

MOLECULAR DYNAMICAL SIMULATION OF TWO-DIMENSIONAL DISCLINATIONS*

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(Received 27 March 1987, final version 8 September 1987)

An investigation is made of the core structure of total positive and negative wedge disclinations of strength $\pm\pi/3$ in two-dimensional crystallites containing up to 476 atoms. The total energy is determined as a function of the size of the crystallite and the position of the disclination in it. A comparison is made between the computer results and predictions of the linear theory of elasticity. The change in structure of the disclination core when vacancies or interstices are introduced into it and when edge dislocations are nucleated in the crystallite is analysed.

The use of disclination ideas has become necessary and is generally accepted in many areas of solid state physics [1-8]. The use of computer simulation, which provides both qualitative and quantitative results, can give important information on the properties of disclinations. Computer simulation of point defects, dislocations, grain boundaries, radiation damage in solids, deformation and failure of crystals has been developed quite extensively [9, 10]. Only trial investigations have been carried out for disclinations [11, 12], but they not only prove the effectiveness of the given method, but also make it possible to predict a number of new effects, such as amorphization of the disclination core when point defects are introduced [12].

In the present work, computer simulation is used to analyze the structure and properties of positive

* *Fiz. metal. metalloved.*, 66, No. 1, 65-72, 1988.

and negative wedge disclinations in two-dimensional crystallites. Since most calculations in disclination theory have been done in the framework of the linear theory of elasticity [2, 7], it is interesting to check the validity of the results of those calculations. That is done below for a model potential with parameters that typify the atomic bond in metals.

CALCULATION METHOD

A wedge point disclination is introduced into a disc as follows (Fig. 1). Along a radius passing through the location of the future disclination ($x=c, u=0$) or ($r=c, \varphi=0$) a cut is made in the range $c \lesssim r \leq R$, where R is the disc radius. A sector of material with angle ω is then inserted into the area of the cut. After that, the sides of the sector and the initial cut are stuck together. This gives rise to a negative disclination of strength $-\omega$, displaced relative to the centre of the disc. A positive disclination can be obtained by taking the sector out of the disc.

We shall compare the computer results with the formulae of the linear theory of elasticity. For an exact comparison, the latter must be obtained for the case of a thin disc, that is, for a planar stressed state. In that case, the total (elastic plus surface) energy of a disc with a disclination which is displaced relative to the centre of the disc through a distance c is equal [7] to

$$E_\gamma = \frac{G(1+\nu)}{16\pi} \omega^2 \frac{(R^2 - c^2)^2}{R^2} + 2\pi R\gamma, \quad (1)$$

where it is necessary to use the shear modulus G and specific surface energy γ relative to the thickness of the disc, that is, with changed dimensionality. In the cases examined below, the Poisson ratio of the isotropic material of the disc or of the triangular lattice $\nu=1/3$, $\omega = \pm 1/3$, and G and γ are found from the parameters of the atomic interaction potential. We note that the elastic fields of disclinations have been

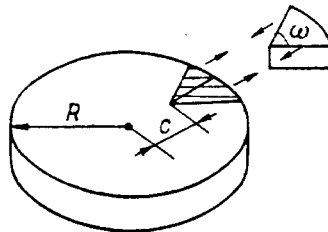


FIG. 1. A disclination in a thin elastic disc, formed after the removal or introduction of a sector of material.

used for a similar purpose in the case of planar strain and, as shown in [13], these cannot properly be used for the description of two-dimensional crystallites.

We consider a two-dimensional crystallite with triangular lattice corresponding to close-packed plane $\{111\}$ of a crystal with f.c.c. lattice, with free boundary conditions. The atomic interaction can be described by the Morse potential

$$U(d) = D [\exp(-2\alpha(d-d_0)) - 2\exp(-\alpha(d-d_0)) - \exp(-2\alpha(r_c-d_0)) + 2\exp(-\alpha(r_c-d_0))]; \quad 0 < d \leq r_c, \quad (2)$$

where d —the interatomic distance; D —energy of dissociation of atomic bond; d_0 , α —parameters of potential; $r_c=2.8d_0$ —cut-off radius of potential, chosen so as to allow for interaction within three co-

ordination spheres. Two sets of parameters are used in the work. For the main one (I) $D = 54.8 \times 10^{-21}$ J, $\alpha = 1.3588 \times 10^{10}$ m $^{-1}$, $d_0 = 2.87 \times 10^{-10}$ m, which is typical of the atomic interaction in metals. The shear modulus for a triangular lattice in this case is equal to $G = 15.8D/d^2$, the potential energy of an atom in an infinite two-dimensional crystal $E_\infty = -3.60D$, the surface energy per unit free surface length of the crystallite $\gamma = 0.084 Gd_0$. The second set of parameters (II) is only used in the investigation of disclinations which are displaced relative to the centre of the crystallite. It differs from the first by the use of $\alpha' = 0.74\alpha$ instead of α . For this softer potential $G = 11.3 D/d^2$.

The initial configurations of crystallites with positive and negative disclinations were created with the method shown in Fig. 1, by respectively removing from the crystallite or inserting into it a sector of perfect lattice with vertical angle $\pi/3$. The sides of the cut were then stuck, introducing uniform angular deformation. A disclination which was displaced relative to the centre was obtained when a circle of the required radius, the centre of which was at a distance c from the centre of the crystallite, was separated from the original crystallite and disclination.

The initial configurations were relaxed using the method of molecular dynamics and atom-by-atom damping. The atomic velocities were assumed to be equal to zero whenever they reached a maximum value. Relaxation ended when the temperature of the crystallite, determined from the mean kinetic energy of atoms, became less than 0.1 K. The equations of motion were integrated by the method of Nordsik of fifth-order accuracy [14].

The different configurations of the disclination cores were obtained by introducing vacancies or interstitial atoms into the core of positive or negative disclinations respectively. The new atoms were taken from, and the removed atoms placed in the surface of the crystallite. The total number of atoms remained unchanged, so that the elastic energies of different configurations could be compared directly.

We note that the free boundary conditions that have been used here are more correct in the investigation of the atomic configurations of defects [13]. At the same time, the presence of a free surface gives

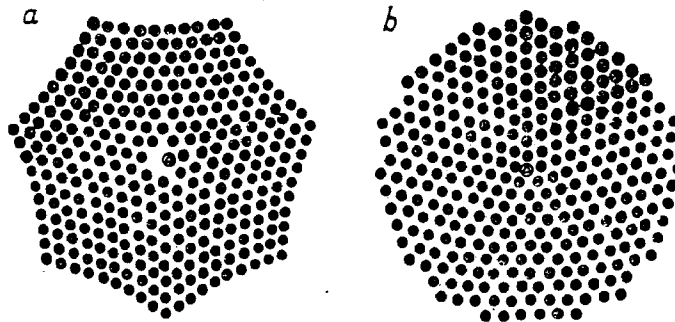


FIG. 2. Examples of atomic configurations of crystals with disclinations: a —316-atom with negative disclination $\omega = -\pi/3$; b —306-atom with positive disclination $\omega = +\pi/3$.

rise to additional pressure in the crystallite, associated with surface tension. As a consequence, the energy E_N and dilation δ_N per atom in an N -atom crystallite depend on the position of the atom and differ from the values in an infinite lattice. Atoms which are further than $4d_0$ away from the free surface have almost constant energy and dilatation. For crystallites containing 200–400 atoms, these parameters are equal to $E_N \approx 0.95 E_\infty$, $\delta_N \approx 0.03$ respectively. The appearance of non-zero dilatation of compression is associated with diminution of the equilibrium atomic distance $a_N = 0.96 a_\infty$. In order to exclude the influence of that effect, the computer calculated parameters of disclinations must be compared with the values of a perfect (disclination-free) crystallite of the same size. In particular, for the relaxed state

of a crystallite with a disclination, the elastic energy inside a circle of radius r can be defined as

$$E(r) = \sum_{i=1}^n E_i - nE_N, \quad (3)$$

where E_i is the potential energy of atom i , and the sum is taken over all atoms in a circle of radius r .

To analyze the simulation results, we need to give an unambiguous definition of a point disclination in a crystal. This can be done with the help of the Dirichlet procedure [15], where the coordination number of each atom is determined. Particles with coordination numbers 5 and 7 are regarded as the centres of positive and negative point disclinations and denoted respectively as \blacktriangledown and \blacktriangle . The Dirichlet procedure can also be used to find dilatation δ_i at the point where atom i is situated, as the relative change of area of the Dirichlet polygon S_i , which is the two-dimensional analogue of the Voronoy polyhedron: $\delta_i = (S_i - S_N)/S_N$, where $S_N = a_N^2 \sqrt{3}/2$.

RESULTS

Disclinations at the centre of a crystallite. The disclinations were introduced into crystallites of different sizes, containing from 16 to 476 atoms. Figure 2 shows the relaxed configurations of crystallites with negative and positive disclinations at the centre. The character of distortions associated with disclinations is already clear from the Figure. For the crystallite with positive disclination, the lattice near the

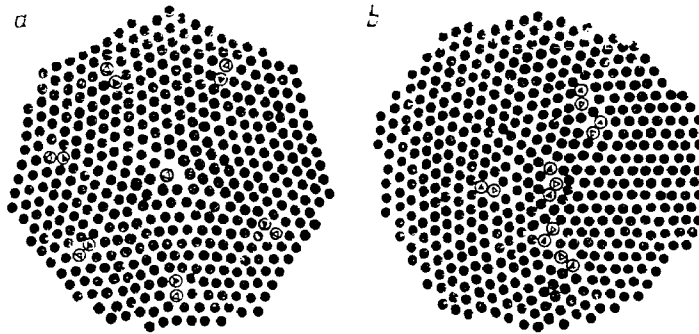


FIG. 3. Screening of disclinations by ensembles of dislocations in large crystallites: *a*—428-atom configuration with negative disclination; *b*—476-atom configuration with positive disclination.

centre is compressed, and extended on the periphery; for the crystallite with negative disclination the opposite is observed. This result is in qualitative agreement with the results of the linear theory of elasticity.

Disclinations for which there is only one atom with destroyed coordination in the crystallite have been called perfect. When the size of the crystallite is increased, the perfection of the disclinations is destroyed. The structure of crystallites proves to be unstable relative to the formation of extra disclination ensembles. For those ensembles typically there will appear disclination dipoles with a shoulder equal to the lattice parameter. These dipoles, as we know [16], are equivalent to edge dislocations. Thus, destruction of the structure of perfect disclinations is associated with the appearance of edge dislocations.

For crystallites with a negative disclination containing more than 250 atoms, edge dislocations

nucleate at the surface. During the relaxation procedure the dislocations move towards the centre of the crystallite and stop at a distance of about seven lattice parameters from it (Fig. 3a). The dislocations are generated on stress concentrators—surface unevenness. After the unevenness has been removed in crystallites with $F \lesssim 350$ atoms dislocations are not nucleated (Fig. 2a). When the size of the crystallite is increased further, dislocations arise whatever the state of the surface (Fig. 3a). Nucleation of dislocations has been observed in crystallites with positive disclinations both at the surface and near the core of the disclination (Fig. 3b).

The dependence of elastic energy of a relaxed crystallite with a disclination on its size, found with the use of (3), is shown in Fig. 4. For comparison we also show the dependence of elastic energy of a continuous disc with a disclination at the centre, calculated with the formula (1), where $c=0$. There is good agreement between the numerical calculations and the results of elasticity theory. The energy of imperfect disclinations, the core of which has been screened by a dislocation cloud, is lower than that of perfect disclinations (cf. Fig. 4).

The total energy of crystallites is observed to fall when point defects are introduced into the disclination core. The corresponding changes of elastic energy when 13 vacancies are introduced into the core of a positive disclination and eight interstitial atoms are introduced into the core of a negative disclination are indicated by arrows in Fig. 4. The energy of the crystal has a curve with a minimum, depending on the number of point defects introduced into the disclination core. The minimum energy is realized with the following quantity of de-

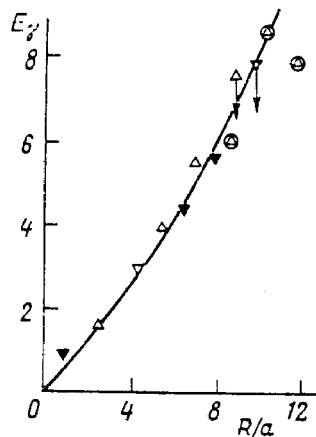


FIG. 4. Computer calculated and theoretical dependences of energy of disclination E_d as function of radius R of crystallite or disc: Δ —results of computer calculations for negative disclinations; \blacktriangledown —for positive disclinations; ———— theoretical curve obtained using formulae of linear theory of elasticity; the open triangle and closed triangle in the circles are the values of the energy for negative and positive disclinations, screened by dislocations; \downarrow —change in energy when point defects are introduced into the disclination core. Energies expressed in units Ga_N^2 .

fects as a proportion of the total number of atoms: 3% for interstices and 5% for vacancies. As shown in [12], the introduction of vacancies into the core of a positive disclination results in amorphization, that is, in loss of short-range order in the atomic arrangement. A similar effect arises when interstitial atoms are introduced into the core of a negative disclination. Non-linear atomic interaction effects lead to non-zero positive dilatation (of the order of several percent) of the crystallite with disclinations.

In the course of computer simulation it has been found that the total dilatation (in the given case, relative change of area) of crystallites with disclinations is not zero, is positive and changes between 0.5–1.5% for positive and 2.5–2.4% for negative defects, depending on the size of the crystallite. We note that the influence of surface effects on dilatation is small and their contribution ($\approx 0.2\%$) falls with growth of the crystallite. The presence of positive dilatation, associated with disclinations, is a purely non-linear effect, which cannot be investigated in the framework of the linear theory of elasticity.

Disclinations, displaced relative to the centre of a crystallite. Crystallites with disclinations which are displaced relative to their centre prove to be less stable than the configurations just described. Even a small (2–3 lattice parameter) displacement of a disclination from the centre of a crystallite results in loss

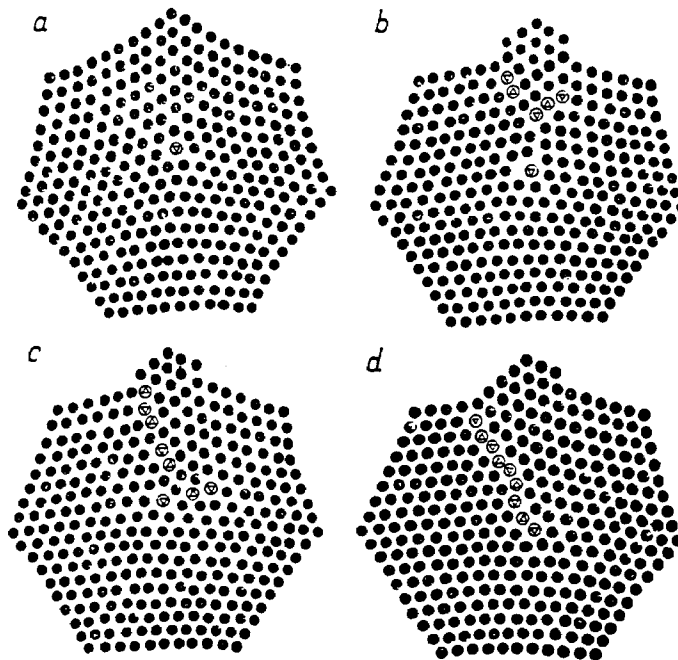


FIG. 5. Relaxation in 307-atom crystallite with displaced negative disclination: *a–d*—successive stages of relaxation.

of stability. During relaxation dislocations are nucleated on the surface of such crystallites and in the disclination core, and these are then moved through the crystallite, creating ultimately a stable disclination-dislocation configuration.

For disclinations (both positive and negative) with small displacement $c=2-3a_N$ a typical stable configuration obtained as a result of relaxation is a disclination, supplemented by a wall of edge dislocations cut-off on it (Fig. 5*d*). The appearance of such a stable configuration for a 307 atom crystallite with negative disclination, which is two lattice parameters away from the centre of the configuration, can be followed in Fig. 5. By analysing the final configuration (Fig. 5*d*) we found that the misorientation of the lattice on different sides of the dislocation wall is $\varphi=18-28^\circ$.

Disclinations which are displaced by large distances relative to the centre of the crystallite ($c=4-8a_N$) move towards the surface as a result of the emission and absorption of dislocations, and leave the crystallite. Ultimately either a perfect crystallite with a complicated surface line, or a configuration containing one or several dislocations is obtained.

Up to now, we have given results obtained using atomic interaction potential I. If the softer potential with parameters II is used, the picture changes qualitatively. For instance, during relaxation of the configuration depicted in Fig. 5a, dislocations are not observed to nucleate in the crystallite, and the disclination turns out to be stable. The influence of rigidity of the potential on stability of two-dimensional disclination configurations in [11] was similar.

DISCUSSION OF RESULTS

As a result of the computer calculations, we have obtained the dependences of the parameters of disclinations on their geometric parameters, agreeing with the predictions of the linear theory of elasticity. We can see from Fig. 4 that the curve of total elastic energy allowing for surface energy, obtained with (1), is in good agreement with the energy values of a crystallite with a disclination found in the computer experiment. The dependence of total elastic energy on the size of a crystallite with a disclination is nearly linear. This means that, for small crystallites, the surface energy proportional to R rather than the elastic energy of a defect, proportional to R^2 , is decisive.

The loss of stability of crystallites with disclinations when their size increases can be explained by rapid growth of the disclination energy with increase in the size of the crystallite (1). The dislocations that are nucleated on the surface screen the elastic field of the disclination and reduce the energy of the system (cf. Fig. 4). For the configuration depicted in Fig. 3a, it can be hypothesized that the distance from the centre of the crystallite to the dislocations is comparable with the maximum size of the crystallite, containing a stable perfect disclination. Dislocations were not observed to nucleate in crystallites of this size or smaller.

When a negative disclination of atoms from the surface is added to the core the energy of the configuration is reduced, and dislocation dipoles are generated near the centre of the crystallite. The introduction of interstitial atoms into the core of a negative disclination results in its amorphization. In such an amorphous core, not only is long-range order in packing of atoms destroyed, but also short-range order, owing to the increase in the number of atoms with coordination number different from six. Amorphization of the core also occurred for a positive wedge disclination when vacancies were introduced into the core [12].

The low-energy (compared with perfect disclinations) disclination-dislocation configurations depicted in Figs. 3 and 5d appear to be typical of disclinations in large crystallites. Similar imperfect configurations have been observed experimentally in the lattice formed by magnetic flux lines in a second-order superconductor and in the bubble model [1].

The lower stability of disclinations with a displaced centre compared with those at the centre of a crystallite can be explained using the linear theory of elasticity. The energy of displaced disclinations falls with increase in the displacement [7]. However, the tangential stresses grow along the line of slip of a dislocation on part of the surface of the disc, in the direction of which the disclination has moved [5]. This also explains the ease with which dislocations are nucleated on the surface of a crystallite with a mixed disclination.

The configuration depicted in Fig. 5d can be interpreted as a partial disclination of strength $\omega_p \approx 25^\circ$. This disclination differs from normal partial disclinations previously examined [2] in that its strength is governed not only by misorientation of the torn-off tilt boundary, but also by strength $\omega = -\pi/3$ of the previously introduced total disclination $\omega_p = \varphi_{ob} + \omega$. Thus, during relaxation an unstable configuration with a total disclination rearranges into a configuration with a partial disclination that is more advantageous in energy terms.

RESULTS

1. The core of perfect positive and negative disclinations is unstable. The core is modified by amorphization when point defects are introduced or when dislocations are nucleated on the surface of the crystallite, or when the total disclination is transformed to a partial disclination. All these processes are accompanied by a reduction in energy of the crystallite.

2. The linear theory of elasticity, supplemented by allowance for the influence of the surface, gives a correct quantitative description of the energy parameters of a disclination in crystallites of finite size. Non-linear atomic interaction effects result in non-zero positive dilation (of the order of a few percent) of the crystallite with disclinations.

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