MECHANISMS OF PLASTIC AND FRACTURE INSTABILITIES OF FUSION STRUCTURAL MATERIALS – N. M. Ghoniem (University of California, Los Angeles)

ABSTRACT

Research progress at UCLA on the DOE grant *#DE FG03-98ER54500 is* outlined in this report, for the period July 15, 1998 through January 14, 1999. The main objectives of the work is to develop new methodologies for modeling a number of mechanisms which control plastic instabilities and fracture of V, Fe and Cu alloys under fusion irradiation conditions. These phenomena appear to be generic, and are believed to present substantial challenges to the structural integrity of first-wall fusion material systems. The main thrust of the modeling effort is to identify the mechanisms which lead to localization of plastic deformation, the accelerated cavitation at grain boundaries, the detrimental influence of helium transmutations, and the loss of ductile crack propagation in irradiated materials. We report here our initial research findings on the problem of accumulation of nano-scale prismatic defect clusters in the vicinity of dislocations. Under irradiation conditions, small defect clusters are produced in collision cascades. These mobile clusters interact with dislocations, hindering its motion. Thus, radiation hardening takes place as a result of these interactions. However, it is shown here that once these nano-phase clusters approach dislocations, they may be trapped in their elastic strain fields. Trapping is shown to occur by elastic interactions within a zone of 10 *nm* in bcc Fe, and 20 *nm* in fcc Cu at RT. If the local stress (i.e. applied plus internal) is high, clusters are absorbed in the core of grown-in dislocations as a result of unbalanced moments, providing sufficient energy for rotation of their Burgers vectors in a zone of 2-3 *nm* in Fe. Near the dislocation core, sessile defect clusters in Cu are shown to convert to a glissile configuration. The current work is performed in collaboration with LLNL (Dr. T. de la Rubia), and is partially supported by the Institute of Materials Research at LLNL. The UCLA group has an active collaboration program on this problem with the Danish RISO National Labs (Dr. B. Singh), and the German Forschungszentrum Julich (Dr. H. Trinkaus). Additionally, collaborative efforts have started with UCSB (Professors Lucas and Odette) on the problem of Ductile-to-Brittle Transition in V and Fe, where our dislocation dynamics method is to be coupled with their fracture mechanics approach at different length scales.

SUMMARY

The main thrust of the current modeling effort is to identify the mechanisms which lead to localization of plastic deformation, the accelerated cavitation at grain boundaries, the detrimental influence of helium transmutations, and the loss of ductile crack propagation in irradiated materials. We report here our initial research findings on the problem of accumulation of nano-scale prismatic defect clusters in the vicinity of dislocations. Under irradiation conditions, small defect clusters are produced in collision cascades. These mobile clusters interact with dislocations, hindering its motion. Thus, radiation hardening takes place as a result of these interactions. However, it is shown here that once these nano-phase clusters approach dislocations, they may be trapped in their elastic strain fields. Trapping is shown to occur by elastic interactions within a zone of 10 *nm* in bcc Fe, and 20 *nm* in fcc Cu at RT. If the local stress (i.e. applied plus internal) is high, clusters are absorbed in the core of grown-in dislocations as a result of unbalanced moments, providing sufficient energy for rotation of their Burgers vectors in a zone of 2-3 *nm* in Fe. Near the dislocation core, sessile defect clusters in Cu are shown to convert to a glissile configuration.

OBJECTIVES

The general objectives of the modeling activities at UCLA are:

(1) To integrate three material length scales for determination of basic mechanisms of plastic and fracture instabilities under irradiation conditions. These length scales are: i- atomistic, using Molecular Dynamics , ii- mesoscopic, using Dislocation Dynamics (DD) and Fokker-Planck (FP) theory approaches, and macroscopic utilizing fracture mechanics.

(2) To apply developed computational tools to the study of four basic types of plastic and fracture instabilities which occur in Fe, V and Cu alloy systems. Those are: (1) transition from a state of uniform deformation (elongation) to localized plastic flow, (2) transition from a ductile mode of crack propagation, associated with extensive plasticity and micro-void formation to a brittle mode associated with cleavage fracture, (3) transition from transgranular crack growth to intergranular crack separation, (4) irradiation effects on thermo-mechanical instabilities.

(3) To focus on important and challenging problems of material deformation under irradiation. Important questions in this regard are: (a) why does plastic flow under irradiation tend to localize in shear bands? (b) what are the effects of material alloying, temperature, neutron irradiation and strain rate on flow localization? (c) What is the connection between radiation hardening and mechanical instabilities? (d) are there any fundamental differences between instabilities occurring in BCC materials (Fe and V) and FCC materials (Cu and steels) ? (e) Is there a relationship between global thermodynamic variables (e.g. stress, temperature, etc) and microstructure transitions from uniform to cellular to banded? (f) what is the relevance of these phenomena to the development of fusion materials? (g) What types of degradation mechanisms does helium

introduce in irradiated alloys?, and what is its role on transition from transgranular to intergranular cracking? (h) What are the exact conditions for the sudden transition in crack propagation from a ductile to a brittle mode? And finally, (i) how do non-metallic interstitial elements influence the ductility of Fe, V, and Cu fusion materials alloys?

(4) To analyze the deformation characteristics of three main fusion material systems; namely reduced-activation ferritic/ martensitic, low-activation vanadium , and copper alloys.

The specific objective of this task is to determine the conditions for the accumulation of nano-scale defect clusters at slip dislocations. Nano-scale defect clusters are produced from collision cascades under irradiation. Their accumulation hinders slip od dislocations, and thus leads to radiation hardening.

BACKGROUND

The deformation behavior of both BCC (e.g. Fe and V) and FCC (e.g. Cu and austenitic steels) metals is sensitive to neutron irradiation, temperature, strain rate and alloying, exhibiting a variety of complex mechanisms which render them brittle. Under low temperature (< 0.4 T_m) neutron irradiation, the flow stress increases because of resistance to dislocation glide on slip planes. At critical neutron fluence, cracks propagate in a brittle fashion, dissipating small amounts of energy in plastic deformation. Resistance to dislocation motion increases as a result of accumulation of dispersed barriers through radiation-induced lattice defects, as well as general mobility reductions at high strain rates through phonon and electron damping mechanisms. Additionally, heavily irradiated fusion materials generally exhibit extreme hardening associated with localized deformation in "dislocation channels", which lead to pre-mature loss of ductility and failure. At higher temperatures, on the other had, helium migration to grain boundaries results in the accelerated formation of gas-filled cavities leading to transition form matrix to grain boundary cracking. Non-metallic interstitial elements (e.g. nitrogen, carbon, hydrogen and oxygen) are transported in the strong stress fields around notches and crack tips, and their segregation results in dramatic weakening and cracking of stressed components. Modeling of the detrimental effects of irradiation on the mechanical properties is required to guide experimental efforts of alloy optimization. Through mechanistic models, one can identify material controlling parameters (e.g. alloying elements, operating conditions (flux, fluence, temperature, stress, etc.), material processing variables, etc.), where the impact could be minimized.

. Under the current DOE grant at UCLA, research on four tasks has been started. The first one: *Atomistic Computer Simulations*, is concerned with the utilization of MD computer simulations to determine defect production and properties, collision cascade effects on dislocation motion and dislocation recovery mechanisms, cascade interactions with radiation-induced barriers to dislocation motion, and the short-range interactions between dislocation segments and dispersed barriers. In the second task: *Atomic Clustering*, we plan to develop efficient computational methods for atomic clustering problems which lead to the formation of dispersed barriers under irradiation. This will include determination of size and composition of precipitate clusters, helium clusters, point defect clusters, as well as their spatial distribution statistics. Task 3: *3-D Dislocation Dynamics,* is concerned with further development of a breakthrough computational method for studying localized plastic instabilities. In this method, the elastic field of dislocations (i.e. displacement, strain, stress, forces, self and interaction energies) is determined on the basis of segmenting arbitrarily curved and oriented dislocation loops into 3D parametric curves. The equations of motion for each loop segment is developed with inertial and viscous drag mobility effects, thus allowing for studies of irradiation effects on plastic deformation. Finally, *Plastic And Fracture Instabilities Under Irradiation* are analyzed in task 4. The onset of flow localization in irradiated materials will be determined by combining the interaction between the hardening effects of radiation-induced barriers and the destruction of these obstacles by leading dislocations in heterogeneous spatial locations. Several other fracture mechanisms will be simulated for Fe, V and Cu alloys, including dislocation-crack interactions, the dynamic structure and size of the plastic zone, and the segregation of interstitial elements under irradiation to crack tips. Coupling of the computational methods developed here with the US experimental program is expected to provide an additional tool for alloy development of fusion structural materials.

SUMMARY OF RESEARCH PROGRESS

Radiation Hardening of FCC and BCC Metals

It has been experimentally established that exposure of all metals to fast-neutron irradiation results in an increase in their flow stress. It has also been established that when BCC metals are irradiated at high temperature, or when they are annealed after irradiation, the stress-strain curve of the unirradiated material is substantially recovered. This is a direct indication of the role of radiation-induced defect clusters on hardening. Several studies discuss the relative roles of both alloying elements in ferritic steels (e.g. Ni, Si, C, Mn, Mo and Co), and intrinsic defect clusters (point defects, dislocation loops, and bubbles) produced by irradiation on the shift in the Ductile-to-Brittle-Transition-Temperature (DBTT) of ferritic alloys [1-4]. Radiation hardening and the shift in DBTT have been qualitatively and phenomenologicaly related to the interaction of mobile dislocations with dispersed barriers as well as with relatively immobile forest dislocations.

Under irradiation conditions of almost all-metallic alloys, localized deformation patterns have been observed. Bloom et al. Observed localized slip traces of {111} planes with type 304 stainless steel specimens, after being irradiated at 120 °C, and deformed to 10%[5]. In FCC alloys, the stress required to unpin small clusters of defects is increased because of the decrease in inter-barrier separation as a result of irradiation. If dislocation pile-ups form behind dispersed barriers, leading dislocations experience a sufficient force on them to break them loose, and with additional dynamic inertia they destroy other irradiation-induced obstacles. The phenomenon is thus intimately related to the dynamics of dislocation motion, and cannot be captured by static considerations alone. Dislocation channels form in a manner similar to avalanche propagation, and the final result is the well-documented plastic instability [5-7]. Plastic deformation in this case is concentrated on slip planes, leading to pre-mature fracture.

Intensive experimental investigations of hardening mechanisms in both FCC and BCC alloys indicated that two types of phenomena govern the increase in flow stress: (1) source hardening; (2) friction hardening. Source hardening operates when the critical resolved shear stress level is low, and is increased slowly until dislocations are unpinned from the influence of small barriers to their motion. The phenomenon is common in BCC alloys, and is related to the fast diffusion rates of impurities, point defects or other elements (e.g. carbon) to dislocation cores. In FCC alloys, impurity atom diffusion is not sufficiently fast to catch up with moving dislocations and result in the associated phenomenon of source hardening. Source hardening is manifest in a yield drop (from upper to lower yield points), and can be observed in unirradiated BCC alloys. The required critical stress to release the dislocation line from a row of carbon atoms has been roughly estimated [6]. When the dislocation is free from the locking action of solute atoms, point defects or impurities, the dislocation can move at a lower stress, causing the drop in the yield point. In FCC alloys, however, source hardening can only be observed under irradiation conditions, where small point defect clusters form the pinning obstacles to dislocation motion.

Friction hardening, on the other hand, is thought to be responsible for the characteristics of plastic stress-strain behavior, as expressed in the work hardening exponent, and several other measures (yield surface, Bauschinger plastic anisotropy, etc.). It can also be decomposed into two parts: (1) flow stress increase by long-range dislocation reactions; (2) flow stress increase by short-range dislocation reactions. Without the influence of irradiation, both types of reactions occur, but irradiation introduces additional features of the microstructure, which can modify or totally change the nature of these types of interactions. Long-range reactions are qualitatively understood by applying simplified elasticity solutions for long, straight dislocations. However, the quantitative predictions of long-range interaction effects on increasing the flow stress are uncertain by factors of 2-4 [8-10]. Several reasons are behind such uncertainties, such as the curved and tangled nature of interacting dislocations, the influence of forest dislocations on the strength of reactions, the formation of dipoles and higher order clusters, and the possible annihilation of close by dislocation segments. On the other hand, the nature and magnitude of short range interactions are not well-understood, because of uncertainties in the applicability of elasticity theory, and uncertainties in estimating the overall energetics of close-range interactions with radiation-induced obstacles (e.g. voids, bubbles, vacancy loops, interstitial loops, and point defect-impurity clusters).

Starting in 1997, a small effort on the development of a new computational method for simulation of dislocation microstructure evolution was initiated at UCLA. Funding for this fundamental work is provided by the ASCI (Accelerated Scientific Computing Initiative) through a collaborative program with LLNL. This research effort is continuing, and has the objective of developing general efficient computational methods for material deformation under general loading conditions. The work is in collaboration with IBM, WSU, and LLNL, and is backed up by a systematic experimental program. Under the current DOE grant, the work is to be extended to the specific conditions of fusion structural materials. This leveraging of knowledge is now leading to wide recognition of the fusion materials problems within the materials science and mechanics communities. There are generic aspects of plastic and fracture instabilities that touch upon many material systems outside the specific conditions of the fusion environment. However, the current effort supported by DOE/OFE is dedicated to the specialized irradiation conditions of the fusion environment. We report here on some of the general methodologies developed at UCLA so far, and point to specific results obtained in collaboration with a number of national and international colleagues.

Development of the Parametric Dislocation Method

In this method, the geometry of dislocation segments is represented in parametric vector form as: $\hat{\mathbf{r}}^{(j)}(u)=\mathbf{q}_i^{(j)}N_i(u)$, where the vector $\hat{\mathbf{r}}^{(j)}(u)$ represents the spatial position of segment (j). A set of parametric functions $N_i(u)$, and generalized coordinates $\mathbf{q}_i^{(j)}$ completely determine the shape of the segment. The displacement vector, **u**, the stress tensor σ_{ij}, and the interaction energy between two loops, E_I, can now be obtained as fast numerical sums, over the number of quadrature points Q_{max}, the loop segments N_s, and the number of loops N_{loop}. These are given by (see our references [11-14] for details):

$$u_i=\frac{1}{4\pi}\sum_{\gamma=1}^{N_{loop}}\{-b_i\Omega+\frac{1}{2}\sum_{\beta=1}^{N_s}\sum_{\alpha=1}^{Q_{max}}w_\alpha(\varepsilon_{ikl}b_lR_{,pp}+\frac{\varepsilon_{kmn}b_nR_{,mij}}{1-\nu})\hat{x}_{k,u}\}$$

$$\sigma_{ij}=\frac{\mu}{4\pi}\sum_{\gamma=1}^{N_{loop}}\sum_{\beta=1}^{N_s}\sum_{\alpha=1}^{Q_{max}}b_nw_\alpha[\frac{1}{2}R_{,mpp}(\varepsilon_{jmn}\hat{x}_{i,u}+\varepsilon_{imn}\hat{x}_{j,u})+\frac{1}{1-\nu}\varepsilon_{kmn}(R_{,ijm}-\delta_{ij}R_{,ppm})\hat{x}_{k,u}]$$

$$E_I=-\frac{\mu b_i^{(1)}b_j^{(2)}}{8\pi}\sum_{\beta^{(1)}=1}^{N_s^{(1)}}\sum_{\beta^{(2)}=1}^{N_s^{(2)}}\sum_{\alpha^{(1)}=1}^{Q_{max}^{(1)}}\sum_{\alpha^{(2)}=1}^{Q_{max}^{(2)}}w_{\alpha^{(1)}}w_{\alpha^{(2)}}[R_{,kk}(\hat{x}_{j,u}^{(2)}\hat{x}_{i,u}^{(1)}+\frac{2\nu}{1-\nu}\hat{x}_{i,u}^{(2)}\hat{x}_{j,u}^{(1)})+\frac{2}{1-\nu}(R_{,ij}-\delta_{ij}R_{,ll})\hat{x}_{k,u}^{(2)}\hat{x}_{k,u}^{(1)}]$$

Comparisons of our method with analytical solutions show that the accuracy of calculating the Peach-Kohler force can be less than 0.5% at distances as close as 1.5 b from the dislocation core. The calculations of the interaction and self-energies (as well as self-forces) are absolutely convergent with increasing the number of segments and/or quadrature. Computational speed tests show that the method is as fast as a purely analytical one for straight segments, hence we describe it as a **fast sum method.**

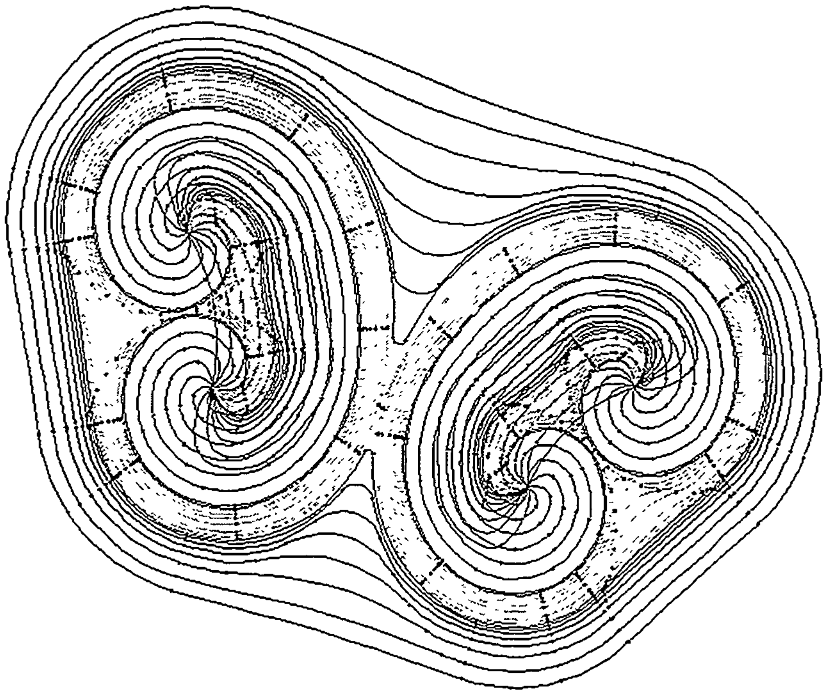

Figure (1); Interaction between Frank-Read sources in Cu

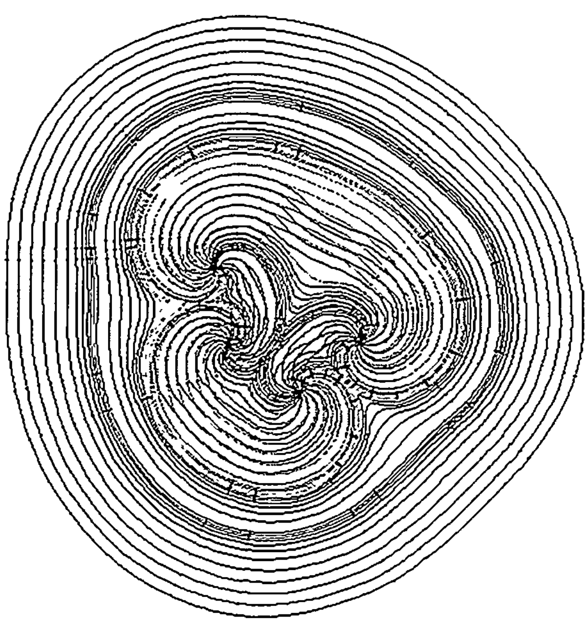

Fig.(2): Formation of Complex Dislocation Loops in FCC Cu.

The equations of motion for dislocation segments have been derived from a Galerkin minimum energy principle, in the same way as customary in FEM techniques in continuum mechanics. The position, tangent and normal vectors of specific nodes on continuous dislocation lines are updated for every time step. Our approach provides a great degree of flexibility in changing the shape and length of each dislocation segment without particular limitations. When additional crystallographic constraints are included, the influence of the crystal structure on dislocation shapes can be clearly seen. Figures (1-3) show the interaction between Frank-Read dislocation sources in FCC Cu. In Figures (1-2), complex loops form as a result of dislocation source interactions, while Lomer-Cottrel junction forms in Figure (3). The time step is adjusted to capture annihilation interaction within one FR source, or junction formation along the common line on two conjugate slip planes.

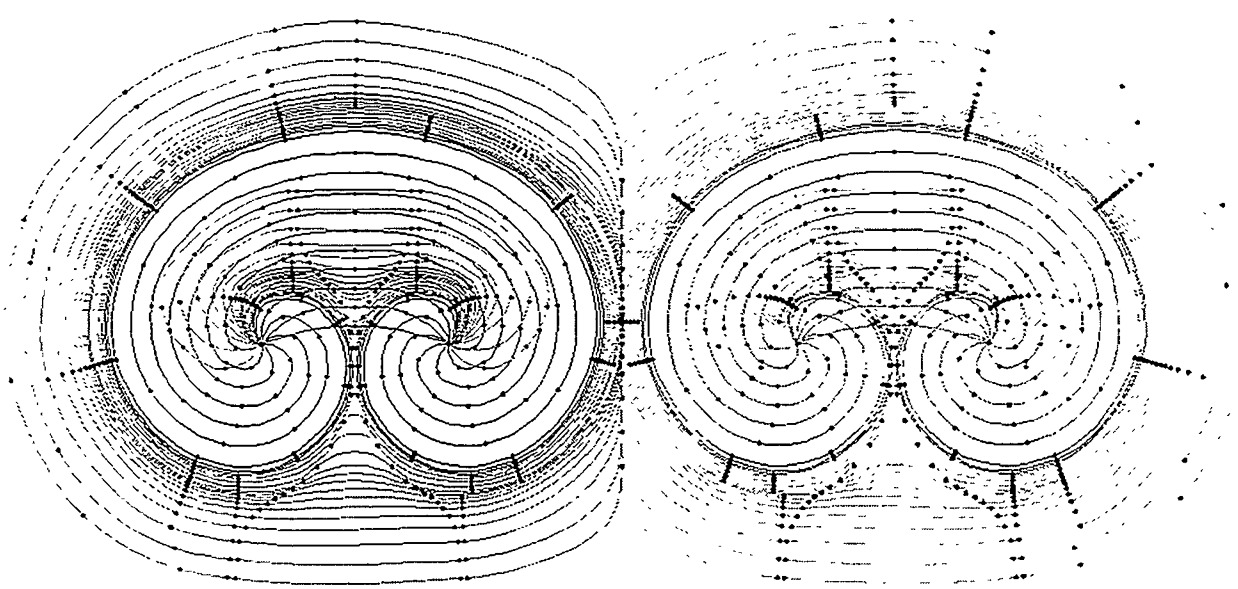

Figure (3): Formation of a Lomer-Cottrel Lock as a result of interaction between two dislocation loops.

Dislocation Decoration with Nano-scale Defect Clusters in Irradiated Metals

Collaborators: N.M. Ghoniem (UCLA), L. Sun (UCLA), B.N. Singh (RISO), and T. Diaz de la Rubia (LLNL)

Under neutron or charged particle irradiation, nano-scale point defect clusters nucleate directly from atomic collision cascades in irradiated materials. Once these clusters nucleate, they assume the shape of small prismatic dislocation loops of radial dimensions in the range of 1-3 *nm*. Molecular Dynamics (MD) computer simulations [15-17], as well as experimental evidence suggest that, at least in bcc metals, these clusters can be rather mobile, and that they migrate predominantly along close-packed crystallographic directions. The most stable clusters in bcc Fe are glissile sets of co-linear <111> crowdions, with a dislocation loop character of $\frac{a}{2}$<111>{111} [15]. In fcc Cu, hexagonal faulted Frank loops of type $\frac{a}{3}$<111>{111} are found to be stable and sessile. Vacancy clusters in Cu are found to be {111}-platelets of Stacking Fault Tetrahedra (SFT's). Experimental evidence [18,19] suggest that under electron irradiation, where defect clusters are not directly produced in collision cascades, grown-in dislocations are not heavily *decorated* with small defect clusters. The work of Sigle et al [18] indicates that only SFT's are found within *20 nm* of dislocation cores, and their position is on the compression side of edge dislocations.

Fig. 4 shows a TEM micrographs of pure single crystal Mo irradiated with fission neutrons at 320 K [19]. Grown-in (slip) dislocations are clearly decorated with small defect clusters, without any preference to either side of pre-existing dislocations. The zone of *attraction* is on the order of 10 *nm* in bcc metals [20], and about 20 *nm* in fcc metals [19]. While defect clusters nucleate homogeneously under electron irradiation, they can be directly produced heterogeneously by collision cascades under ion or neutron irradiation. Experimental evidence of their interaction with dislocations is consistent with a high degree of cluster mobility. The decoration of existing dislocations with nano-scale defect clusters appears to be a consequence of in-cascade nucleation, followed by coherent transport along closely packed crystallographic directions.

Fig. 4: Dislocation decoration and ``raft" formation in single crystal molybdenum irradiated at 320 K to a neutron fluence of 1.5x 10^{21} n/m^2 (E> 1 MeV). After ref. [20].

It is well established that neutron irradiation leads to a substantial increase in the yield strength and hardening of metals. This phenomenon is particularly severe at low temperatures (i.e., below recovery stage V). The decoration of slip dislocation with defect clusters appears to be the controlling mechanism for blocking dislocation motion on its glide plane. Moreover, once plastic deformation commences, it is observed to be rather heterogeneous and concentrated in ``soft" deformation channels, while the vast majority of the matrix is in a state of elastic deformation. The onset of this type of plastic instability is thus associated with the initiation and propagation of dislocation channels that are nearly free of defect clusters. Decoration of dislocations with irradiation-produced defect clusters is possibly the root cause of localized plastic deformation, leading to premature fracture. At low applied stress levels, defect clusters (of both vacancy and interstitial type) inhibit dislocation mobility by acting as barriers to their motion. As the stress is increased in a local region, clusters are absorbed in the dislocation core, and are hence cleared from the glide plane of a moving dislocation loop. This qualitative picture can explain the initial radiation hardening, and the subsequent onset of flow localization. However, quantitative determination of the detailed mechanisms by which the phenomenon occurs remain largely unexplored [21].

We consider here the conditions for the interaction and accumulation of small, prismatic-type point defect clusters with grown-in (deformation) dislocation loops. In particular, we provide theoretical estimates for the attractive elastic interaction region around dislocations, and compare the results to experimental observations. In addition, we give theoretical results for the spatial structure of the accumulation, or elastic trapping, region around dislocation loops. The interaction of point defects with slip loops is also analyzed and compared to the case of nano-scale defect clusters. In fcc metals of low stacking fault energy, small defect clusters are faulted, and are hence sessile. We wish to show that, as a result of their elastic interaction with the internal stress field of dislocations, these clusters can acquire enough energy to convert to a more glissile configuration. We first present the main features of a new the computational model for accurate evaluation of the elastic field of dislocation aggregates. We describe the geometry of interacting dislocations of arbitrary 3-D shapes. The stress, interaction energy, interaction forces, and moments on the small defect clusters are then outlined. Results of the model are given next, and compared to existing experimental observations.

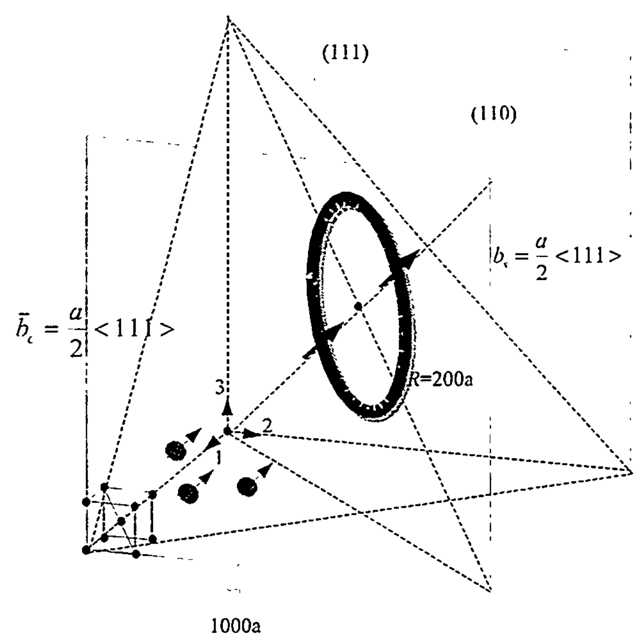

Fig. 5: Geometric arrangement of a proto-typical slip loop and interacting defect clusters in bcc crystals.

Fig. 5 shows a typical geometric representation for interaction between prismatic defect clusters and deformation slip loops on the primary glide plane of bcc crystals. The medium is assumed to be infinite and elastically isotropic, but the cube size of Fig. 5 is taken as (1000 a), where (a) is the lattice parameter. The slip loop is at the center of the cube, and has a diameter of (400 a), while the clusters have a diameter of 3 *nm*. For fcc crystals, the slip loop is assumed to be on the <111>-plane, with Burgers vector $\frac{a}{2}$<110>. The habit plane of defect clusters in fcc is (110), while their Burgers vector is of the $\frac{a}{2}$<110>$-type. Several combinations of loop and cluster Burgers vectors have been studied. Our analysis indicates that are only four independent interaction energy surfaces between slip loops and defect clusters existing in bcc crystals.

A dislocation loop of arbitrary 3-D shape is discretized into parametric segments. For each segment (j), we choose a set of generalized coordinates, and the corresponding shape functions to represent the configuration of the segment. In this case, the generalized coordinates are just the position and tangent vectors, associated with the beginning and end nodes on segment (j). Following Kroner [22] and DeWit \cite [23], the stress field of a dislocation loop is given by a line integral over the dislocation loop. We extend their treatment to the specific case of parametric geometric representation. An efficient numerical integration scheme has been developed to solve for the stress field at any point of the material as a fast summation over quadrature points, as indicated in section 2.2. above. The interaction energy of two dislocation loops over is calculated by equation (3). However, if one of the loops is infinitesimal, the interaction energy can be simplified, as shown by Kroupa [24]. We assume here (the elastic dipole approximation) that the stress tensor of a grown-in dislocation loop is constant over the cross-section of a small point-defect cluster. In case we treat one single vacancy or interstitial atom as a center of dilatation, the interaction energy simplifies to the method of Bullough and Willis [25].

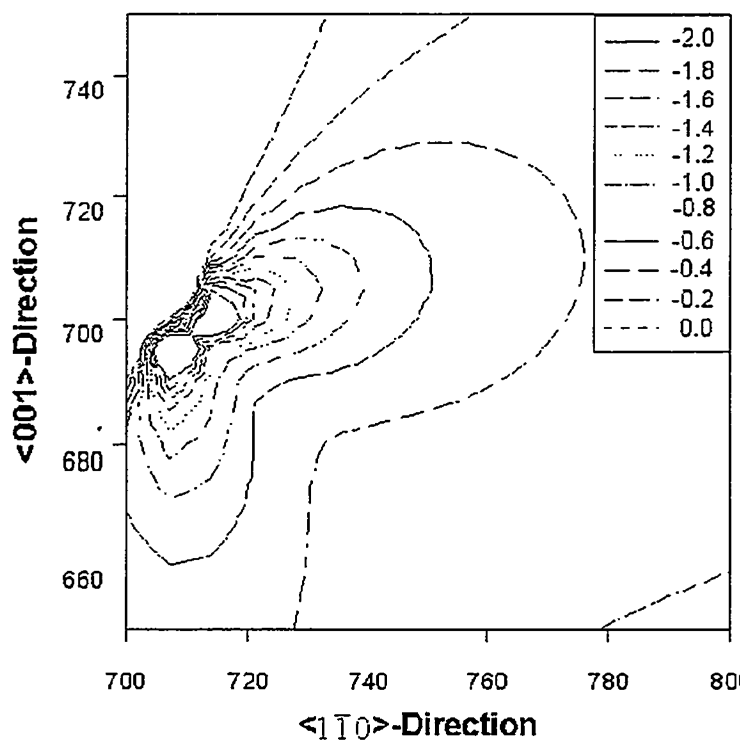

Fig. 6: Interaction Energy Contours (in units of kT) for Cu

Fig. 6 shows a cut in the interaction energy surfaces between interstitial defect clusters of Burgers vector $\frac{a}{2}$<111> and a proto-typical slip loop on the <110>-plane in bcc-Fe at RT. The vectors<001> and <110> define the plane of the contours, and the energy units are in (kT). In this particular orientation of the cluster's Burgers vector, the iso-energy surfaces are anti-symmetric with respect to the $<001>$-direction. The symmetry properties of the iso-energy surfaces depend on the relative orientations of the slip loop and cluster Burgers vectors. Generally, the surface bounding a value of {- *kT*} is considered a trapping surface, and clusters which enter into this zone will oscillate within the surface. A 3-D picture of one of the four trapping zones in bcc at RT is shown in Fig. 7. It is clear that the zone assumes a {\it crescent}-shape, of maximum width around the edge component of the slip loop. The trapping zone size diminishes for mixed character segments on the slip loop, and vanishes at the purely screw component. These results are consistent with experimental observation [20].

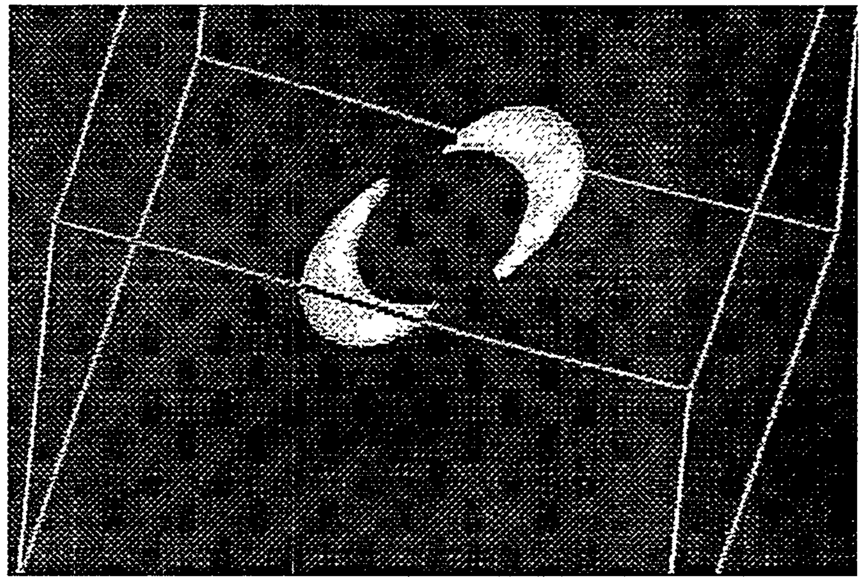

Fig. 7: 3-D picture of one of the four trapping zones in bcc at RT

The total force and its moment on the cluster due to the slip loop can also be computed (see reference 14 for details). They are derived on the basis of the infinitesimal loop approximation of Kroupa [22], where we extended his formulation by introducing geometric parameterization of the loops. As the defect cluster moves closer to the core of the slip loop, the turning moment on its habit plane increases. If the amount of mechanical work of rotation exceeds a critical value (taken as 0.1 *eV/crowdion*, as a result of MD calculations [26], it will change its Burgers vector and habit plane and move to be incorporated into the dislocation core. The mechanical work for cluster rotation is equated to this critical value. The critical surface for cluster rotation and hence subsequent absorption into the dislocation core has been determined. It is found that this *stand-off* zone is about one cluster diameter 3 *nm*. Fig. 7 indicates that the maximum capture zone size (at the edge component) decreases with temperature, and is greater for fcc-Cu as compared to bcc-Fe. Both observations result from an increase in the cluster thermal energy, and a decrease in its modulus with temperature.

In fcc metals of low stacking fault energy, small clusters may exist in the form of faulted Frank loops. However, if the cluster size is large enough, it is energetically more favorable to unfault and become glissile. Another unfaulting mechanism is by assistance of large local stress fields. An *induced surface tension* can change the critical unfaulting radius, depending on whether it adds or subtracts from the stacking fault energy. For a circular Frank loop to unfault, the loop containing the fault and its perfect counterpart is attained by an additional Schokley partial $\frac{a}{6}[1\bar{1}2]$. If clusters are produced very near dislocation cores, it is found that the critical unfauling radius can be as small as 6 *nm* in fcc-Cu (see Ref. 14 for details). This point is illustrated in Fig. 8, where the critical unfaulting radius is plotted against distance along the <001>-direction in Cu. The stress-free unfaulting radius of 22 *nm* is dramatically altered near the core of the slip loop. On the compressive side, the stress field shrinks the critical radius to 6 *nm*, while it expands it significantly on the tensile side.

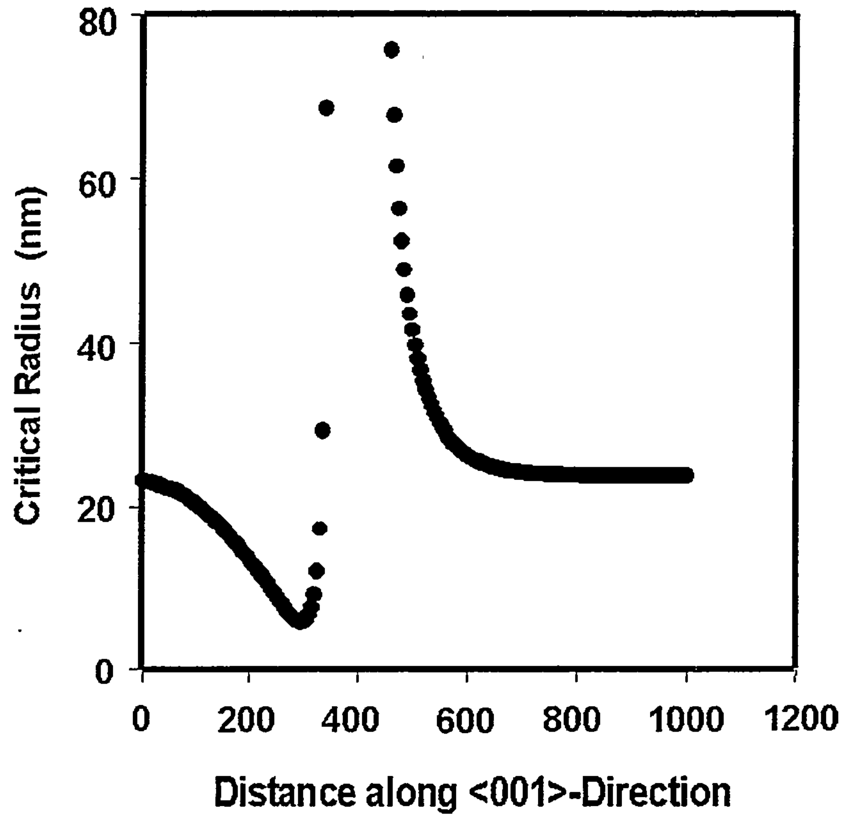

Fig. 8: Dependence of the critical unfaulting cluster radius on its distance from the core of the slip loop

It is concluded that the interaction between nano-scale clusters and slip loops is highly orientation dependent, unlike the situation with defect dilatation centers used in calculations of dislocation [25]. The size of the elastic capture zone is primarily determined by the interaction between the edge components of slip loops, and is not very sensitive to cluster-cluster interaction. Calculated trapping zone sizes are in reasonable agreement with experimental results. On the other hand, clusters that are very near dislocation cores (within 3 *nm*) can be absorbed into the core by rotation of their Burgers vector as a result of unbalanced moments. Clusters that glide on prismatic cylinders are trapped above and below the slip plane in a *crescent* shape, obstructing the motion of edge components. The expansion of loops is thus anisotropic upon further deformation, where screw components will first propagate. It appears that the initiation of a dislocation channel on the slip plane is associated with the stress required for the dislocation to overcome the collective elastic potential of trapped clusters, rather than by cutting through dispersed obstacles on the glide plane in the normal Orowan hardening mechanism.

RECENT RELEVANT PUBLICATIONS & PRESENTATIONS:

Publications:

(1) N.M. Ghoniem and M. Bacaloni, "Finite Segment Method for 3-D Dislocation Dynamics," Eng. Report No. {**UCLA/MATMOD-97-01**}, (1997).
(2) H. Huang, N.M. Ghoniem, T. Diaz de la Rubia, M. Rhee, H. Zbib and J. Hirth, "Stability of dislocation short-range reactions in bcc crystals," *J. Eng. Mat. & Tech.*, in the press, April 1999.
(3) N.M. Ghoniem, "Curved parametric segments for the stress field of 3-D dislocation loops," *J. Eng. Mat. & Tech.,* in the press, April 1999.
(4) N. M. Ghoniem, L. Sun, "A Fast Sum Method for the Elastic Field of 3-D Dislocation Ensembles," *Phys. Rev.*, Submitted.
(5) N.M. Ghoniem, B. N. Singh, L. Z. Sun, and T. Diaz de la Rubia, "Dislocation Decoration with Nano-scale Defect Clusters in Irradiated Metals," Submitted, *J. Nucl. Mater.*

Conference Presentations:

(1) M. Ghoniem, "Three-dimensional Dislocation Dynamics with Parametric Dislocation Segments," Second Euro-Conference on Fracture and Plastic Instabilities in Materials, Thessaloniki, Greece, September 1997.
(2) N.M. Ghoniem, "Principles of 3-D Dislocation Dynamics," 13^{th} US Congress on Applied Mechanics, Gainesville, Florida, June 1998.
(3) N.M. Ghoniem, " Stability of short-range Reactions in 3-D Dislocation Dynamics, " Society of Engineering Science Conference, Pullman, Washington, September 1998.
(4) N.M. Ghoniem, "Simulations of Dislocation Loop Interactions in Single and Multiple Slip," Seventh International Symposium on Plasticity and Its Current Applications, Cancun, Mexico, January 1999.

RESEARCH COLLABORATIONS

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(1) Dr. Tomas Diaz de la Rubia, Lawrence Livermore National laboratory.
(2) Dr. Klaus Schwarz, IBM Watson Research Center.
(3) Professors H. Zbib and John Hirth, Washington State University.
(5) Dr. Bachu N. Singh, RISO Danish National Laboratory.
(5) Dr. Helmut Trainkaus, German Forschungszentrum Julich.

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