

Cooperative generation of dislocation loops and the brittle-to-ductile transition

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Abstract

A mechanism of cooperative generation of dislocation loops above a critical temperature in loaded solids is described. We model the massive dislocation activity which commences near the crack tip at the brittle-to-ductile transition temperature in terms of this mechanism and show that it can explain the main features of the transition. © 1997 Elsevier Science S.A.

Keywords: Cooperative dislocation generation; Brittle-to-ductile transition; Dislocation loops

1. Introduction

The brittle-to-ductile transition (BDT) is ubiquitous in crystalline materials [1] and yet, the underlying mechanism is not well understood. Two characteristic features of the BDT are: (i) The dramatic increase of the fracture toughness in a narrow temperature interval around the brittle-to-ductile transition temperature (BDTT) accompanied by a sudden onset of extensive plasticity leading to crack blunting and arrest; and (ii) the strain-rate dependence of the BDTT and the variation of dislocation velocity with temperature are both of the Arrhenius type with similar activation energies. These distinct features have been the focus of numerous models of the BDT [2–4]. An issue that remains unresolved is how very extensive dislocation generation commences suddenly in the region near the crack tip above a certain temperature.

We have recently proposed a model which describes how massive dislocation activity can take place above a certain temperature in a loaded solid and give rise to extensive plasticity [5,6]. In two dimensions (2D), this occurs by a thermally-driven, stress-assisted cooperative dissociation of many atomic-size dislocation dipoles. In this paper, we describe how a similar mechanism operates in three dimensions (3D) leading to the cooperative

generation of dislocation loops and discuss its application to the BDT. We show that the density of glissile dislocation loops can increase by many orders of magnitude in a small temperature interval well below the melting temperature when the applied loads are of the order of $\mu_0/100$, where μ_0 is the shear modulus.

2. Cooperative process of dislocation generation

Dislocation loops of atomic sizes have finite formation energies in the range 0.1–2.0 eV in most materials and can therefore form by spontaneous fluctuations at finite temperatures. The density of loops of radius r at a temperature T is proportional to the Boltzmann factor, $\exp[-H(r)/k_B T]$, where $H(r)$ is the formation enthalpy of the loop and k_B is the Boltzmann constant. Under applied loads, the formation enthalpy is reduced by an amount equal to the work done by the external stresses. Consequently, the density of loops at a given temperature is higher in a loaded solid. When the applied stress is below the ideal shear strength of the material, the activation energy needed to expand an individual dislocation loop to the critical radius beyond which the dislocation can glide freely, is generally very high, of the order of 10 eV or more. Thus, even at high temperatures, thermally-activated generation of glissile dislocations is considered improbable. The cooperative instability process describes an alternative mechanism

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by which many dislocation loops of sub-critical sizes can undergo unstable expansion in a collective manner at finite temperatures.

This process is facilitated by two distinct factors which enable the formation of increasing numbers of sub-critical loops as the temperature increases for a given value of the applied stress. First, there is a direct exponential increase of the density of loops with temperature due to the Boltzmann probability factor. The second, and more important reason, is the lowering of the total self-energy of the loops as more sub-critical loops form in the solid. This was first demonstrated by Kosterlitz and Thouless (K-T) in the context of phase transitions in a 2D solid [7]. It is based on the fact that the energy of a dislocation loop or dipole is determined not only by the elastic properties of the medium defined in the absence of dislocations but is indirectly influenced by the presence of all other dislocation loops or dipoles. For example, when a dislocation loop or a dipole is formed in a medium containing other loops or dipoles, a rearrangement of the existing loops and dipoles takes place by contraction or expansion under the influence of the stress field of the newly formed loop or dipole. Under applied loads, there is a net plastic strain associated with such rearrangement. This additional plastic strain induces a decrease of the 'effective moduli' relating stresses and total strains in the medium. The self energy of the newly formed loop or dipole is proportional to the effective moduli and is therefore lower than the energy of an isolated loop or dipole which is proportional to the elastic moduli.

At low temperatures, the difference between the effective and elastic moduli is very small and the self-energy of N dislocation loops differs only marginally from the sum of the self-energies of individual loops. At a constant applied load, as the temperature increases, the probability of formation of dislocation loops increases, which in turn, increases the plastic strain in the medium. Concomitantly, the lowering of the self-energy (and formation enthalpy) increases the probability of forming more dislocation loops. This further increases the plastic strain and a positive or 'cooperative' feedback is set up between the formation of additional sub-critical dislocation loops and the continued reduction of the effective moduli.

The entropy of the dislocation loops is also enhanced owing to the increase of the density of loops. Hence, the free energy of the system of many dislocation loops decreases with increasing temperature. Ultimately, when the free energy becomes comparable to the thermal energy, there is a significant probability of many loops attaining the critical radius needed for collective unstable expansion. This critical size is substantially smaller than the critical radius of an iso-

lated dislocation loop under similar applied loads. There is a dramatic increase of the density of glissile loops in this temperatures range. The plastic strain in the medium increases rapidly due to the macroscopic glide of dislocations and, consequently, the effective moduli converge to zero. When the free energy of many loops becomes negative it becomes possible for even the smallest dislocation loops of atomic sizes to expand and glide under the applied loads. The temperature above which the collective expansion occurs is well below the melting temperature when the applied stresses are large and is just below the melting temperature when the solid is not loaded [7,8]. Thus, the behavior of many small dislocation loops at finite temperatures in a loaded solid differs significantly from that of a single dislocation loop under similar conditions.

The collective behavior of many dislocation loops at a temperature T in a 3D loaded solid can be formulated using statistical mechanics and linear elastic description of dislocations; the procedure is analogous to that in 2D [5]. The set of 'renormalization group' equations describing the cooperative generation of many loops is

$$\begin{aligned}\frac{dh}{d\ell} &= h - h^2 y \pi^3 / 96; \\ \frac{dy}{d\ell} &= [6 - h(\ell + c + 1)/4 + 2\sigma b \pi r^2 \beta] y\end{aligned}\quad (1)$$

where

$$\begin{aligned}\ell &= \ln(r/r_0); \quad y(\ell) = (r/r_0)^6 \exp((-U(r) + \sigma b \pi r^2) \beta); \\ h(\ell) &= K_0 r / r_0 \varepsilon(r) \\ K_0 &= \beta \mu_0 (2 - \nu_0) b^2 r_0 / (1 - \nu_0); \\ \beta U(r) &= \int_{r_0}^r (K_0 / 4 r_0 \varepsilon(r')) \left\{ \ln\left(\frac{r'}{r_0}\right) + c + 1 \right\} dr' \\ \varepsilon &= 1 + (\mu_d^{-1} + B_d^{-1}) / (\mu_0^{-1} + B_0^{-1})\end{aligned}\quad (2)$$

Here $\{\mu_0^{-1}, B_0^{-1}\}$, and $\{\mu_d^{-1}, B_d^{-1}\}$ are the shear and bulk components of the elastic and plastic compliance tensors, respectively; ν_0 , the Poisson's ratio; b the Burgers vector; r_0 , the elastic inner cut off radius; $\beta = (k_B T)^{-1}$; c , a constant that defines the core energy per unit length of the loop; and σ , the shear stress in the slip plane (M. Khantha and V. Vitek, unpublished). $\varepsilon(r)$ is a dimensionless quantity (expressed in terms of the effective moduli) which determines the energy reduction of a test loop of radius r amidst loops of radii smaller than r . For example, the energy coefficient of the test loop is proportional to $K_0 \varepsilon(r)$ while it is proportional to K_0 for an isolated loop. $y(\ell)$ is proportional to the probability of forming a test dislocation loop of radius r in the presence of loops of smaller sizes.

3. Results and discussion

We use parameters (summarized in caption of Fig. 1) that are in the same range as for typical materials to illustrate how the collective instability of many dislocation loops differs from the thermally activated expansion of a single loop. The probability of forming a test loop of radius r as a function of r at different temperatures, taking into account the presence of loops of radii smaller than r , is shown in Fig. 1. At 300 K, the probability of forming a loop of radius 4.5 Å (r_0) is 0.008 while the probability of forming a loop of radius 5.5 Å is approximately 15 orders of magnitude smaller. The reduction of the total self-energy of loops is negligible compared to the sum of their individual energies. The critical radius for unstable expansion is almost the same as that of an individual loop (~ 25 Å). However, if such a large loop could form and expand freely, the subsequent probability of forming loops of size larger than the critical radius increases because the rapid increase of the plastic strain when the critical loop expands makes the effective moduli converge to zero. The above scenario is, however, extremely unlikely because the probability of forming the critical size loop is nearly forty orders of magnitude smaller than that of a loop of radius r_0 . In other words, there is a very large activation barrier (~ 12 eV) for the expansion of individual loops. At 700 K, the critical radius for collective expansion is considerably smaller than for an individual loop (~ 13

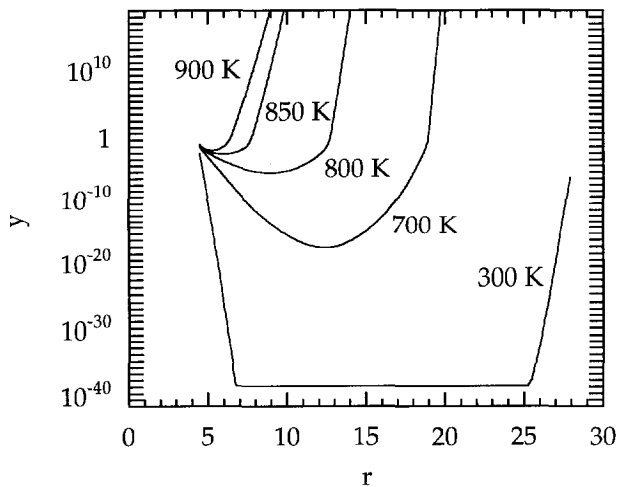


Fig. 1. $y(r)$ which is proportional to the probability of forming a test loop of radius r plotted as a function of r (in Å) at different temperatures. The parameters used are $\mu_0 = 70$ GPa, $\nu_0 = 0.26$, $b = 2.224$ and $r_0 = 4.48$ Å, $c = 0.33$ and $\sigma = 2$ GPa. The value of c is such that the formation energy of a loop of size r_0 is less than 2 eV and σ is chosen such that the difference in behavior between the collective expansion of many loops and that of a single loop is apparent at temperatures between 300–1000 K. This temperature range encompasses the BDTT of many materials.

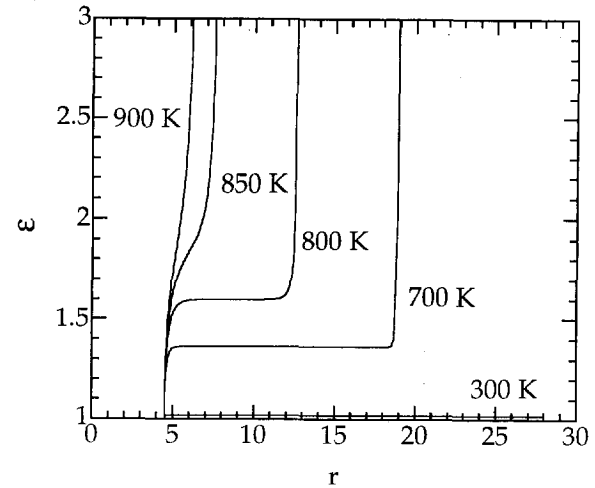


Fig. 2. The variation of $\varepsilon(r)$ with r (in Å) for the same values of parameters as in Fig. 1.

Å) but the probability of forming such a loop remains fifteen orders of magnitude smaller than that of a loop of radius r_0 . Thus, almost negligible density of ‘free’ dislocations can be generated at this temperature. At $T = 800$ K, the critical radius for collective expansion is ~ 9 Å and the probability of forming such a loop amidst other loops is approximately five orders of magnitude smaller than that of a loop of radius r_0 . The scenario is dramatically different for $T \geq 850$ K. The critical radius for collective expansion at 850 K is less than 6 Å and the probability of forming such a loop is only one order of magnitude smaller than that of a loop of radius r_0 . The activation barrier for collective expansion at 850 K is less than 0.2 eV and the barrier disappears above 900 K. The density of ‘free’ glissile dislocations increases by several orders of magnitude in the temperature interval 850–900 K. For stresses smaller than $\mu_0/100$, the reduction of the total self energy is very small even at high temperatures (~ 1000 K) and the loops need to expand to almost the same radius as do individual loops before collective expansion can take place.

Fig. 2 shows the variation of ε as a function of the radius of the test loop for the same temperatures as in Fig. 1. At 300 K, ε increases from 1 to 1.01 while at $T = 700$ and 800 K, ε increases to 1.3 and 1.5, respectively and saturates for large values of r . When r is greater than the critical radius for collective expansion, ε diverges, but for $T \leq 800$ K, as seen from Fig. 1, the probability of forming a test loop of critical size is vanishingly small. Above $T = 800$ K, ε increases continuously as a function of r and diverges with increasing values of r . This is consistent with the behavior seen in Fig. 1, where the probability of forming larger loops increases dramatically after a small initial decrease.

In the present model, the density of glissile dislocations remains virtually zero up to a certain temperature and thereafter it increases dramatically by several orders of magnitude in a temperature interval of less than 50 K. This is similar to the sudden onset of dislocation activity that develops in a narrow temperature interval around the BDTT. We propose that the cooperative generation of many dislocations gives rise to the extensive plasticity at the BDTT. The stresses in the crack tip region are usually very high, of the order of $\mu_0/100$. Thus, the crack tip environment is especially suited for this mechanism to operate.

This is a preliminary model of dislocation generation in homogeneously stressed solids at finite temperatures under static loading. The model is being developed further to take into account the variation of the stress field in the vicinity of the crack under dynamic loading conditions.

Acknowledgements

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References

- [1] J.F. Knott, *Fundamentals of Fracture Mechanics* (Revised), Butterworths, London, 1979.
- [2] J.R. Rice, R. Thomson, *Phil. Mag.* 29 (1974) 73.
- [3] P.B. Hirsch, S.G. Roberts, J. Samuels, *Proc. R. Soc. Lond. A* 421 (1989) 25.
- [4] J.R. Rice, *J. Mech. Phys. Solids* 40 (1992) 239.
- [5] M. Khantha, D.P. Pope, V. Vitek, *Phys. Rev. Lett.* 73 (1994) 684.
- [6] M. Khantha, D.P. Pope, V. Vitek, *Scripta Metall. Mater.* 31 (1994) 1349.
- [7] J.M. Kosterlitz, D.J. Thouless, *J. Phys. C: Solid State Phys.* 6 (1973) 1181.
- [8] F. Lund, *Phys. Rev. Lett.* 69 (1992) 3084.