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DISCLINATION MODEL OF HIGH ANGLE GRAIN BOUNDARIES

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Since the grain boundary is a rotational defect and so is a disclination, it is proposed here that a grain boundary may be made of disclinations instead of dislocations which are translational defects. The excess elastic energy for a symmetric tilt boundary whose orientation is between two low energy orientations is calculated by using this model. Such calculation cannot be easily performed using dislocations.

1. Introduction

For low angle grain boundaries, the dislocation structure is well accepted[1]). The dislocations have been observed[2]), their Burgers vectors determined[3]), and their spacings measured[4,5]). The energy-angle relations have been derived theoretically[1]) as well as confirmed experimentally[6,7]).

However, for high angle grain boundaries the dislocation model is no longer satisfactory. When the spacing between dislocations is so small that the core regions overlap[8]), the grain boundary becomes virtually structureless elastically. The Burgers vectors may be referred to either grain or the transition lattice and many choices are possible. Furthermore, the dislocation model breaks down completely for a twin boundary or coincidence boundaries in which the atoms fit well at the boundary without dislocations.

Yet a high angle boundary is not structurally homogeneous[9]). It behaves anisotropically in diffusion[10,11]). Such inhomogeneity must introduce elastic fields which extend beyond the boundary thickness. How do we describe them? Although a proper choice of dislocation distribution probably could achieve the purpose, it is proposed here to use disclinations. One of the main reasons is that the disclination is a rotational defect while the dislocation is a translational defect. A grain boundary, being a rotational defect, should be described more simply by disclinations.

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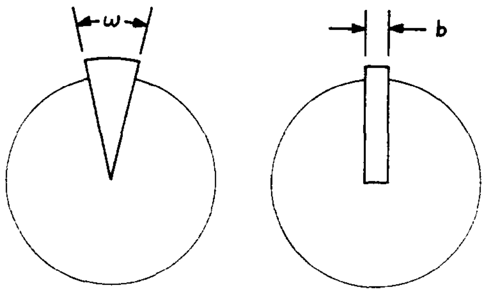
2. Disclinations

As shown in fig. 1, a disclination is simply a Volterra dislocation in which the two surfaces of the cut *rotate* with respect to each other instead of *displacing* parallelly with respect to each other as in the case of a conventional dislocation. If the rotation is a symmetry operation, no fault is created at the cut surfaces just as in the case of a dislocation if the displacement is a lattice

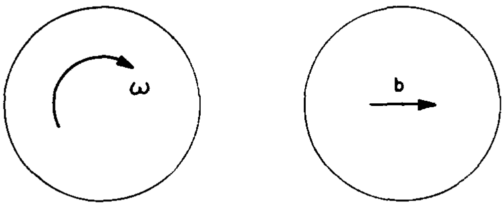


(a) (b)

Fig. 1. (a) Wedge disclination; (b) edge dislocation.

translational vector. Thus the disclination is also a line defect which delineates the boundary of the cut. On the other hand, if the rotation is not a symmetry operation, a fault is created at the cut. Then the disclination is a *partial* disclination.

When the axis of rotation is parallel to the disclination line, as in the case shown in fig. 1, the disclination is a *wedge* disclination or a screw disclination. The term "wedge" is preferred because it is more descriptive, while the term "screw" seems misleading. On the other hand, when the axis of rotation is perpendicular to the disclination line, as in the case shown in fig. 2, the disclination is a "twist" disclination or an edge disclination. Here again, the term "twist" is preferred.



(a) (b)

Fig. 2. (a) Twist disclination loop; (b) shear dislocation loop.

Disclinations can be considered as continuous distributions of dislocations. For example, as shown in fig. 3, a wedge disclination can be constructed by using a wall of edge dislocations. If the Burgers vector has a component b' perpendicular to the wall and the spacing is h', the rotation or the strength of the disclination, ω, is given by

$$\tan(\omega/2) = b'/2h', \tag{1}$$

or when ω is small, $\omega = b'/h'$. The model is more accurate the smaller the b' or h'. However, the model breaks down when ω is a symmetry operation. Similarly as shown in fig. 4, the twist disclination loop can be constructed by

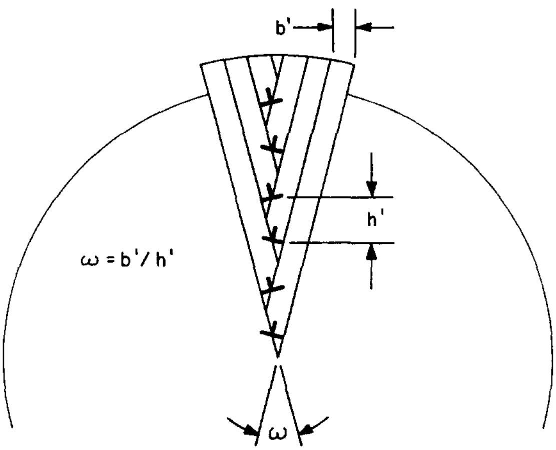


Fig. 3. A wedge disclination made of edge dislocations.

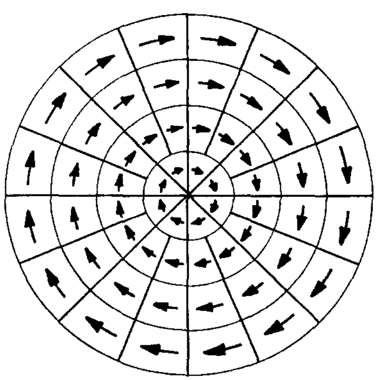


Fig. 4. A twist disclination loop made of screw dislocations.

using a network of screw dislocations[12]), although the Burgers vectors vary from place to place. Here also, the model breaks down when ω is a symmetry operation.

Since disclinations can be considered as continuous distributions of dislocations, a disclination dipole of small separation can be approximated as a dislocation. Conversely, each dislocation can be considered as a disclination dipole. However, it is to be noted that the rotation axes in the disclination dipole are separated in the same way as the disclination lines. There are other disclination dipoles which do not represent a dislocation.

3. Stress fields of disclinations

The stress field of the wedge disclination of fig. 1 is given by Huang and Mura[13]). Let the disclination be the z axis, the only non-vanishing components are, in units of $\mu\omega/2\pi(1-\nu)$:

$$\sigma_{rr} = \ln(R/r), \tag{2a}$$

$$\sigma_{\theta\theta} = \ln(R/r) - 1, \tag{2b}$$

$$\sigma_{zz} = \nu[2\ln(R/r) - 1], \tag{2c}$$

where R is the size of the specimen which is assumed to be much larger than the size of the core, r_0. The stress is at a point with cylindrical coordinates (r, θ, z). The strain field at the same point is, in units of $\omega/4\pi(1-\nu)$,

$$\varepsilon_{rr} = (1-2\nu)\ln\frac{R}{r} + \nu, \tag{3a}$$

$$\varepsilon_{\theta\theta} = (1-2\nu)\ln\frac{R}{r} - 1 + \nu, \tag{3b}$$

$$\varepsilon_{zz} = 0, \tag{3c}$$

$$\frac{\Delta V}{V} = (1-2\nu)\left(2\ln\frac{R}{r} - 1\right). \tag{3d}$$

It is seen that all the stresses and the strains are independent of θ, as expected from the way the wedge disclination is constructed. In rectangular coordinates, the stress field is, in units of $\mu\omega/2\pi(1-\nu)$:

$$\sigma_{xx} = \tfrac{1}{2}\ln\frac{R^2}{x^2+y^2} - \frac{y^2}{x^2+y^2}, \tag{4a}$$

$$\sigma_{yy} = \tfrac{1}{2}\ln\frac{R^2}{x^2+y^2} - \frac{x^2}{x^2+y^2}, \tag{4b}$$

$$\sigma_{zz} = \nu \left(\ln \frac{R^2}{x^2 + y^2} - 1 \right), \tag{4c}$$

$$\sigma_{xy} = \frac{xy}{x^2 + y^2}. \tag{4d}$$

Eqs. (4) can be used to find the stresses of a wedge disclination dipole. When the separation of the two parallel wedge disclinations of opposite sign is small, such as δy, the stresses can be obtained by differentiating with respect to y:

$$\sigma_{xx} = \frac{-y(3x^2 + y^2)}{(x^2 + y^2)^2}, \tag{5a}$$

$$\sigma_{yy} = \frac{y(x^2 - y^2)}{(x^2 + y^2)^2}, \tag{5b}$$

$$\sigma_{zz} = -2\nu y/(x^2 + y^2), \tag{5c}$$

$$\sigma_{xy} = x(x^2 - y^2)/(x^2 + y^2)^2, \tag{5d}$$

in units of $\mu\omega\delta y/2\pi(1-\nu)$. Eqs. (5) are the stresses of a single edge dislocation[14]) as shown in fig. 1 with a Burgers vector equal to $\omega\delta y$. This illustrates the possibility that a disclination dipole of small separation is equivalent to a dislocation.

When the separation between the two wedge disclinations of opposite sign is large, such as $2L$, the stresses can be obtained by using eqs. (4) twice, one for each disclination. Let the position of the positive disclination be $(0, -L)$ and that of the negative disclination be $(0, L)$. Then the stresses of the large dipole are

$$\sigma_{xx} = \tfrac{1}{2} \ln \frac{x^2 + (y-L)^2}{x^2 + (y+L)^2} + \frac{x^2}{x^2 + (y+L)^2} - \frac{x^2}{x^2 + (y-L)^2}, \tag{6a}$$

$$\sigma_{yy} = \tfrac{1}{2} \ln \frac{x^2 + (y-L)^2}{x^2 + (y+L)^2} - \frac{x^2}{x^2 + (y+L)^2} + \frac{x^2}{x^2 + (y-L)^2}, \tag{6b}$$

$$\sigma_{zz} = \nu \ln \frac{x^2 + (y-L)^2}{x^2 + (y+L)^2}, \tag{6c}$$

$$\sigma_{xy} = \frac{x(y+L)}{x^2 + (y+L)^2} - \frac{x(y-L)}{x^2 + (y-L)^2}, \tag{6d}$$

in units of $\mu\omega/2\pi(1-\nu)$. Eqs. (6) are the stresses of a finite edge dislocation wall[15]) in which the Burgers vectors are b' and the spacings are h' provided $\omega = b'/h'$. The stress component σ_{xx} for $x=0$ is shown in fig. 5 for both a single edge dislocation, eq. (5a), and a wedge disclination dipole, eq. (6a). It is seen that at large distances they approach each other provided $b = 2\omega L$.

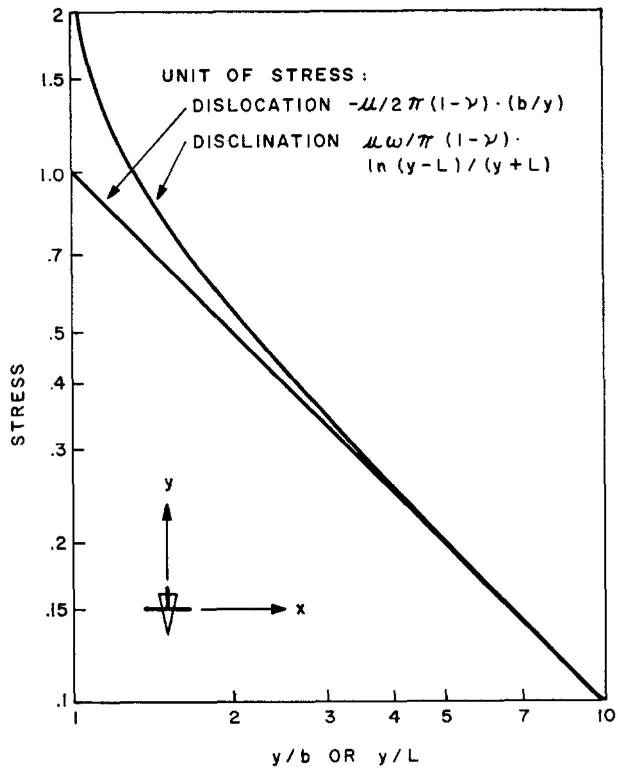


Fig. 5. The normal stress, σ_{xx}, in the plane $x=0$, for an edge dislocation and a wedge disclination dipole.

4. Energy of disclinations

The strain energy of the wedge disclination shown in fig. 1 is given by Huang and Mura[13]). Per unit length of disclination line it is given by

$$E = \mu\omega^2 R^2 / 16\pi (1 - \nu). \tag{7}$$

The average strain energy density is then $\mu\omega^2/16\pi^2(1-\nu)$ independent of R. Eq. (7) is really a limiting form in which R is assumed to be much larger than the core radius r_0 of the disclination.

The strain energy of wedge disclination dipole is the same as that of a finite edge dislocation wall and is given by Li[15]):

$$E = \frac{\mu\omega^2 L^2}{\pi(1-\nu)} \ln \frac{R}{2L} \quad \text{per unit length} \tag{8}$$

for $R \gg L \gg r_0$. To see whether a single edge dislocation would transform spontaneously into a wedge disclination dipole, consider the equivalent Burgers vector $b = 2\omega L$. The total energy of a single edge dislocation is shown in fig. 6 where C is the core energy per unit length. Also shown in fig. 6 is the total energy of a wedge disclination dipole including a surface energy γ per

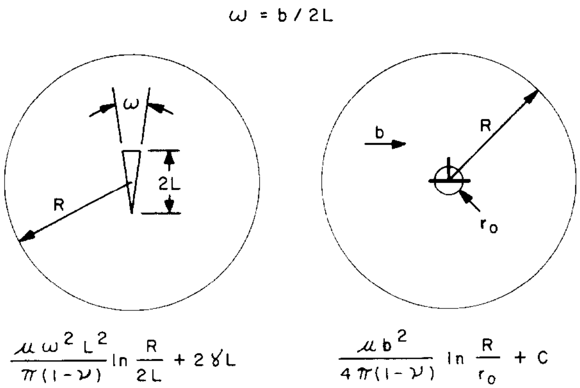


Fig. 6. Energies of a disclination dipole and of a dislocation.

unit area. Hence an edge dislocation may be transformed into a wedge disclination dipole if the following quantity is positive:

$$\Delta E = \frac{\mu b^2}{4\pi(1-\nu)} \ln \frac{2L}{r_0} + C - 2\gamma L. \tag{9}$$

Such quantity is obviously positive if ω is a symmetry rotation for which $\gamma = 0$. Even if ω is not a symmetry rotation, as long as γ is small, an edge dislocation may be transformed spontaneously into a wedge disclination dipole.

5. Interaction between disclination dipoles

Even if a single edge dislocation tends to be transformed into a wedge disclination dipole, this may not happen in the grain boundary if such transformation affects the interaction energy. By using continuous distribution of edge dislocations of infinitesimal Burgers vectors, the force between two wedge disclination dipoles is found to be

$$f = \frac{\mu\omega^2 L}{\pi(1-\nu)} \left[\left(\frac{y}{2L} - 1\right) \ln\left(1 - \frac{2L}{y}\right) + \left(\frac{y}{2L} + 1\right) \ln\left(1 + \frac{2L}{y}\right) \right], \tag{10}$$

which is compared with that between two edge dislocations in fig. 7. It is seen that the interactions are quite similar.

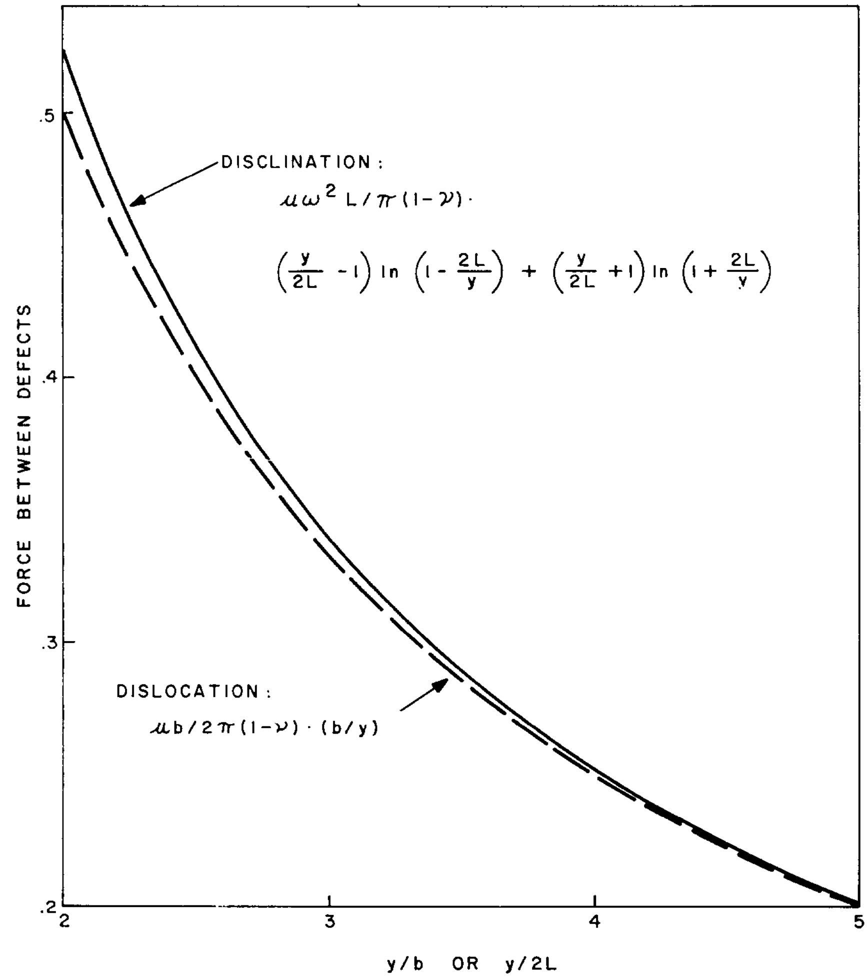


Fig. 7. Forces between dislocations and between disclination dipoles.

6. Disclination structures of grain boundaries

The foregoing considerations suggest that a disclination model of grain boundary is possible for high angle as well as low angle boundaries. The case of a simple tilt symmetric boundary is illustrated in fig. 8. Each dislocation is transformed into a wedge disclination dipole. Some advantages are obvious: The concept of Burgers vector is no longer needed. The rotation axis of the disclination is the common direction of the two grains. The angle ω could be a symmetry rotation so that the misfit energy in the dipole disappears. The size $2L$ does not have to be b/ω; it could be adjusted to minimize

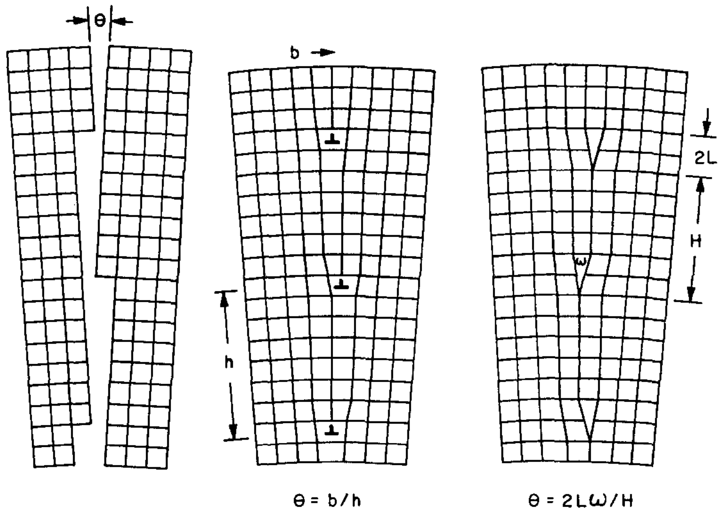


Fig. 8. A simple tilt boundary made of dislocations or disclinations.

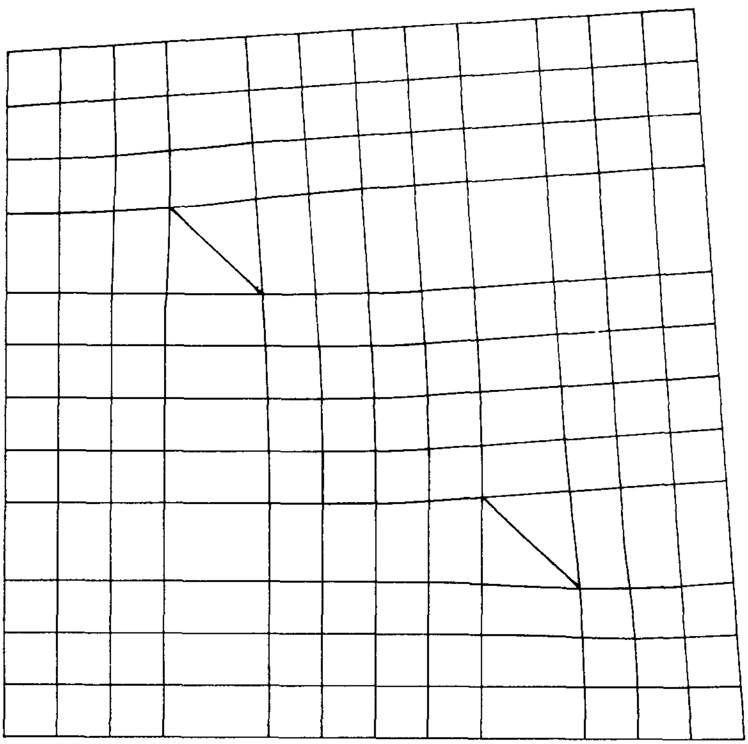


Fig. 9a

the energy. If the low energy plane of the disclination dipole does not coincide with the plane of the boundary, the boundary may show a ledge structure as frequently observed in the electron and field ion microscopes[16,17]).

A square lattice is shown in fig. 9a in which a periodic structure of fit and misfit regions is shown. The misfit region could be a low energy coincidence boundary.

A tilt boundary in a hexagonal lattice is shown in fig. 9b. Again a periodic structure of fit and misfit regions is seen. The misfit region is shown by a pentagon followed by a heptagon. Since a pentagon in a hexagonal lattice is

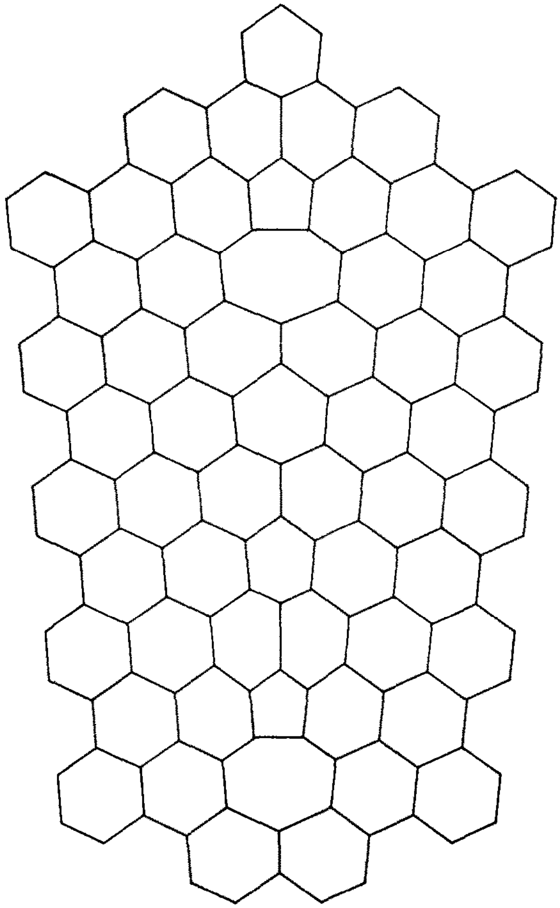


Fig. 9b

Fig. 9. A symmetric tilt boundary made of wedge disclinations: (a) lattice with four fold symmetry; (b) lattice with six fold symmetry.

a negative wedge disclination while a heptagon is a positive wedge disclination, the misfit region is thus a wedge disclination dipole.

The excess elastic energy for a simple tilt boundary whose orientation is between two low energy coincidence (or any other type) orientations is shown in fig. 10. The wedge disclination dipoles are approximated by finite walls of edge dislocations. The calculation was performed by adding one by one low angle infinite dislocation walls of Burgers vector b' and spacing H which is also that between the finite walls. The result is

$$E = \frac{-\mu b'^2}{4\pi(1-\nu)H}\left[M \ln \frac{2\pi r_0}{eH} + 2\sum_{I=1}^{M-1}(M-I)\ln\left(2\sin\frac{I\pi}{N}\right)\right] \quad (11)$$

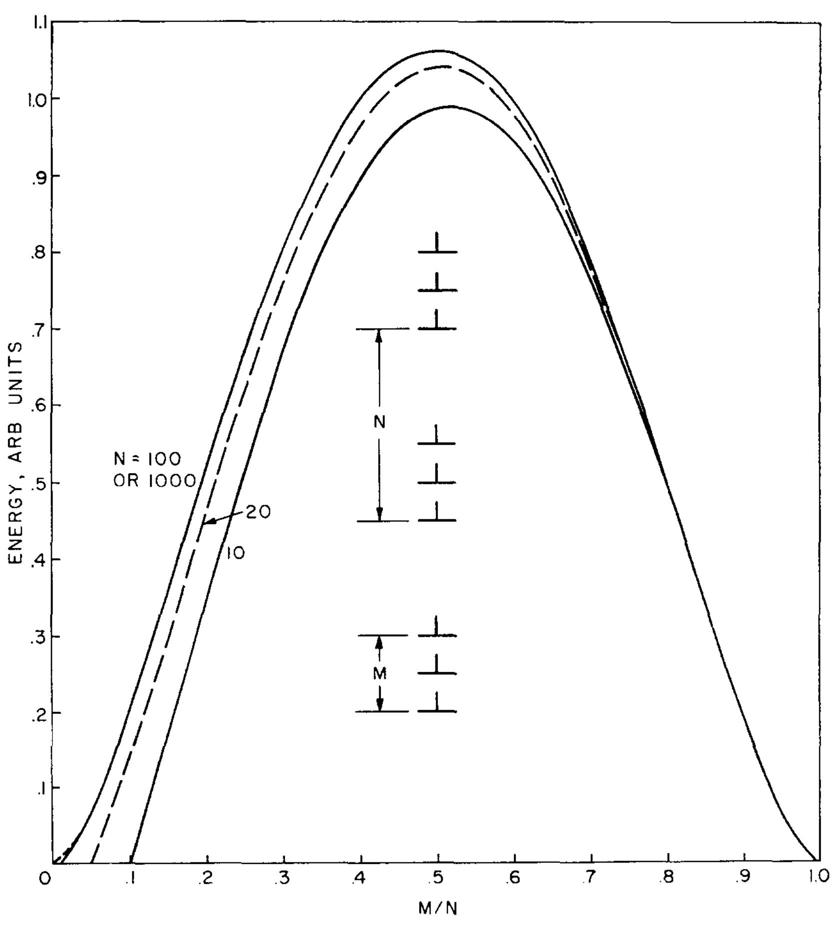


Fig. 10. Energy of a wall of wedge disclinations.

per unit area. Eq. (11) is, of course, more accurate the smaller the b' and the larger the N and M. However, since the angle of the boundary is $\theta = Mb'/H$ and the strength of the disclination is $\omega = Nb'/H$, the products Mb' and Nb' stay finite when b' approaches zero. Furthermore, since the separation of the disclination dipole is $2L = MH/N$, the angle of the grain boundary can be increased by maintaining constant either H or L or a relation between H and L. The situation shown in fig. 10 is for the case in which H is kept constant. When L is kept constant, the curve at the low angle end would look like that of dislocation walls.

7. Summary and conclusions

A disclination dipole is equivalent to a dislocation[18,19]) when the separation is small and to a dislocation wall when the separation is large. These facts are used to replace dislocations in the grain boundary by disclinations. In the disclination model, the concept of Burgers vector is no longer needed. Instead, a rotation vector of the disclination is introduced which is along the common direction of the two grains. A general grain boundary thus consists of regions of low energy separated by disclinations. The elastic energy caused by the presence of these disclinations is calculated, and it is proposed that such elastic energy represents the excess energy between energy cusps in the energy misorientation relations.

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Discussion

G. BISHOP (Army Materials and Mechanics Research Center, Watertown, Massachusetts): First, I do not agree that the cores overlap. They are separated by a series of coincidence sites in the boundary. The second thing is the distinction you make between the dislocation and disclination representation. For it to be operationally significant you should suggest an experiment that would distinguish between the two descriptions. Can you?

J. C. M. LI: Well, as I just described, with this model one can calculate the energy of all the orientations between two low energy orientations. One can't do this with the dislocation model. However, to compare with experiments, I do need very accurate measurements.

BISHOP: You can calculate the boundary energy for misorientations between two cusp misorientations by superposing an array of secondary dislocations on the primary grain boundary dislocation array.

LI: From which grain and with what Burgers vector?

BISHOP: The Burgers vectors can be well defined geometrically. However, I agree with you that defining the physical size of the Burgers vector in the dislocation model is a problem because you do have a situation in which the two crystals can relax inward or outward normal to the grain boundary.

LI: Right. So what you end up doing is to introduce disclinations rather than dislocations. Now what was your first objection?

BISHOP: Well, the first objection was that if the cores do not overlap, in fact the regions of misfit are separated by a series of coincidence sites. That is in the highest angle grain boundary. When you go to low angles you assume the cores are separated by lattice.

LI: Well, you are actually describing the disclination structure. The series of coincidence sites is nothing but a disclination dipole. Now when I say the cores overlap, that is strictly in the sense of the dislocation model. If you are going to separate them by coincidence sites, then it is equivalent to describing the grain boundary by disclinations.

W. BOLLMANN (Batelle Institute, Geneva, Switzerland): I am sorry that I do not agree with your introductory remarks. I hoped to show in my talk that it is possible to describe boundaries by a fully consistent dislocation story.

With respect to your remark that a Burgers vector cannot be defined because you do not know to which grain to refer to, I should like to remind you that F. C. Frank defined the Burgers vector with respect to a reference lattice and not with respect to a crystal. This means that the Burgers vector of a dislocation in the boundary is an invariant coordinate difference which can be referred to the coordinate system of either of the two crystals (considered as reference lattice). The two coordinate systems related by the transformation A of the 0-lattice theory are considered as equivalent.

A dislocation in a single crystal has many properties; it is a line with a core, a stress field, a Burgers vector which is invariant along the line and continuous on branching (Frank's node condition), etc. When you extend this concept into the boundary you have to decide which of the properties you want to conserve by all means. I decided to conserve the fact that a dislocation is a line which has attributed to it a Burgers vector with its invariance and continuity properties. The stress field, the subdivision into core and good material, etc., may change or even get lost. In this way, you can obtain a complete balance between dislocations in the crystals, and primary and secondary dislocations in the boundary. I have nothing against your saying that you *can* describe the boundary by a disclination story, but I have something against your saying that it is not possible to describe it by means of dislocations.

LI: You can not really. Geometrically you can. You can do all the things you just said until you try to calculate the elastic energy or the interaction of a boundary with other things. Then you will have to know what is the actual Burgers vector among all the possible ones. Since we want to know the properties of grain boundaries, we have to do more than just to describe them geometrically.

M. E. GLICKSMAN (Naval Research Laboratory, Washington, D. C.): Jim, is the wedge disclination array equivalent then to a tilt island? Is there an equivalency there to the structure you generate by taking a cut within a crystal followed by a rotation?

LI: A wedge disclination dipole is a tilt island.

GLICKSMAN: Now, at lower angles where people have seen that the misfit is taken up locally, is it not by a series of equivalent edge dislocations?

LI: Yes, especially when the angle is low.

GLICKSMAN: Those would be sets of edge dislocations that one might see in an electron micrograph.

LI: Correct.

GLICKSMAN: Now, since you can essentially produce something very similar to the disclination loop is there some way that you could distinguish – or perhaps there is no distinction – between a disclination loop and what I consider to be just a set of edge dislocations?

LI: Well, it really depends on how wide is the separation of the disclination dipoles. If the separation is very wide, then you should be able to see it in the electron microscope just as you see the separation of partial dislocations. But if the separation is too small, then I think the contrast is probably the same as a dislocation.

R. de WIT (National Bureau of Standards, Washington, D. C.): I liked most of your talk but I disagree when you say that a disclination is identical with a wall of dislocations. It is not. The way I would modify your statement is as follows: If you have a disclination you can conceive of a dislocation model which has the same stress. In other words, a tilt boundary which ends in a crystal has the same stress pattern as a wedge disclination. This statement can be generalized: For an arbitrary disclination loop there exists a dislocation model on any surface whose boundary is the loop, which gives exactly the same stress and strain. However, other things may be different; for instance, for a disclination we cannot have a single-valued distortion field, whereas for the dislocation wall that gives you the same stress, there exists a unique distortion.

LI: Thank you.

G. F. BOLLING (Ford Motor Co., Dearborn, Michigan): In your last slide you left us with an intriguing idea. Do you have any preference for the number of units. When you go from a very low angle, simple boundary that you can analyze in dislocations (to a higher angle one) would you then expect the next package, where you would talk about disclinations, to be described in terms of two unit dislocations? In other words, do you see this as occurring in steps? Is the disclination to be taken down first of all into a single dislocation, then a package of two, then three, or what? Do you have a preference? Since you have looked at this do you have a preference from the calculations?

LI: I do not think it goes by steps. It is either a dislocation or a wedge disclination dipole. But when the angle gets higher, the grain boundary may take different low energy orientations or different wedge disclination dipoles. That is, the structure of the grain boundary may change discontinuously when the angle rises across a coincidence (low energy) orientation, as the boundary will take a mixture of nearby orientations. However, for all the orientations between two low energy orientations, the structure should change continuously.

BOLLING: But then as a criterion would you not expect, if you were very close to certain coincidence orientations, and using the idea of disclinations, that you should be able to predict a span of orientations over which you might have special characteristics. I am trying to search for a criterion to distinguish between the two elements – dislocations and disclinations.

LI: I guess I do not quite understand. This model cannot predict the low energy orientations. All it can do at the moment is to describe the situation between two low energy orientations. We need atomistic calculations for coincidence (low energy) boundaries.