of such irradiated materials takes increasingly long time because of limited availability of test conditions. These studies are assisted by the theoretical studies involving multi-scale material models which help us in understand basic mechanisms of material damage and the related radiation embrittlement and hardening. In the present work, a dislocation dynamics (DD) study of irradiation hardening in ferritic/martensitic steels is studied.

INTRODUCTION

The future reactor structural materials are expected to operate at severe operating conditions such as high temperature and high radiation doses, for e.g., the ferritic/martensitic (FM) steels in fusion reactor structural applications. Understanding the changes in properties of such materials has been a great challenge for many years. This is due to the fact that the microstructure of irradiated materials evolves over a wide range of length and time scales, making radiation damage an inherently multi-scale phenomenon. Due to the cascading effects, small nano sized defects like voids, bubbles and prismatic loops are formed which completely govern the microstructure of irradiated materials. Under the external loads, the existing network of dislocations interacts with the irradiation defects causing the increase in observed flow behavior. Experimental investigation of these features in irradiated materials pose challenges in terms of cost, cooling time, number of samples and size (volume) of samples that can be tested. Understanding mechanical behavior of such materials through experimental investigation can well be supplemented by rapidly evolving multi scale material modeling methodologies.

With rapid development of computational capabilities, it is becoming increasingly possible to look inside materials and understand plastic behavior of materials at various length scales. Some authors used this approach to determine the mechanical properties of materials under irradiated and un-irradiated conditions [Naveen Kumar et.al (2012) and references therein]. For example, Diaz de la Rubia et al (2000) used MD and DD simu-lations to explain the plastic flow localization in irradiated Cu. Queyreau (2008) used DD simulations to predict the irradiation hardening in reactor pressure vessel steel, where a scale transition law is used to link nano and meso-scales. Wirth et al (2001) successfully coupled the spatial distribution of defects to three dimensional DD simulations to investigate the corresponding mechanical behavior of irradiated Cu and Pd. Groh et.al (2009) showed the complete multi-scale approach to determine the stress strain curve for single crystal aluminum under un-irradiated condition explaining the successful linking of nano-scale to meso-scale and meso-scale to micro-scale. Naveen Kumar et.al (2012) used this multiscale approach to understand effect of nano sized voids and bubbles on plastic behavior of irradiated FM steels. In their paper, results from atomistic simulations of dislocation-defect interactions in Fe-Cr-He systems are transferred to DD simulations and change in flow strength of irradiated materials is analyzed. In a recent paper, Arsenlis et.al (2012) used dislocation dynamics simulations to study heterogeneous deformation in bcc iron due to irradiation defects. In their work, they used the interactions of prismatic loops formed due to irradiation with a network of existing dislocations to understand deformation behavior.

In the present work, an attempt is made to find changes in mechanical properties of irradiated FM steels using DD simulations with prismatic loops as irradiation defects. The dose dependence of change in flow stress is analyzed through a combined effect of defect density (N) and defect loop size (d). In the next sections, details of brief theory behind DD simulations, computational details used and results and discussions on FM steels are presented.

DD SIMULATIONS: COMPUTATINAL DETAILS

Dislocations are the line defects in continuum space, which are characterized by their line direction and Burgers vector. The Burgers vector has two components – edge, perpendicular to line sense and screw, parallel to line direction. The stress and displacement fields around the dislocation lines can be obtained from elasticity theory. Based on these stress fields and the external loads, evolution of dislocations is obtained. Various rules are framed to incorporate for nucleation, annihilation, pinning, cross-slip, junction formation, etc. With these set of rules, DD simulations can be used to study the role of dislocation microstructure in strain hardening, low-strain fatigue, creep and fracture.

The formulation for DD simulations and the necessary input are described now. The dislocations are assumed to move in a viscous medium with a drag coefficient either derived experimentally or by lower length scale simulations. The driving force on the dislocations is derived from the Peach-Koehler equation in terms of the stresses acting on the dislocation segments due to all other dislocations and any external stresses. Various stresses/forces seen by dislocation segments are: a) drag force, B.v where B is the drag tensor, v velocity vector, b) Peirels stress or the friction stress, c) External applied stress, Dislocation-obstacle interaction forces, d) Osmotic forces resulting from non-conservative motion of dislocations (climb) which results into generation of point defects, etc. Along with these, the other input in DD simulations are: a) slip systems information- slip plane normal, slip direction, b) dislocation line direction along with Burgers vector defined mutually together, c) shear modulus, poisson's ratio, d) dislocation density, defect density where defects may be obstacles because of alloying elements or loops/voids/bubbles generated by irradiation. The DD simulations in the present work are performed by using a highly scalable parallel code PARADIS [Arsenlis(2007)], which is available as open source. More details of which can be found in [Arsenlis(2007) and Arsenlis (2012)].

Equations of dislocation motion

Firstly, various forces on dislocation segments are obtained. Forces on segments due to all other segments are obtained from elastic stress fields of dislocations by Peach-Koehler equation.

$$\mathrm{f} = [\sigma.\mathrm{b}] \times \mathrm{t}$$

where, f is the force vector, σ is the stress tensor on centre of dislocation segment with contributions from stresses due to all other segments and any external stress fields. B is the Burgers vector, t is the dislocation line direction. Once forces are obtained, the velocity of dislocation segment is computed from drag relation,

$$\mathrm{f=B.v}$$

where, B is the drag coefficient tensor given by

$$\mathrm{B} = \mathrm{B_g}(\mathrm{m} \otimes \mathrm{m}) + \mathrm{B_c}(\mathrm{n} \otimes \mathrm{n}) + \mathrm{B_l}(\mathrm{t} \otimes \mathrm{t}),$$

where, B_g and B_c are the temperature dependent drag coefficients for motion along the glide and climb directions, and B_l is the drag coefficient related to configurational forces responsible for equilibrium line shape defined by vector t. The vectors n, m are unit vectors defined from following relation,

$$\mathrm{n} = \frac{\mathrm{b} \times \mathrm{t}}{|\mathrm{b} \times \mathrm{t}|}, \ \mathrm{m} = \mathrm{n} \times \mathrm{t}$$

The dyads $m \otimes m$, $n \otimes n$, $t \otimes t$ shown in the above equations will give the direction of force vectors in the directions along m, n and t vectors respectively when operated on velocity vector. The velocity vector v is then obtained from inverting B to get mobility function M, i.e., $M = [B]^{-1}$ and multiplying M with force vector. The velocity here is the first order differential equation which is integrated by forward Euler or trapezoidal integration schemes to obtain time evolution of dislocation segments.

For the present simulations, bcc iron is chosen as representative system for FM steels. The slip system considered is the {110}<111> type dislocations. Various other computational details are as given below:

- The computational domain is a cubic cell with length = 1.3 μm.
- The Burgers vector has a magnitude = ½ (111) equal to 0.25 nm.
- Initial dislocation micro structure contains a network of screw dislocations with density = $2x10^{13}$ m^{-2} which represents a well annealed crystal. Periodic boundary conditions are used for the analysis.
- Material constants are shear modulus = 86 GPa and Poisson's ratio = 0.291,
- Temperature = 300 K
- Loading direction, tensile along [001] direction with strain rage of 100 s^{-1}.

DD SIMULATIONS ON IRRADIATED FM STEELS

Due to irradiation particularly in Fe, self-interstitial atom (SIA) dislocation loops with sizes of 4 nm or less are formed [Zinkle(2006)]. The SIA-type dislocation loops are perfect and prismatic, and therefore stable and glissile. Further, it is believed that they are the main contributors to irradiation hardening in the absence of strengthening particles [Singh (1997)]. The prismatic loop size distribution can be consolidated into much larger average sizes (10–50 nm) by post-irradiation annealing and thermal treatments [Rau (1969) and Eyre (1971)]. The dislocation dynamics simulations taking into effect of these loops will thus help us to understand theoretically the flow behavior of irradiated FM steels. In the present work, DD simulations are used to study the flow behavior of irradiated FM steels taking into consideration of interaction of such loops with existing network of dislocations. With these parameters, increase in flow stress due to change in size (d) and loop density (N) is determined. In this analysis, an attempt is made to find dose dependence of change in flow stress through a combined effect of N and d.

After doing some nitial parametric studies on unirradiated material, few parameters are taken for subsequent analysis on irradiated materials. The drag coefficient for glide is set as B_g = 1.0 Pa.s which gives rise to a initial flow stress of 440 MPa. Effect of irradiation is considered in simulations by taking nano sized prismatic loops in the domain for different density of loops which correspond to various irradiation doses. The prismatic loops will have glide path along the glide prism developed by the loops along the burgers direction. The present studies on irradiated steels is restricted for cases with density of prismatic loops as N=0 (unirradiated), $N=8.15x10^{20}$ m^{-3}, N=1.63 $x10^{21}$ m^{-3} and $N=3.26x10^{21}$ m^{-3} considering the large computational time involved. The initial calculations used diameter of prismatic loops d=25 nm for all cases of N. The flow behavior of irradiated steels is shown in Figure.1. The flow stress values corresponding to these loop densities at 0.15% strain are 558 MPa, 610 MPa and 738 MPa. There is an increase in flow stress of $\Delta\sigma$ = 104 MPa for prismatic loops density of $N=8.15x10^{20}$ m^{-3} and an increase of $\Delta\sigma$ = 172 MPa with $N=1.63x10^{21}$ m^{-3} and an increase of $\Delta\sigma$ = 298 MPa with $N=3.26x10^{21}$ m^{-3} loop density.

The variation of total density of dislocation network including prismatic loops is shown in Figure.2. It can be seen that rate of increase in total dislocation density is small compared to that of unirradiated materials. The corresponding dislocation microstructure at strain of 0.0% and 0.5% is shown in Figure.3. A combined effect of loop density (N) and loop diameter (d) with various combinations of N and d on flow behavior is shown in next section.

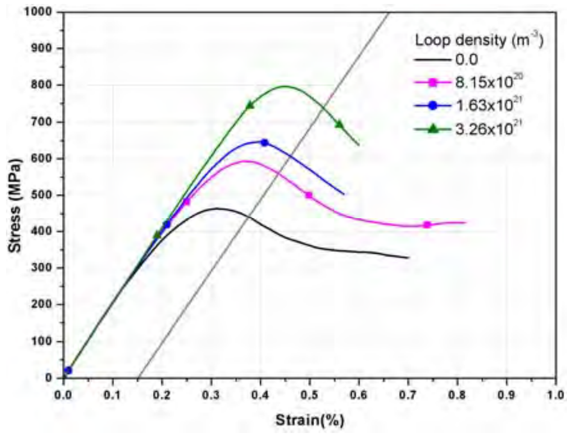


Figure 1. Global stress-strain behavior as function of density of prismatic loops (N) for a fixed loop size of d=25nm. The straight line represents stresses at 0.15% strain.

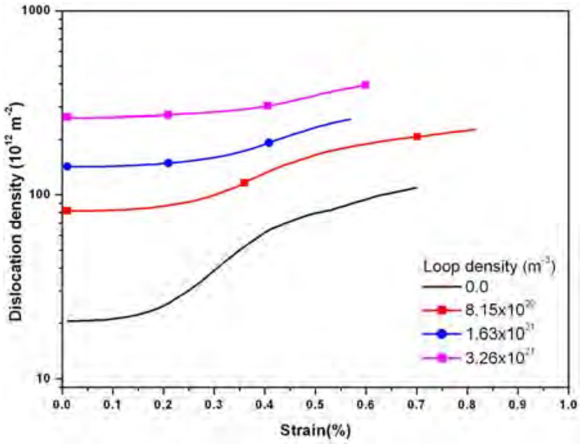
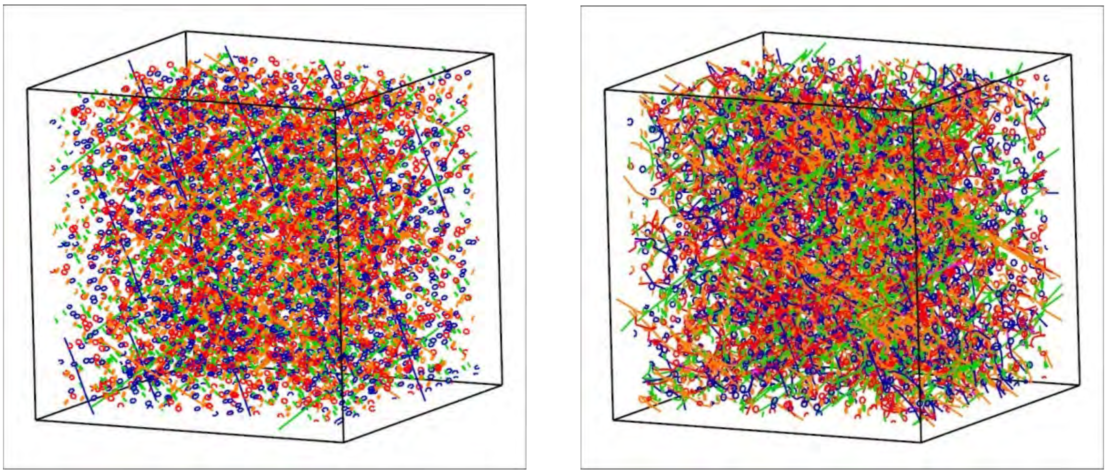


Figure 2. Dislocation density variation for various loop densities(N)



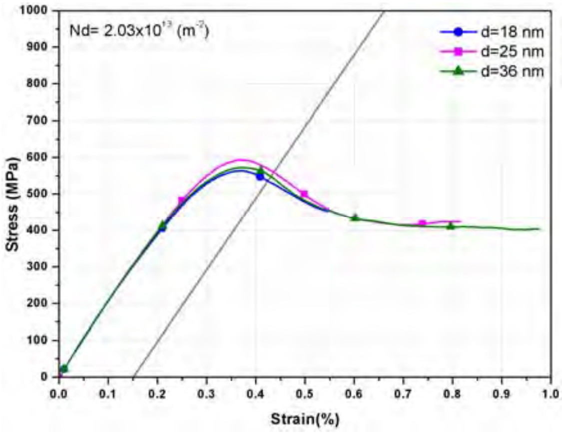
(a) (b)

Figure 3. Dislocation microstructure at strain=0% and 0.7% for N=3.26×10^{21} /m^3 with d=25nm

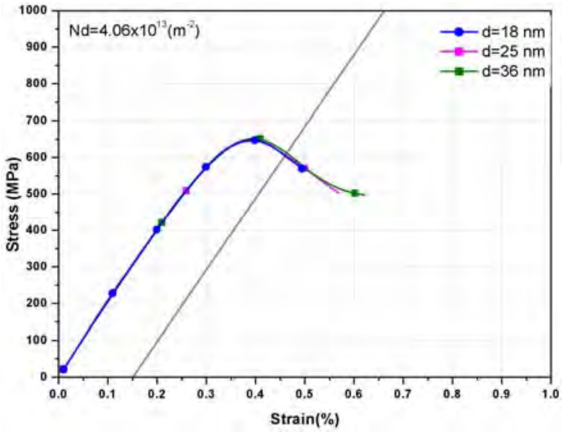
Combined effect of loop density (N) and loop size (d) on flow behavior.

In the previous section, the general trend of increase in flow stress because of irradiation (in terms of defect density) for a fixed loop diameter (d=25 nm) was shown. Arsenlis et.al (2012) used a similar study in quantifying the effect of defect density N on flow behavior by taking a fixed loop diameter 'd'. In their study, they also studied transition from homogenous to heterogeneous deformation when the defect density is very high. The present section deals with a combined effect of N and d by considering simulations with different N and d values, however keeping product of N and d, i.e., N*d = constant (k). The choice of this function N*d is rational because, the effect of irradiation in generation of a total number of point defects and subsequent amalgamation of them in to loops of different sizes (d) with loop density (N) essentially keeps N*d as constant.

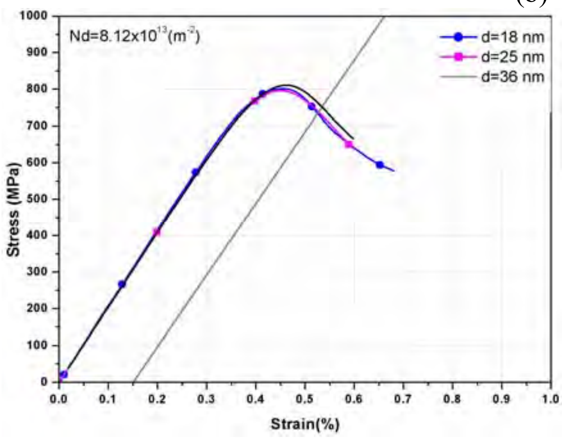
The flow behavior of irradiated material for different values of N*d is shown in Figure. 4a-c. For convenience, d is taken to have three values 18, 25 and 36 nm and the loop density is changed accordingly to make N*d = k. Different N*d values considered are a) k= $2.03 x 10^{13}$ m^{-2}, b) k= $4.06 x 10^{13}$ m^{-2} and c) k= $8.12 x 10^{13}$ m^{-2}.



(a)



(b)



(c)

Figure 4. Flow behavior for various N*d =k with values: a) k= $2.03 x 10^{13}$ m^{-2}, b) k= $4.06 x 10^{13}$ m^{-2} and c) k= $8.12 x 10^{13}$ m^{-2}.

The flow stress values at 0.15% strain for all these cases are summarized in Figure.5 as increase in flow stress $\Delta\sigma_f$ as a function of N for different values of loop size d. The important observation that can be made from these results is that for each of constant k, the flow stress is same for different sets of N and d that make the product N*d as constant. The above observation motivates to study flow behavior of irradiated materials as function of N*d rather than N and d independently. This also helps to tackle DD simulations of large N*d values by taking large loop diameter *d* but with a relatively lower defect density N. One such simulation study is performed for k=3.6x10^{14} m^{-2} with d=36nm. Flow behavior for this simulation along with previous k values is shown in Figure.6a. The increase in flow strength for different N and d values from Figures 5&6 can be summarized by taking single parameter of N*d as shown in Figure.6b. An approximate fit of increase in flow stress due to defect loops can be obtained as

$$\Delta\sigma_f = 3\times10^{-5}\sqrt{Nd}\ \text{MPa}$$

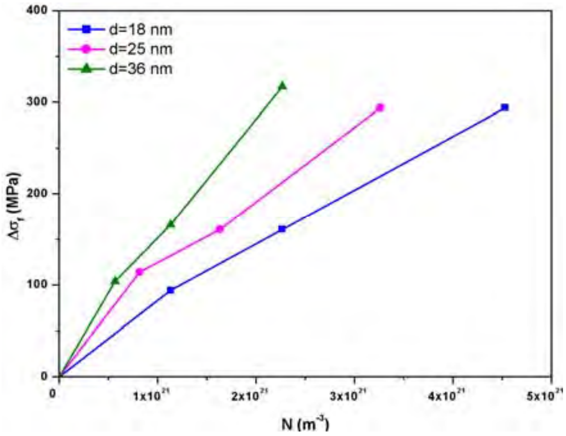


Figure 5. Change in flow stress due to irradiation (as function of loop density N) for various loop diameters.

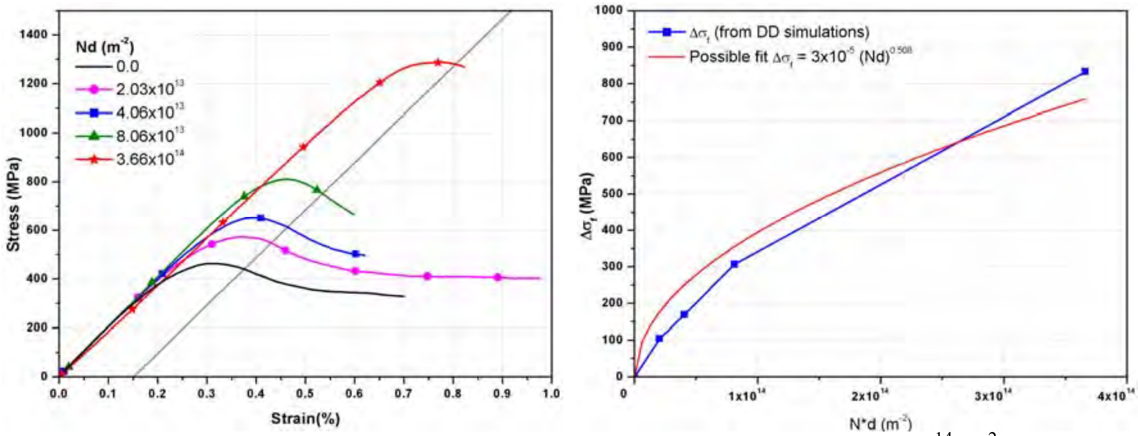


Figure 6.(a) Flow behavior for various N*d values including a larger value of 3.6x10^{14} m^{-2} (b) Increase in flow stress showing a combined effect of N and d on flow behavior and a possible curve fit for the same.

Irradiation strengthening analysis

Radiation effects in terms of hardening in materials are traditionally treated by two dislocation barrier models [Zinkle(2004)]. The dispersed barrier hardening model (DBH) is based on geometrical considerations for obstacles intersecting dislocation glide plane which is most suitable for hard obstacles. The other model known as FKH model is used for treating weak obstacles such as radiation-induced small defect clusters. These two models give the functional dependence of polycrystalline flow stress on defect density and defect size as given below:

$$\text{DBH: } \Delta\sigma_f = M\alpha\mu b\sqrt{Nd}$$

$$\text{FKH: } \Delta\sigma_f = \frac{1}{8} M\mu b N^{\frac{2}{3}} d$$

In these equations, $\Delta\sigma_f$ is increase in flow stress, M is the Taylor factor (3.06 for BCC and FCC metals), α is the defect cluster barrier strength (0.4 or higher for BCC metals), μ is the shear modulus, b is the Burgers vector, and N and d are defect cluster density and diameter. With α =0.5 and other used parameters in the simulations, the DBH model predicts $\Delta\sigma_f = 3.29\times10^{-5}\sqrt{Nd}$ which shows a nice agreement with the current computed results.

DEPENDENCE OF FLOW STRESS ON IRRADIATION DOSE

A lot of research is under progress all over the world to correlate the irradiation dose in terms of dpa (displacements per atom) to size (d) and density (N) of defects generated. Getting such correlations involve lot of experimental observations on micro-structural changes due to irradiation. Other alternative is to use computational radiation cascade analysis using Kinetic Monte Carlo models. Chaitanya Deo et.al (2008) used relations of the form given below to obtain N and d in terms of dpa:

$$N = A\sqrt{dpa}$$
$$d = B\sqrt{dpa}$$

where A = 10^{-3} nm^{-3} and B=8 nm for doses less than 1 dpa. Taking product of N and d gives a relation for dpa in terms of product Nd as

$$N\times d = (AB)\ dpa = 8\times10^{-3}\ nm^{-2}\ dpa = 8\times10^{15}\ m^{-2}\ dpa\ .$$
$$dpa = Nd/8\times10^{15}$$

In the present analysis, using the (Nd) values considered, this relation gives an irradiation dose of 0.01 dpa for Nd=8.12×10^{13} m^{-2} and Nd=3.66×10^{14} m^{-2} gives a dose of about 0.5 dpa.

SUMMARY

DD simulations are used to study the irradiation hardening in FM steels. The irradiation hardening is studied in terms of increase in flow stress due to presence of irradiation induced prismatic loops which are quantified by defect density and defect size. A combined effect of N and d on flow behavior is reported which allows us study them as a single parameter such as product of N and d. For various values of N and d with N*d=constant *k*, the flow behavior is obtained for this material. An important observation that can be made from these results is that for each of constant k, the flow stress is same for different sets of N and d that satisfies N*d=*k*. This allows us to solve for relatively higher N*d values by taking higher d for the same N*d value keeping computational cost the same. One such simulation is performed with higher N*d value. Finally, an attempt is made to correlate the N*d parameter to irradiation doses in terms of dpa.

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