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Critical misfit for generation of dislocations at second-phase particles

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The generation of dislocation loops around spherical second-phase particles by various models is examined. A theoretical lower limit to the critical misfit is obtained and it is found to agree with the experimentally observed values.

I. INTRODUCTION

In the past considerable attention has been given to the generation of dislocations due to misfits around second-phase particles.[1-4] Ashby and Johnson[2] have proposed a model for generation of a shear loop around a spherical particle and showed that a prismatic loop forms by double cross slip of the shear loop. A quantitative criterion for generation of dislocations is given by Ashby and Johnson by defining an upper limit to the misfit for which the energy barrier for the formation of a dislocation loop vanishes and a lower limit for which the energy change during the formation of a dislocation loop as a function of size of the loop becomes negative. The upper limit is the same as that given by Weatherly.[1] The lower limit gives the misfit due to which a stable loop can form. In this paper the model offered by Ashby and Johnson is reexamined and a theoretical lower limit to the critical misfit is given. The discussion is extended to the generation of climb loops by a mechanism suggested by Matthews and Mader.[4]

II. EXPERIMENTAL EVIDENCE

The experimentally observed values of critical misfit for dislocation generation in a Cu-SiO_2 system by Ashby *et al.*[5] and in a Cu-Co system by Philips[6] and by Brown *et al.*[3] are much lower than the theoretical values obtained by Ashby and Johnson.[2] Conclusions on recent experimental observation on the formation of dislocation loops around nitride particles in niobium by Dahlstrom and Eyre[7] have shown that the mechanism of generation of loops is closely akin to that given by Ashby and Johnson.[2] In addition, formation of two dislocation loops simultaneously on both sides of the second-phase particle is observed instead of a single loop that is assumed to form in the model of Ashby and Johnson. It is this experimental observation that motivated the authors to reexamine the changes in the energy of formation of dislocation loops.

III. THEORETICAL MODELS

A. Two dislocation loops form simultaneously on either side of the particle and on the same slip plane (model 1)

Consider, as shown in Fig. 1, two dislocation loops formed on either side of the particle on a slip plane of maximum shear stress which is situated at a height of $z=R_p/\sqrt{2}$. The spherical particle with its center at the origin has a radius R_p. The curved dislocation loops are approximated by rectangular loops ABCD and EFGH as in the model of Ashby and Johnson. The energy change during generation of the two dislocation loops consists of the following three terms:

(a) The work done by the shear stress (in this case the τ_{xz} component) around the misfitting particle decreases the energy of the system. This term is the same as that given by Ashby and Johnson, but in the present model two dislocation loops should be considered in calculating the total work done. Work done by the shear stress in the formation of a single dislocation loop is

$$W=\int_{\text{loop area}} b\tau_{xz}\,dA = -6G\epsilon z R_p^3 b\int_{-c_1}^{c_1}\int_{c}^{c+c_1}\frac{x\,dx\,dy}{(x^2+y^2+z^2)^{5/2}}, \qquad (1)$$

where $c_1=\frac{1}{2}\sqrt{\pi}\,r_l$, r_l is the loop radius, b is the Burgers vector of the loop, dA is the element of area, ϵ is the misfit around the particle, G is the shear modulus, and c is the distance from the origin on the x axis at which the loop is generated on the slip plane ($c=R_p/\sqrt{2}$). Evaluation of the integral by using $z=R_p/\sqrt{2}$ gives the work done in terms of the loop size.

(b) The self-energy of the dislocation loops increases the energy of the system. The self-energy in the formation of a single dislocation loop is

$$E_s=\frac{Gb^2 r_l}{4}\left(\frac{2-\nu}{1-\nu}\right)\left[\ln\left(\frac{8r_l}{b}\right)-2\right], \qquad (2)$$

where ν is Poisson's ratio.

(c) The interaction energy between the two dislocation loops ABCD and EFGH decreases the energy of the system. This term is calculated by considering the piecewise interaction of the dislocation segments (see, for example, Hirth and Lothe[8]). This procedure, which gives sufficiently accurate values, has been adopted to simplify the lengthy numerical calculations involved in using the theory of curved dislocations. The interaction energy between the two dislocation loops ABCD and

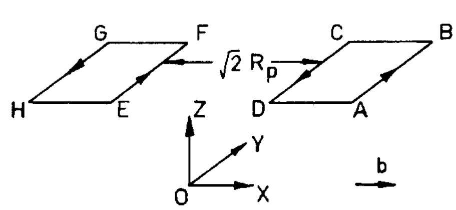

FIG. 1. Coordinate system and position of the dislocation loops in model 1 when they form on the same slip plane. The particle is situated at the origin. Coordinates of the points: A $(R_p/\sqrt{2}+r_l\sqrt{\pi}/2, -r_l\sqrt{\pi}/2, R_p/\sqrt{2})$; B $(R_p/\sqrt{2}+r_l\sqrt{\pi}/2, r_l\sqrt{\pi}/2, R_p/\sqrt{2})$; C $(R_p/\sqrt{2}, r_l\sqrt{\pi}/2, R_p/\sqrt{2})$; and D $(R_p/\sqrt{2}, -r_l\sqrt{\pi}/2, R_p/\sqrt{2})$.

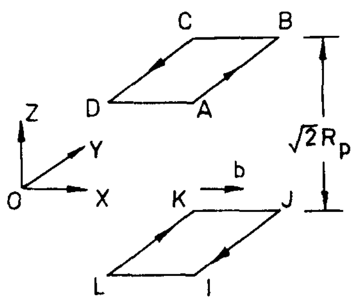

FIG. 2. Coordinate system and position of the dislocation loops in model 2 when they form on two parallel planes. The particle is situated at the origin. In this model the loops are on one side of the particle. The coordinates of the points are same as for Fig. 1.

EFGH is

$$E_{\text{int}} = 2[E(\text{AB},\text{EF}) + E(\text{BC},\text{GF}) + E(\text{DA},\text{GF})] + E(\text{CD},\text{EF}) + E(\text{AB},\text{GH}). \quad (3)$$

In the above equation, $E(\text{AB},\text{EF})$ is the interaction energy between the segments AB and EF and the other terms have the same significance. The interaction energy between other segments of the two loops is found to be zero. Expressions for the interaction energy between various segments are obtained from the formulas given by Hirth and Lothe.[8] However, for simplicity, the lengthy expression for the total interaction energy between the two loops is not given here. The interaction energy E_i^1 with the system considered to be one dislocation loop is taken as one-half the value of E_{int}. The net change in the energy of the system in considering one dislocation loop is

$$E^{(1)} = E_s + E_i^{(1)} - W, \quad (4)$$

where the superscript within parentheses is used to indicate the change in energy calculated by model 1.

B. Two dislocation loops form simultaneously on one side of the particle but on two different slip planes (model 2)

Consider, as shown in Fig. 2, two dislocation loops formed on one side of the particle on slip planes of maximum shear stress which are situated at $z = \pm R_p/\sqrt{2}$. The curved dislocation loops are again approximated by rectangular loops ABCD and IJKL. The energy change during the generation of the two dislocation loops again consists of the same three terms as given in model 1 except that now the interaction energy between the loops is

$$E_{\text{int}} = 2[E(\text{AB},\text{IJ}) + E(\text{AB},\text{LK}) + E(\text{DA},\text{LI}) + E(\text{DA},\text{KJ})]. \quad (5)$$

The interaction between the other segments is found to be zero. The lengthy expression for the total interaction energy between the loops is not given for the reason mentioned earlier. The interaction energy E_i^2 in the system considered to be one dislocation loop is taken as one-half the value of E_{int} given by Eq. (5). The net change in the energy of the system considered to be one dislocation loop is given by

$$E^{(2)} = E_s + E_i^{(2)} - W, \quad (6)$$

where the superscript 2 in parentheses is used to indicate the change in energy calculated by model 2.

C. Four dislocation loops form simultaneously on all four sides of the particle and on two parallel slip planes (model 3)

This model is a superposition of the two previous models, and therefore it is not considered separately. In this case an additional interaction energy term arises due to the interaction between the loops situated diagonally opposite to each other, —e.g., between IJKL and EFGH.

IV. DISCUSSION

The results obtained in Sec. III will now be analyzed numerically to determine whether the lower limit to the critical misfit required for the generation of dislocations is further lowered as a result of including the additional interaction energy term that arises in models 1 and 2. The change in the energy given by Eqs. (4) and (6) differs from that given by Ashby and Johnson[2] because they did not consider the formation of two dislocations loops. Therefore, the change in energy as given by Ashby and Johnson[2] is

$$E = E_s - W, \quad (7)$$

where the interaction energy term is absent. The values of misfit at which E, given by Eqs. (4), (6), and (7) becomes negative at some value of loop size as the size increases, have been evaluated numerically and reported in Fig. 3. The experimentally observed values of critical misfit are also shown.[3,5,6,9] It can be seen that the lower limit to the misfit obtained by the model of Ashby and Johnson is much higher than that obtained by models 1 and 2. It is also seen that all the experimentally observed values of misfit including the Cu-Co

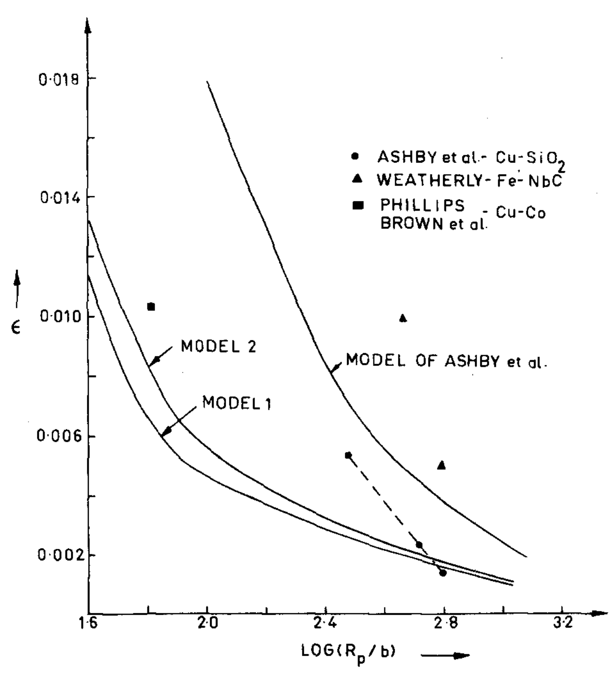

FIG. 3. Lower limit of the misfit around the particle, shown as a function of loop size. Experimentally observed values are also shown.

system appear very near or above the theoretically derived values, which give support to the present calculations. The difference between the values of misfit obtained by models 1 and 2 and that obtained by Ashby and Johnson[2] decreases as the particle size increases because then the interaction energy between the loops also decreases.

The above considerations can also be applied to the generation of climb loops around second-phase particles. Matthews and Mader[4] gave a mechanism by which a climb loop nucleated on one side of a spherical particle grows either by emission of vacanciies or by absorption of interstitials to form a single loop surrounding the particle. The critical misfit required for the generation of a stable loop has been given in terms of the particle size and interstitial supersaturation in the matrix. Further improvement of the model suggested by Matthews and Mader[4] will be to consider the formation of two interstitial dislocation loops on either side. Under sufficient supersaturation of the point defects, the loops grow towards each other and form a single loop. It is expected that, at the same level of supersaturation of point defects, formation and growth of two loops can occur at a lower critical misfit than the formation of a single loop.

SUMMARY

The generation of dislocation loops due to misfit around second-phase particles is reexamined. The lower limit to the values of the misfit required for generation of stable dislocation loops is obtained after taking into account the interaction energy between the two loops that are assumed to form. The following conclusions have been arrived at:

(i) The values of the critical misfit required for generation of stable dislocation loops are much lower when two dislocation loops are considered to form simultaneously than when a single loop forms.

(ii) The difference between the values of the misfit obtained by using models 1 and 2 and that obtained by Ashby and Johnson[2] decreases with increasing particle size.

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