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Dislocation dynamics and multiplication via atomistic simulations

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Abstract: Molecular Dynamics simulations of edge dislocation mobility under stress in ordered L1₂ Ni₃Al have been performed between 10K and 1000K, and at applied shear stresses ranging from 0.01 to 0.08 C₄₄. In this way it has been possible to determine the Peierls stress and mobility parameters as a function of stress and temperature. $\langle 001 \rangle \{ 100 \}$ edge dislocations were studied, which split into closely spaced partials under stress. Under all levels of applied stress (and at lower temperatures) the initial partial dislocations would intermittently stop moving and recombine, then dissociate and move again. In all cases the dislocations exhibited a soliton-like behavior: infinite acceleration at the onset of movement, and further movement at a steady velocity (which was only weakly dependent on stress) on the order of 25% of the acoustic shear velocity. Non-classical, highly non-linear behavior was observed indicating the probability that a soliton picture of dislocation motion is more appropriate than the classical, "massive string" model that is traditionally used. Furthermore, as both the temperature and the stress were increased, dislocation multiplication became increasingly frequent, ultimately resulting in a spontaneous amorphisation transition which has signs of being a percolation process.

1. Introduction

The minimum stress to initiate and maintain the motion of dislocations (the Peierls stress), and the mobility of dislocations (as measured by their steady state velocity under stress) are quantities that frequently enter equations predicting different properties of materials, yet they are numbers that are extremely difficult to measure directly by experimental means. In addition, theoretical estimates of these quantities heretofore have depended on the inherent approximations of linear continuum elasticity theory which are known to seriously fail in describing the details of the dislocation core, and consequently err in predicting properties dependent on the core structure, such as the Peierls stress. As a result, only a very few crude estimates are available in the experimental or theoretical literature for these numbers at this writing¹.

Furthermore, it is now generally agreed^{2,3} that the actual atomistic structure of dislocations may produce very significant effects in the plasticity of crystalline materials, with the possible exception of the most ductile fcc metals where it is believed that the Peierls stress is so low that thermal fluctuations effectively wash out any significance of the core structure⁴. The symptoms which generally signal the importance of the core structure in material plasticity are the appearance of at least one of the following: (a) a strong temperature dependence of the flow stress, (b) a crystallographic orientation dependence of the critical resolved shear stress (crss), (c) different, or multiple, slip systems operating at different temperatures.

Another issue of considerable current interest and debate revolves around the question of whether the core configuration of a static dislocation is a good representation of the same dislocation in motion. A related question is whether the core configuration at absolute zero (0 K) remains stable at finite temperatures, or whether important configurational transformations might occur as the temperature is increased and be a significant contributing factor to the well known ductile-brittle transition that occurs in a wide variety of materials? Virtually all of the current predictions regarding the relative mobility of different dislocations at finite temperatures are based on static 0 K core configuration calculations and so may require substantial revision.

The "classical" theory of dislocation dynamics¹ based on continuum mechanics concepts asserts that the steady state velocity (V_s) of a dislocation under an applied resolved shear stress (σ) will be:

$$V_s = b \sigma / B \quad (1)$$

where b is the Burger's vector of the dislocation, and B is a material dependent damping coefficient. The magnitude of B is postulated to be governed by a combination of phonon damping, electron damping and "flutter radiation" contributions, with the phonon damping thought to be the dominant mechanism at temperatures above about 10% of the Debye temperature. Efforts have been made to calculate the interaction of the moving non-linear displacement field of a dislocation core with the linear elastic vibrational waves (phonons) in order to estimate the phonon contribution to B . This is an extremely difficult calculation, requiring many approximations which leave the validity of the final result in some question. The general trend of such calculations however is to indicate that B should increase approximately linearly with absolute temperature.

An additional prediction of the classical theory is that dislocations possess inertia (arising from the strain energy field carried along by the dislocation), so that when the external stress is first applied there will initially be an acceleration stage which proceeds until the terminal velocity given in Eq. (1) is reached. Thus the velocity-time characteristics are projected to be of the form:

$$V(t) = V_s [1 - \exp(-t/T)] \quad (2)$$

where t is the time, and T is a relaxation time proportional to the "mass" of the dislocation.

Although some attempts to experimentally determine the dynamics of individual dislocations have been made, this is in principle a very difficult measurement. Almost any sample investigated will have a rather large number of different kinds of dislocations, which will interact in varying ways with an unknown distribution of crystalline defects and pinning points. One of the most frequently cited measurements is

that of Johnston and Gilman⁵ in LiF, where they used the technique of monitoring the change of the surface etch pit patterns to deduce how far the dislocations had moved when under stress. These measurements showed quite a strong dependence of velocity on stress. However, subsequent measurements by Baker⁶ on the same material using an ultrasonic internal friction technique found a very different velocity versus stress relationship, which he ascribed to the average velocity of dislocations as they bowed out between fixed pinning points on successive stress cycles. He assumed that at the low applied stress levels used in the ultrasonic measurements, no dislocations broke free from their anchors, and that the population of dislocations contributing were the number that could be seen from etch pit determinations. The inferred velocities could change by orders of magnitude if either of these assumptions in his analysis were wrong. However, the fact that dislocations were obviously moving at stresses an order of magnitude or more below those used in the Johnston-Gilman study does strongly suggest that the latter were not measuring the instantaneous dislocation velocities between pinning points, but primarily some average velocity of the pinning points themselves. One must conclude that even in this much cited system, the instantaneous velocity of dislocations moving at stresses in excess of the Peierls stress is not known, even to within several orders of magnitude, nor can the velocity versus stress characteristic be given any measure of validity.

More direct visual measurements of dislocation dynamics have been made by Louchet in Si⁷ and Ge⁸ by in situ straining in a high-voltage electron microscope. In the case of Si, he was able to obtain the velocity versus stress (and temperature) characteristic, and his Arrhenius plot of the dislocation velocity versus inverse temperature gave an activation energy of about 1.9 eV, which he asserted could be associated with the activation energy for double kink nucleation (although such double kinks were not resolvable in the microscope images). The model for dislocation motion at these stress levels was then proposed in terms of a kink nucleation limited process requiring thermal activation of a double kink, followed by rapid spreading of same, thus producing an advance of the dislocation by 1 b. Each advance of the dislocation would require repeating this basic nucleation process. The velocities measured were on the order of 10^{-6} cm/s and clearly in the sub-Peierls stress regime, given the importance of thermal activation and the very low resulting velocities. Thus, one still does not have any sort of reliable measurement of the dynamic characteristics of individual dislocations in the super-Peierls stress regime, a regime which is bound to be of great importance in the understanding of dislocation behavior in metals (where Peierls stresses are thought to be very low) or near crack tips in any material (where stresses can become very high).

The Peierls stress itself has only been very crudely inferred from scattered measurements with rough estimates {ref. 1, p. 241} being in the range of about 1% of the shear elastic constant for covalently bonded crystals to 0.01% of the shear constant for close packed metals, with bcc metals and ordered alloys lying somewhere in between. There appears to be no direct experimental method of obtaining this quantity with any degree of accuracy, despite its considerable importance as a fundamental parameter in theories of dislocation motion. In addition, there is virtually no experimental information bearing on the question of whether the Peierls stress increases or decreases if the lattice is put under compression, nor can the continuum mechanics theories address this problem since the answer depends very sensitively on the anharmonic nature of the atomic interactions.

2. Computer Simulations

A number of computer simulations have been carried out over the past twenty five years or so to investigate different aspects of dislocation dynamics. Reviews of the field have appeared periodically^{9,10,11} and two excellent reviews including this topic have appeared lately^{2,3}. Until fairly recently simulations were carried out on small arrays of a few hundred atoms, were often two dimensional, and employed simple pair potentials. Even so, some very significant advances have been achieved with these limited means. For instance, the essential correctness of Hirsch's hypothesis¹² that the $1/2\langle 111 \rangle$ screw dislocation core in bcc metals would not be confined to the slip plane, but extend into several $\{110\}$ planes, thereby causing it to be sessile was confirmed (at least at 0 K) by a series of static relaxation

simulations^{13,14,15}. This result also appeared to be relatively insensitive to the specific details of the interatomic potential used¹⁶, which added additional confidence to the demonstration, and provided a reasonable basis for understanding the large Peierls stresses, and complex orientation dependences of the critical resolved shear stress (crss) in bcc metals. Although one may conjecture that this complex core structure may also provide the key to understanding the strong temperature dependence of the flow stress observed in bcc metals, simulations at temperatures above absolute zero largely remain to be done.

More recently, the ability to accurately simulate specific metals and alloy systems has been very significantly improved by the advent of the Embedded Atom Method¹⁷ (or the very similar Finnis-Sinclair method¹⁸). These are semi-empirical approaches, incorporating some of the fundamental theoretical concepts of first principles quantum mechanical calculations, which can be used to construct interatomic potentials (including volume dependent many body interactions), based upon experimental (and other) data of a given binary alloy system. Then by using a supercomputer equipped with a Molecular Dynamics program to simulate the motion of an atomic array interacting according to the fitted EAM potentials, many different details of atomistic behavior can be observed and predicted. Considerable success has been achieved in predicting (via simulation) such properties as bulk and surface phonons, surface structure, impurity segregation, phase stability, liquid structure, grain boundary structure and thermal expansion^{19,20,21}. As a result, it should now be possible to simulate the motion of individual dislocations in specific metallic systems and derive reasonably accurate dynamic properties as a function of temperature and stress. Perhaps the most extensive "modern" study of this kind was performed via Molecular Dynamics simulations by Daw, Baskes and co-workers^{19,21} on $\langle 1-10 \rangle (111)$ edge dislocations in pure fcc Ni and in H and He doped Ni. They used arrays of about 700 atoms in a slab approximately $75 \times 25 \times 4 \text{ \AA}$ with periodic boundary conditions in all directions, except that normal to the (111) glide plane. The edge dislocation was found to split into Shockley partials separated by about $12-15 \text{ \AA}$, and when a sufficient external shear stress was applied to the top and bottom (111) planes, the partials would move at an ever increasing velocity until some limit was reached depending upon the stress level and temperature. They found that by using four adjustable parameters these dynamic characteristics could be well described by the classic equations of dislocation motion (including phonon damping and relativistic effects), i. e.:

$$\frac{d}{dt} \frac{mv}{\sqrt{1-(v/c)^2}} = (\sigma - \sigma_0)b - \frac{3\alpha kT}{10b^2} \frac{(v/c)}{\sqrt{1-(v/c)^2}} \quad (3a)$$

or from Eq. (3a), when the left hand side is zero, (and with the variable replacement: $\omega \equiv 3\alpha kT / 10b^3$) one has for the steady state velocity, V_s :

$$V_s = \frac{c(\sigma - \sigma_0)}{\sqrt{\omega^2 + (\sigma - \sigma_0)^2}} \quad (3b)$$

where m is the dislocation mass per unit length, c is a limiting velocity, σ is the applied stress, σ_0 is the friction stress (or Peierls stress), b is the magnitude of the Burger's vector of the dislocation, and α is a dimensionless constant. b and σ were known and the other four parameters were fit to the simulation results. They reported the values, $c = 2000 \text{ m/s}$, $m = 0.2 \text{ atoms/b}$, $\alpha = 0.98$, and $\sigma_0 = 4 \text{ MPa}$, which they argued were sensible numbers although only c (the transverse sound velocity) is known with any accuracy experimentally. That number is about 3340 m/s in a macroscopic sample, but would be reduced to about 1840 m/s in the very small sample size used in the simulations, thus achieving reasonable agreement. We were thus encouraged to follow this same approach, but to use larger arrays in order to minimize the possible size and boundary effects.

Our first results have been dramatically different from those to be expected from classical dislocation theory and suggest an entirely different mechanism for dislocation motion, at least in some stress and temperature regimes, as we shall detail in the next section.

3. First Simulation Results

A limited set of Molecular Dynamics simulations of edge dislocations in $L1_2$ Ni_3Al using Voter-Chen EAM potentials²² has been carried out. The edge dislocation $\mathbf{b} = \mathbf{a}_0\langle 100 \rangle$ moving on a $\{001\}$ glide plane was studied between the temperatures of 10 K and 1000 K with levels of applied shear stress ranging from 0.01 to 0.08 in units of C_{44} (where $C_{44} = 131$ GPa). The $\mathbf{a}_0\langle 100 \rangle$ type of edge dislocation, although not seen experimentally in Ni_3Al , in the simulations formed a stable dislocation core only slightly spread out along the glide plane with an easily recognizable structure. It therefore seemed to represent a good example of the Peierls model of a dislocation (in that the core was relatively compact and essentially confined to the glide plane), and so was used as a "starter case" to simplify the analysis and to test pattern recognition routines. The equilibrated structure projected along the dislocation line is shown in Fig. 1, and consisted of 6,720 atoms ($24 \times 14 \times 5$ unit cells). The array extended 5 unit cell distances ($5a_0$, where $a_0 = 3.57$ Å) along the dislocation line before periodic boundary conditions were applied in that direction. Free surface conditions were used in the two other orthonormal directions, thereby permitting a natural bending of the crystal. We felt this was a better choice than imposing periodic boundary conditions on the end surfaces, which would have the effect of warping the array back to an approximately straight configuration and lead to very large artificial tensile and compressive stresses in the vicinity of the dislocation core.

Fig. 1 - Relaxed stress free configuration of Ni_3Al edge dislocation with $\mathbf{b} = \mathbf{a}_0[100]$ on (001) glide plane after 12,000 time steps (300 atomic vibration periods) of thermal equilibration at $T = 10$ K. Solid circles = Ni atoms; open circles = Al atoms. Without stress the core remains undissociated.

After the array was fully equilibrated (about 5000 time steps, each being 4.0×10^{-16} s, and the total being equivalent to about 100 atomic vibrational periods) shear stresses were applied instantaneously on

the four outer free surfaces by the application of tangential atomic forces to the two outer atomic layers in such a manner that there was zero net torque on the array. The applied stress was held constant for the duration of the run, and a "temperature clamp" which rescaled the velocities of all atoms at each step by $1/33$ of the value necessary to reach the target temperature exactly was used to keep the temperature approximately constant, without introducing noticeable transients in the vibration spectrum. Also, it was found to be important to allow the array to adjust to its correct equilibrium lattice parameter at each temperature before applying the stress. It was found that a stress of about 1,310 MPa (or 1% of C_{44}) was necessary to get the dislocation to move at all, so this would appear to be about the magnitude of the Peierls stress for a straight edge dislocation of this type in Ni_3Al .

Immediately after the application of the stress no motion occurred for about 600 time steps, which corresponds almost exactly with the time necessary for a shear wave initiated at the surface to reach the position of the dislocation core. A plot of the displacement of both the leading and trailing partial as a function of time thereafter (see Fig. 2) shows essentially no sign of an acceleration stage, indicating that the dislocation is behaving as a massless object. At the lower stress levels, the partial dislocations would occasionally recombine into a compact core which is apparently more sessile and causes a temporary interruption of forward motion, as seen in Fig. 2. After a certain time the core would redissociate and the partials would move on as before. This "interruption time" was subtracted out in the calculation of the dislocation velocities. The dislocation was only observed to separate into partials while being driven under stress, but this separation is never more than about $1 a_0$ (see Fig. 3).

Fig. 2 - $[100](001)$ edge dislocation mobilities in Ni_3Al at $T = 10$ K versus applied shear stress.

Fig. 3 - $[100](001)$ glissile edge dislocation in Ni_3Al under stress showing dissociation of the core structure into partials. $T = 1000 \text{ K}$ and $\sigma = 1\%$ of C_{44} .

The dislocation dynamics data for temperatures at 300 K and above was difficult to analyse because in the higher stress ranges multiple dislocation generation often occurred, emanating from the original core and/or glide plane. An example of this phenomenon is shown in Fig. 4. An even more dramatic manifestation of dislocation multiplication was the appearance (at temperatures of 600 K and above) of an amorphisation transition, as shown in Fig. 5. We do not offer here any theoretical explanation for either of these phenomena, other than to point out that very high strain rates, easily in the realm of shock loading, are being used in the simulations. However, these complications did not arise at 10 K or 100 K, and the data from these temperatures is displayed in Fig. 6.

Fig. 4 - Multiple nucleation of dislocations from the original (001) glide plane onto $\{110\}$ glide planes. MD time step = 9,900; $T = 300 \text{ K}$; $\sigma = 8\%$ of C_{44} .

Fig. 5 - Partial amorphisation of the array as a result of copious dislocation generation. MD time step = 13,500; $T = 600$ K; $\sigma = 8\%$ of C_{44} .

Fig. 6 - Velocities of the partials of a Ni_3Al $\mathbf{b}=\mathbf{a}[100]$ edge dislocation gliding on a (001) plane versus stress at $T = 10$ K and 100 K. The partials, with $\mathbf{b} = (\mathbf{a}/2)[110]$, remain within a unit cell distance of each other during the simulation.

Several surprising features appear in these low temperature simulations of individual straight dislocations in Ni_3Al . First, the velocity at 10 K shows only a very weak dependence on stress. A previous study on edge dislocation motion in B2 NiAl , which however had the complicating interference of a martensitic transformation, also found quite similar phenomena²³. Second, for a given stress level (in the higher stress range) the velocity at 100 K is greater than at 10 K, contrary to expectations from classical damping concepts. Third, there is a lower velocity regime which apparently is forbidden, and attempts to fit the data to the classical Eq. 3b (the solid lines in Fig. 6), lead to absurd parameter values, such as negative numbers for the Peierls stress.

4. Conclusions

Neither the stress nor temperature dependence of dislocation velocities predicted by the standard continuum mechanics theories of dislocation dynamics are observed in molecular dynamics simulations of edge dislocation motion in Ni_3Al . Furthermore, in the simulations, the dislocations reach their terminal velocities virtually instantaneously, violating the classical concept that dislocations should act as if they have a mass. All of these phenomena together suggest that the motion of straight edge dislocations may be more satisfactorily modelled with soliton concepts^{24,25,26}. At the very least, these initial results are quite provocative and we believe are worth exploring much more extensively, as we propose to do in the near future.

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