ATOMIC-LEVEL INTERACTION OF AN EDGE DISLOCATION WITH LOCALIZED OBSTACLES IN FCC AND BCC METALS - Yu. N. Osetsky (Oak Ridge National Laboratory) and D. J. Bacon (Department of Engineering, The University of Liverpool, UK)

SUMMARY

Interaction between a moving dislocation and localized obstacles determines microstructure-induced hardening. The mechanisms and parameters of such interactions are necessary inputs to large scale dislocation dynamics modelling. We have developed a model to investigate these characteristics at the atomic level for dislocation-obstacle interactions under both static (T=0K) and dynamic (T>0K) conditions. We present results on hardening due to pinning of edge dislocations at obstacles such as voids, coherent precipitates and stacking fault tetrahedra in bcc-iron and fcc-copper at temperatures from 0 to 600K. It is demonstrated that atomic-scale simulation is required to determine the effects of stress, strain rate and temperature and that such effects cannot always be rationalized within continuum theory.

PROGRESS AND STATUS

Introduction

Materials subjected to different treatments may suffer degradation of mechanical properties, e.g. hardening, loss of ductility and plastic instability. In many cases, for example under irradiation, the main reason is formation of localised obstacles to dislocation motion. The typical radiation defects affecting mechanical properties are defect clusters of both vacancy and interstitial types and secondary phase precipitates. Three-dimensional dislocation dynamics (3DDD), as a part of multiscale materials modelling approach, can be used to predict mechanical properties on the basis of the microstructure present but suffers from lack of understanding of short-range interactions between moving dislocations and obstacles, which makes 3DDD approximate in some cases. This gap can be filled using atomic modelling techniques at large enough scale to overlap with the continuum approach, and hence provide mutual validation and parameterization of the mechanisms considered. Another essential advantage of the atomic modelling is the possibility for direct study of thermal effects, which is impossible by other techniques. Recent achievements in atomic-scale modelling of dislocation dynamics [1-5] have demonstrated the importance of this approach. In this paper we review new modelling where a variety of obstacles, such as vacancy voids, stacking fault tetrahedra (SFTs) and coherent precipitates, to the glide of edge dislocations was studied in Cu and Fe over a range of temperatures. We focus mainly on mechanisms of dislocation-obstacle interaction, differences observed for different metals and temperature effects.

Model

The model for simulating the dynamics of the edge dislocation is described in detail in [4]. It is based on the approach of Baskes and Daw [1] using a periodic array of dislocations. An advantage of the model described in [4] is that is allows the stress-strain curve to be obtained under both statics (T=0) and dynamics (T>0) conditions. The results discussed here were obtained from bcc-Fe and fcc-Cu model crystals. Edge dislocations ½<111><112> (Fe) and ½<110><112> (Cu) were simulated in crystallites having from ~2,000,000 to ~8,000,000 mobile atoms over the temperature range from 0 to 600K. Voids or coherent copper-precipitates in Fe and voids or SFTs in Cu were created in the vicinity of the previously relaxed dislocation, the crystal was relaxed again and then loaded by applying strain or stress. Two approaches were used. Static modelling provides information on equilibrium structure under a given strain, which can be compared directly with continuum modelling of dislocation line shape for example. Dynamic modelling by molecular dynamics (MD) allows temperature effects as well as kinetic properties of moving dislocations to be investigated. The stress-strain curve can be obtained with both approaches and its dependence on strain rate studied in dynamics.

Results

Voids and copper precipitates in iron

An example of stress-strain curves obtained for an initially straight edge dislocation overcoming a periodic row of voids (diameter D, spacing L) in Fe at T=0K is presented in Fig. 1. According to [4] the total process of dislocation-void interaction can be divided into four stages of dislocation motion, first before it meets the void, second as it enters the void, third as it glides over the void surface and fourth after it breaks away. These stages can be seen clearly in Fig. 1 for all the voids. The maximum stress for each void size gives the corresponding critical resolved shear stress (CRSS) at which the dislocation breaks away and, provided the strain is increasing, gives further plastic deformation in the fourth stage. Data on CRSS obtained for D=0.7-5nm and L=41-82nm versus harmonic mean $(D^{-1}+L^{-1})^{-1}$ are presented in Fig. 2 (empty circles) together with the results of continuum dislocation dynamics modelling for voids and Orowan particles from [6,7]. It can be seen that atomic scale modelling data are qualitatively similar to the result for voids in the continuum treatment, suggesting that the dependence :

$$\tau_{Void} = \frac{Gb}{2\pi L}\left[\left(D^{-1}+L^{-1}\right)^{-1}+1.52\right] \qquad (1)$$

can be used for estimation of CRSS in higher level continuum modelling of void strengthening.

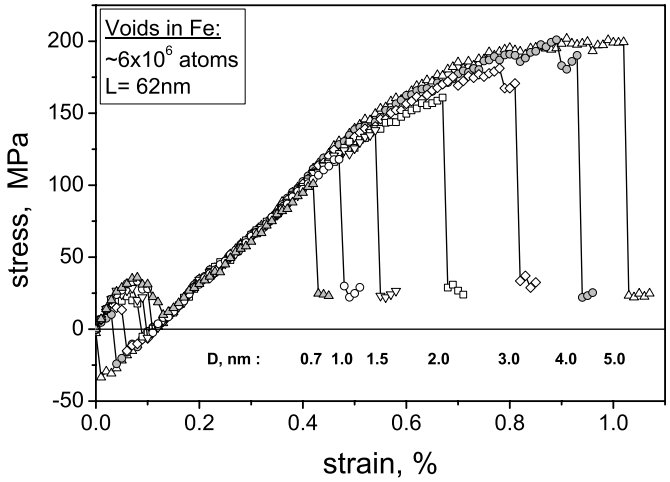

Figure 1. Stress-strain curves obtained for dislocation-void interaction by static modelling in Fe. The number of mobile atoms in the simulated crystal, void spacing, L, and void diameter, D, are indicated.

However, the mechanism of dislocation-void interaction observed by atomic modelling in Fe has some differences from that expected from continuum modelling in [7]. The main difference is that at atomic level this interaction is accompanied by dislocation climb, to an extent that depends on the void size (see e.g. [5]). As a result of this climb, the effective size of a void decreases and it becomes a weaker obstacle for the following dislocation.

MD modelling has demonstrated that stress-strain curves are strongly temperature dependent and the CRSS decreases as T rises. An example of CRSS temperature dependence for the 2nm void is presented in Fig. 3 by open circles. One can see that at T=600K the CRSS drops to 60% of its zero temperature value.

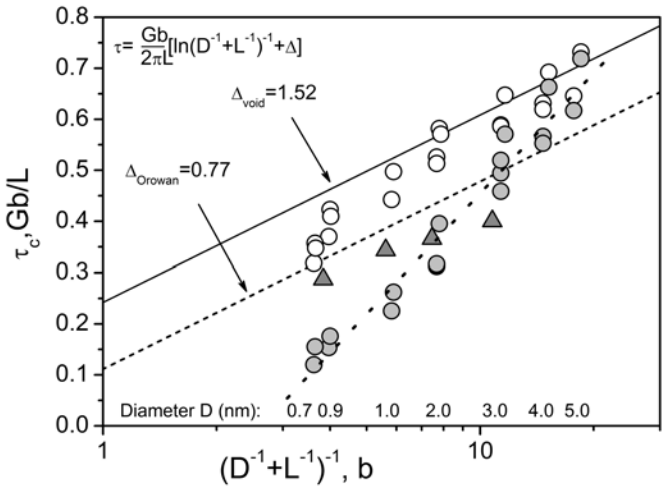

Figure 2. Critical resolved shear stress obtained for different defects as function of harmonic mean of obstacle size D and spacing L. G is the shear modulus and b is the magnitude of the Burgers vector. Open circles – voids in Fe, dark circles – Cu-precipitates in Fe, triangles – voids in Cu. Dashed and solid lines are results obtained in [6,7] by continuum modelling of an edge dislocation passing through a row of Orowan particles and voids respectively, dotted line is interpolation of precipitate results by the dependence $Gb/1.3L[\ln(D^{-1}+L^{-1})^{-1}-0.44]$.

The above data were obtained at strain rate $\dot{\varepsilon}=5\times10^{6}s^{-1}$ at which, for the model size used, the dislocation moves with the steady state velocity $V_d\approx15$m/s, which is a rather low velocity for atomic scale modelling. It was found that the stress at which the dislocation cuts the void depends on its velocity. As an example, consider the following data for the same 2nm void in a crystal under different $\dot{\varepsilon}$. At zero temperature the CRSS was found to be 207MPa and it drops to 179MPa at 100K. However, if simulation at T=100K is made at constant applied stress equal to 100MPa, at which $V_d\approx900$m/s, the dislocation cuts the void. Notice, this kinetic effect depends on temperature and crystal size, e.g. higher stress should be applied at high temperature but lower stress is sufficient for the dislocation to cut the void in a larger crystal (i.e. lower dislocation density). This effect could be explained in terms of kinetic energy associated with a moving dislocation. More detailed discussion and explanation of kinetic effects can be found in [8]. We also note here that a fast dislocation climbs more than a slow one.

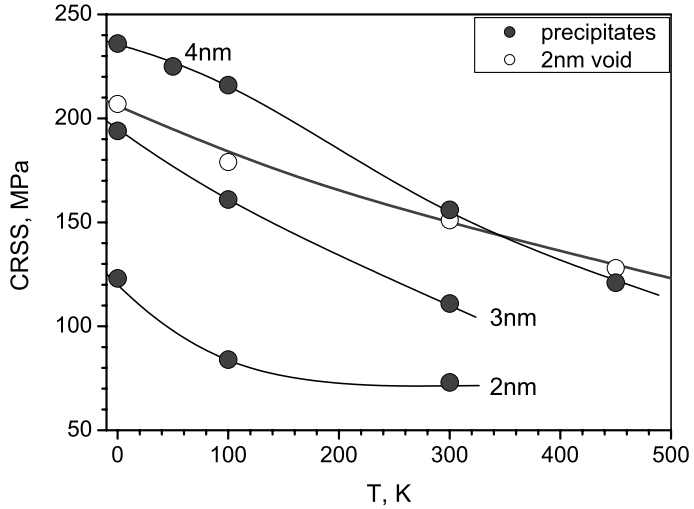

Figure 3. Temperature dependence of the CRSS due to coherent Cu-precipitates of different size and 2nm voids in Fe at applied strain rate $5\times10^{6}s^{-1}$.

Copper-precipitates

Results for the CRSS at zero temperature due to a periodic row of coherent spherical Cu precipitates in Fe are presented in Fig. 2 by dark circles. The dependence of the CRSS on $\ln(D^{-1}+L^{-1})^{-1}$ can be approximated by a linear function (indicated by dotted line) with a slope significantly steeper than that for voids, i.e. ~1/1.3 compared with $1/2\pi$. However, the mechanism of dislocation-precipitate interaction depends on precipitate size. Thus small precipitates, D<3nm, suffer simple shear, whereas in the case of large precipitates partial transformation towards the more stable fcc structure inside precipitates and dislocation climb are observed.

It is common to attempt to describe precipitate hardening on the basis of the constant line tension approximation. For this the critical angle, φ, between dislocation segments as they break away from a precipitate are required, e.g. it is estimated from the Cu-Fe modulus difference in [9]. It is obtained accurately in our modelling and is >0 for $D \leq 3$nm and equal to zero for larger precipitates. This angle was used to estimate the corresponding stress in the line-tension treatment, and gave values up to twice the true value estimated in atomic-scale modelling (see [5]). In other words, in order to give correct stresses, the line-tension model has to use incorrect angles.

The temperature dependence of the CRSS due to Cu precipitates in Fe under a constant applied strain rate of $5\text{x}10^{6}\text{s}^{-1}$ is presented in Fig. 3 by full circles. The dependence is strong relative to that of voids. Thus, a row of 2nm voids is weaker at T=0K than 4nm precipitates, they have similar strength at T=300K and at higher temperature the voids are stronger obstacles. Another effect observed for precipitates is an increase of dislocation climb: the higher the temperature the more vacancies are left inside a precipitate.

Voids and SFTs in copper

Examples of stress-strain curves for dislocation-void interaction at T=0K in copper are presented in Fig. 4. It can be seen that the dependences are qualitatively different from those obtained for Fe (see Fig. 1). The explanation lies in the difference of the dislocation core structure in the two metals, for unlike that in Fe, the dislocation in Cu is dissociated into two Shockley partials linked by a stacking fault ribbon of width $\approx$13a for the edge dislocation. As a result each partial dislocation interacts with an obstacle individually. The first stress peak at yield in Fig. 4 for voids of each size corresponds to the stress when the leading partial breaks away, whereas the second peak is related to the same process for the trailing dislocation. The corresponding partial dislocation line shapes for D=2nm are presented in Fig. 5. It is interesting to note that the relative height of the two stress peaks in Fig. 4 depends on void size. Thus, when the dislocation cuts small voids the stress at the first peak is lower than that at the second, whereas for the

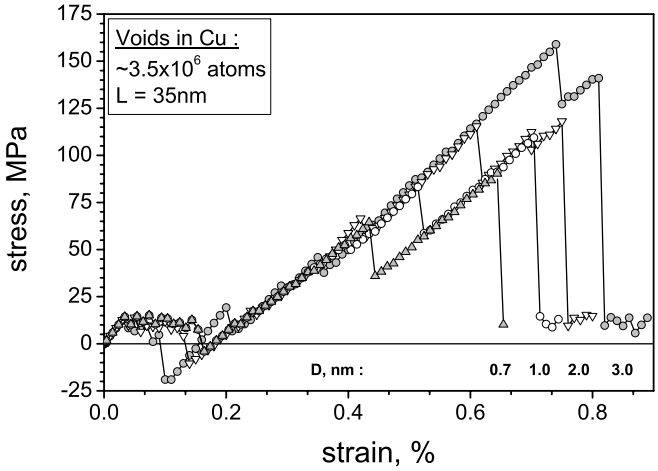

Figure 4. Stress-strain dependence for dislocation-void interaction in Cu at T=0K.

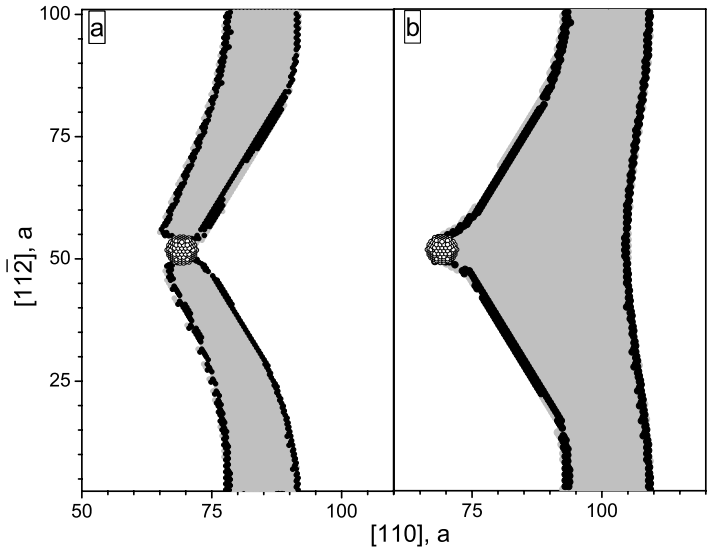

Figure 5. Critical shape of partial dislocations interacting with a 2nm void in Cu at T=0K: (a) leading partial at shear stress 115MPa; (b) trailing partial at 118MPa. The core region of partials is shown by black symbols, the stacking fault is grey and the void surface atoms are indicated by hollow spheres.

largest void studied (D=3nm) the leading partial breaks away at maximum stress. This size-dependent effect is presumably related to the pulling force the leading partial can provide for the trailing one if the area of the stacking fault increases significantly at such a high stress. The assistance of the leading partial may also explain the overall weaker strengthening due to voids in Cu in comparison with Fe, as seen in Fig. 2. Another feature of the dislocation-void interaction mechanism in Cu is the absence of climb and defect absorption, for only pure shear of voids has been found in all the cases studied.

Temperature effects have been studied in dynamic modelling of interaction of a gliding dislocation with 2nm (369 vacancies) and 3nm (1205 vacancies) voids and 2.5nm (45 vacancies) and 3.0nm (78 vacancies) SFTs in Cu. A significant drop in CRSS occurs when temperature is increased from 0 to 100K. Further increase of temperature gives only a weak additional decrease of CRSS, as shown by the data in Fig. 6. Note that the 2.5nm SFT demonstrates very similar strengthening to that of a 2nm void, despite the fact that it contains only 45 vacancies against 369 in the void. Moreover, the 2.5 nm SFT is a stronger obstacle than the 3.0nm one. A detailed analysis of dislocation-SFT interaction sheds light on this paradox. The data presented in Fig. 6 were obtained when the dislocation glide plain cuts an SFT through the centre of mass. In this geometry the glide plane is closer to the parallel face for a smaller SFT than a larger one. By varying the position of the glide plane, we have found that maximum strengthening occurs when a dislocation glide plain coincides with the stacking fault of one of the faces.

The larger the distance between the face and the glide plane, the lower the CRSS. Moreover, when the larger SFT (3nm) is cut though the centre of mass at all temperatures above T=10K it recovers its regular structure via a thermally-activated propagation of a jog on the stair-rod partial dislocations of its edges. This recovery does not occur for the smaller SFT whose regular structure remained disturbed after being cut by the dislocation. Similar damage of a small SFT by a dissociated dislocation at T=0K was observed earlier [10].

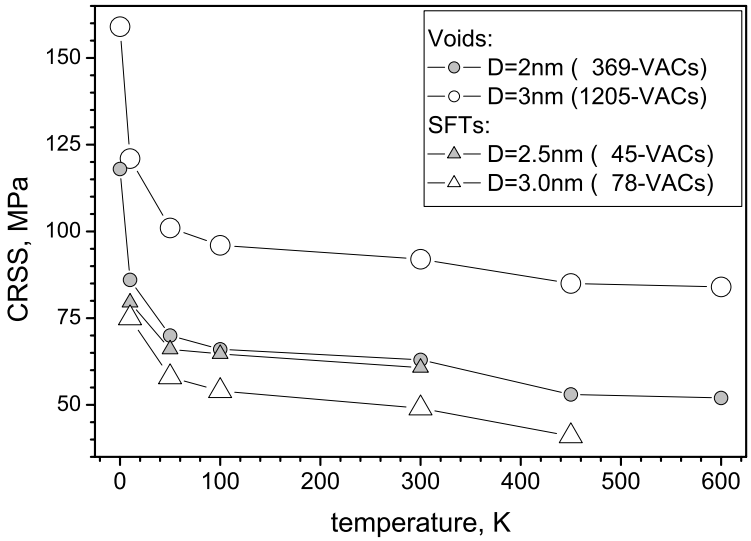

Figure 6. Temperature dependence of the CRSS of voids and SFTs in Cu obtained by molecular dynamics modelling at strain rate $5x10^6s^{-1}$. Void diameter, SFT size and the corresponding number of vacancies is indicated.

Summary

Atomic-scale modelling with a choice of static (T=0K) and dynamic (T>0K) conditions, together with different types of crystal loading, i.e. applied strain increment or strain rate or applied stress, allows a wide range of features of dislocation-obstacle interactions to be studied. Static modelling reveals many general features which can be treated and understood within continuum dislocation theory. An example is presented in Fig. 2 where stress values for voids and precipitates in Fe are close to the linear dependence of CRSS on logarithm of harmonic mean of obstacle size and spacing found earlier in simulations based on elasticity theory [6,7]. The data for voids in Cu can be described as a linear dependence in principle, but due to the dissociated character of the dislocation the mechanism is more complicated and void-size dependent: strengthening by small voids is controlled by breakaway of the trailing partial whereas that of large voids is controlled by the leading partial. Dissociation also reduces the total strength of these obstacles. Static modelling can also provide information on dislocation line shape in equilibrium at different stress levels (see e.g. [5]), and this can be used for fitting parameters required in continuum dislocation dynamics models. One of the conclusions on dislocation line shape revealed here and in [5] is that the simple constant line tension model widely used in estimations of CRSS (e.g. for hardening due to Cu precipitates in Fe [9]) provides an incorrect relationship between applied stress and line shape.

Atomic-scale details of dislocation-obstacle interactions depend strongly on dislocation core structure, as demonstrated here by comparison of Fe and Cu. The low stacking fault energy in Cu causes wide separation of the partial dislocations and leads to absence of dislocation climb in interactions with obstacles of vacancy type. The perfect edge dislocation in Fe, in contrast, may climb and absorb defects in all the cases considered.

The dynamic simulations demonstrate a strong temperature effect in the stress-strain characteristics for all the obstacles studied. The nature of this is not yet fully understood. Based on the results presented, we can conclude that the temperature enhancement mechanisms may be different for different obstacles,

e.g. stronger for coherent precipitates than voids in Fe (see Fig. 3), and for different metals, e.g. the temperature dependence of the CRSS for voids is different in Fe and Cu (see Figs. 3 and 6).

Kinetic effects in dislocation-obstacle interactions have been observed in all the cases treated and this seems to be important for explanation of plastic instability and creation of cleared channels in irradiated metals [11]. In fact, we have demonstrated that a dislocation moving at high speed can cut and breakaway from an obstacle at a stress significantly lower than the CRSS. Moreover, the change in structure of the obstacle due to the fast dislocation is more significant. More studies are necessary to understand these effects and to reveal mechanisms suitable for incorporation in higher level dislocation dynamics applications.

ACKNOWLEDGMENT

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