Pergamon

Scripta Materialia, Vol. 35, No. 11, pp. 1331-1333, 1996
Elsevier Science Ltd

1359-6462/96 $12.00 + .00

PII S1359-6462(96)00300-4

NUCLEATION OF SMALL-ANGLE BOUNDARIES

F.R.N. Nabarro
Condensed Matter Physics Research Unit, University of the Witwatersrand, Private Bag 3, Wits 2050, Johannesburg, and Division of Materials Science and Technology, CSIR, P.O. Box 395, Pretoria, South Africa

D.K.-Wilsdorf
Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA 22903, USA

(Received May 22, 1996)
(Accepted July 8, 1996)

Abstract

The internal stresses induced by the strain gradients in an array of lattice cells delineated by low-angle dislocation boundaries are partially relieved by the creation of new low-angle boundaries. This is shown to be a first-order transition, the new boundaries having finite misorientations. The calculated misorientations both of the new boundaries and of the existing boundaries which provoke the transition agree well with observations.

Introduction

When polycrystals of face-centered cubic metals of moderate or high stacking-fault energy are deformed plastically into stages III and IV, the grains develop a characteristic microstructure of cell blocks subdivided into cells, recently studied in (1,2) for rolled or channel-die compressed aluminum. The cell block boundaries have mutual misorientations of order 5°. They are usually elongated, with aspect ratios up to ten or more. Within each cell block the dislocation cells are delineated by small-angle boundaries with mutual misorientations of the order of 0.7° (1). These are low-energy dislocation structures, essentially rotation boundaries with no long-range stresses. On account of imperfect dislocation arrangements and redundant close dislocation dipoles, the total dislocation density in these low-angle boundaries may exceed the minimum density required to effect the rotation by a modest factor $M \simeq 2$. The relative misorientations, both across cell-block boundaries and across small-angle boundaries, increase with increasing strain while their spacing decreases. Evidently the misorientations across dislocation boundaries can increase simply by the capture of glide dislocations. The origin of the constantly increasing number of dislocation boundaries is a transformation of elastic strain energy into dislocation energy (3). The present paper shows that this transformation is of first order.

Theoretical Considerations

A given increase in the misorientation between the opposite faces of a cell may be accommodated elastically, or by the formation of a new small-angle boundary or by a combination of these mechanisms. In fact, new small-angle boundaries are continually nucleated. According to (1), these new boundaries are generated with finite misorientations, always greater than 0.1°. One of the present authors (3) has explained the origin of the new small-angle boundaries as follows.

Each cell is modeled as a bent beam of length L and thickness $D = L/\lambda$, with its ends relatively rotated by an angle X. We shall take X to be the mean misorientation between neighboring cells. This gives rise to an energy density, averaged over the beam, proportional to $G(DX/L)^2$, where G is the shear modulus. Suppose a fraction f of the rotation, equal to an angle fX, is accommodated by a single new small-angle boundary. Then, as shown in the derivation of eq. 14 in (3), the resulting energy density U in the cell is given by

$$U/G = (1 + \nu)(X/\lambda)^2 (1 - f)^2/12 - \{Mb(X/\lambda)f/[4\pi(1 - \nu)D]\} \ln(fX) \quad (1)$$

where b is the Burgers vector and ν is Poisson's ratio.

For a given value of X, i.e. a (substantially) fixed external shape of the beam, the equilibrium value of f will be that which minimizes U, independent of the spatial distribution of the strain energy. Differentiating eq. 1 with respect to f at constant X, we find

$$2\pi(1 - \nu^2) D X (1 - f) / (3M\lambda b) = - \ln (fX) - 1 \quad (2)$$

Write

$$2\pi(1 - \nu^2) D / (3M\lambda b) = Q \quad (3)$$

and write

$$\Phi = fX \quad (4)$$

for the angle of the single small-angle boundary. Then eq. 2 may be written

$$Q\Phi - \ln \Phi = QX + 1 \quad (5)$$

Now the function $Q\Phi - \ln \Phi$, where Φ is assumed to be positive, is positive infinite for $\Phi = 0$ and for $\Phi = \infty$. It has a single minimum at

$$\Phi = 1/Q \quad (6)$$

with the value

$$(Q\Phi - \ln \Phi)_{min} = 1 + \ln Q \quad (7)$$

Thus eq. 5 has no roots, and there is no equilibrium value of Φ, if

$$Q X + 1 < 1 + \ln Q \quad (8)$$

i.e. if

$$X < (\ln Q)/Q. \quad (9)$$

If X > (ln Q)/Q, there are two roots in Φ. We may distinguish them as follows: When the first dislocation is introduced, there is a finite decrease in the first term in U, but a large increase in the second term, because the strain field of the dislocation is not screened. Therefore $dU/d\Phi$ is positive at $\Phi = 0$. As Φ approaches X the second term in U is still increasing, because X is a fairly small angle. However, the

first term hardly decreases, because the relief of strain occurs in a region which is now almost free of stress. Therefore, $dU/d\Phi$ is also positive at $\Phi = X$. It follows that if U possesses both a maximum and a minimum, the turning point at the smaller value of Φ is a maximum of U and that for the larger value is a minimum, corresponding to a stable state.

Consider now what happens as X gradually increases. As long as $X < (ln\ Q)/Q$, the formation of a new small-angle boundary cannot reduce the total energy. When X reaches $(ln\ Q)/Q$, a boundary of small angle of $\Phi = 1/Q$ forms suddenly. Within the present approximations there is no activation barrier.

Numerically, Q depends on ν, which we may take to be 1/3, and on the quantities D/b, M and λ, which are known only empirically (however, the empirical relationship $D = KGb/(\tau - \tau_o)$ with $(\tau - \tau_o)$ the effective flow stress and $K \approx 10$ follows from the theory of (3)). For the reasonable case of D/b = 500, M = 2, $\lambda = 3/2$ one finds from eq. 3

$$Q \approx 310, \qquad ln\ Q \approx 5.74. \tag{10}$$

From eq. 9, the theoretical critical value of X is then 5.74/310 radians ≈ 1.06°, while from eq. 6 the minimum value of Φ is 1/310 radians ≈0.18°. These angles both increase as the deformation increases. We assume that in the experimental histograms of (1) the boundaries of smallest angle are the newest. They appear to have angles of about $\Phi = 0.15°$, while the mean misorientation between adjacent cells increases from about X = 0.4° to about X = 1° as the rolling reduction increases from 5% to 30%, with an average of ≈0.7°. In view of the roughness both of our model and of the experimental measurement of the smallest values of Φ, the agreement between the theoretical and observed values of X and Φ is perhaps fortuitously good.

A quantity less sensitive to the value of Q is

$$X/\Phi = ln\ Q \approx 5.74 \tag{11}$$

It is the ratio of the misorientation between the ends of an existing cell and the angle of a new small-angle boundary at the instant the latter is formed. The observed ratio of

$$0.7°/0.15° = 4.7 \tag{12}$$

is in reasonable agreement with eq. 11.

Acknowledgment

F.R.N. Nabarro is grateful to the University of Virginia for hospitality during the course of this work. D. Kuhlmann-Wilsdorf thanks the National Science Foundation, (Surface Engineering and Tribology Program, Division of Civil and Mechanical Systems, Dr. Jorn Larsen-Basse) for sponsorship of this research.

References

1. Q. Liu and N. Hansen, Scripta Metall. et Mater. 32, 1289 (1995).
2. S. Panchanadeeswaran, R. D. Doherty and R. Becker, Acta Metall. et Mater. 44, 1233 (1996).
3. D. Kuhlmann-Wilsdorf, Scripta Mater. 34, 641 (1996).