Plastic deformation and decay of dislocations in quasi-crystals

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Abstract

The motion of special (mobile) partial dislocations is proposed as being an effective micromechanism of plastic deformation in quasi-crystalline materials. The decay of perfect topological dislocations into partial dislocations, which serves as a source of mobile partial dislocations, is theoretically examined.

1. Introduction

Quasi-crystals—solids with a long-range orientational order and a long-range quasi-periodic translational order—are the subject of intensive theoretical and experimental studies (for a review, see for instance refs. 1–5). Of special interest is the investigation of dislocations in quasi-crystals [5–14], since such defects essentially influence the physicomechanical properties of quasi-crystals. At present, mainly perfect topological dislocations in quasi-crystals, being analogues of perfect topological dislocations in conventional crystals, have been studied. However, perfect dislocations in crystals often decay into partial dislocations. This leads us to think that the perfect-dislocation decay can also occur in quasi-crystals. The above statement is supported by experimental data [13]. The main purpose of the present paper is to analyse theoretically the decay of perfect topological dislocations into partial dislocations in quasi-crystals and to discuss the role of partial dislocations in plastic deformation in quasi-crystals.

2. Decay of topological perfect dislocations

Consider a perfect dislocation in a three-dimensional icosahedral quasi-crystal. Such a dislocation is characterized by a (six-dimensional) Burgers vector $\boldsymbol{B}$ and induces elastic and phason distortions in the quasi-crystal. In doing so, the six-vector $\boldsymbol{B}$ can be decomposed into a "translational" Burgers three-vector $\boldsymbol{b}$ and a "phason" Burgers three-vector $\boldsymbol{\beta}$ ($\boldsymbol{B}=(\boldsymbol{b}, \boldsymbol{\beta})$) which define the dislocation-induced fields of elastic and phason distortions respectively [6–9].

Let us consider the decay of a perfect straight dislocation into two partial dislocations in an icosahedral quasi-crystal (Fig. 1). For geometrical reasons, each partial dislocation bounds a plane stacking fault in the quasi-crystal [8]. As a corollary, as with crystals, the decay of the perfect dislocation in the quasi-crystal is followed by the formation of a plane stacking fault between two partial dislocations (Fig. 1).

The change in the phason distortion field is a very slow process which is conditioned by the diffusion in the quasi-crystal [4, 5, 7, 8]. Therefore dislocations characterized by Burgers vectors with a non-zero "phason" three-component $\boldsymbol{\beta}$ are immobile in the quasi-crystal, since their motion requires considerable changes in the "quenched" phason field [7, 8]. Under

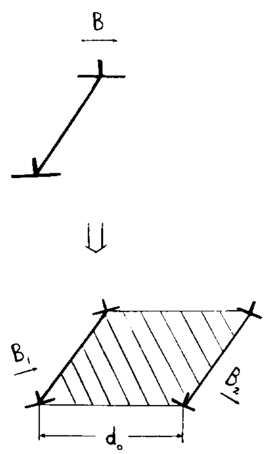

Fig. 1. The decay of the perfect dislocation into two partial dislocations, mobile and immovable, is accompanied by the formation of the plane stacking fault (shaded region). $\boldsymbol{B}$, $\boldsymbol{B}_1$ and $\boldsymbol{B}_2$ are (schematically) the Burgers six-vectors of the dislocations. d is the distance between the partial dislocations.

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these circumstances, we think that only the following scenario is possible for the perfect-dislocation decay. When the decay of the perfect dislocation with a Burgers six-vector $\boldsymbol{B}=(\boldsymbol{b}, \boldsymbol{\beta})$ occurs, the first resultant partial dislocation is characterized by a Burgers vector $\boldsymbol{B}_1=(\boldsymbol{b}_1, \boldsymbol{\beta})$ (having the same "phason" three-component $\boldsymbol{\beta}$, as with the perfect dislocation) and is immobile, while the second resultant partial dislocation with a Burgers vector $\boldsymbol{B}_2=(\boldsymbol{b}_2, \boldsymbol{0})$ (having a zero "phason" three-component) moves through a distance d (Fig. 1). In terms of Burgers vectors the above perfect-dislocation decay is characterized by

$$\boldsymbol{B}(\boldsymbol{b},\boldsymbol{\beta})\rightarrow\boldsymbol{B}_1(\boldsymbol{b}_1,\boldsymbol{\beta})+\boldsymbol{B}_2(\boldsymbol{b}_2,\boldsymbol{0}) \quad (1)$$

When such a scenario of the perfect-dislocation decay is realized, only elastic-field changes occur, whereas the "quenched" phason field is invariable.

Let us consider the energy characteristics of the above-discussed perfect-dislocation decay process (Fig. 1). (In doing so, hereafter the translational Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ of the partial dislocations are assumed to be parallel ($b=b_1+b_2$) for simplicity.) The perfect-dislocation decay is accompanied by a change in the unit-length dislocation energy, which is as follows:

$$\Delta F=\Delta F^{\mathrm{d}}(\boldsymbol{B},\boldsymbol{B}_1,\boldsymbol{B}_2)+F^{\mathrm{SF}}+F^{\mathrm{el\text{-}el}}(\boldsymbol{b}_1,\boldsymbol{b}_2) + F^{\mathrm{el\text{-}ph}}(\boldsymbol{\beta},\boldsymbol{b}_2) \quad (2)$$

where ΔF^{d} denotes the difference between the proper energies of the partial dislocations and the proper energy of the perfect dislocation, F^{SF} the stacking fault energy, $F^{\mathrm{el\text{-}el}}$ the energy of elastic interaction between the partial dislocations, $F^{\mathrm{el\text{-}ph}}$ the energy of the interaction between the phason field of the immovable partial dislocation and the elastic field of the mobile partial dislocation. If the energy change $\Delta F<0$, the perfect-dislocation decay is energetically profitable.

Let us now discuss the structure of ΔF in detail. During the decay process, the phason field of the decaying dislocation remains constant. Therefore the property-energy change ΔF^{d}—the first component of ΔF—is related to only translational Burgers vectors of the perfect and partial dislocations and, as with conventional crystals [15, 16], is approximately defined by the formula

$$\Delta F^{\mathrm{d}}\approx\frac{\mu}{4\pi(1-\nu)}(b_1^{\,2}+b_2^{\,2}-b^2) \quad (3)$$

where $b=b_1+b_2$, μ is the shear modulus and ν is the Poisson ratio.

The stacking fault energy F^{SF}—the second component of ΔF—is defined as follows:

$$F^{\mathrm{SF}}=\gamma d \quad (4)$$

where γ and d are the specific energy of the stacking fault and the distance between the partial dislocations (Fig. 1) respectively.

Let us now discuss the elastic-interaction energy $F^{\mathrm{el\text{-}el}}$ which is the third component of ΔF. The theory of elastic distortions in quasi-crystals is identical with that in conventional crystals [4, 6–8]. As a corollary, $F^{\mathrm{el\text{-}el}}$ is defined via the ordinary formula for elastic interaction between two dislocations separated by the distance d in a conventional crystal:

$$F^{\mathrm{el\text{-}el}}(b_1,b_2)\approx\frac{\mu b_1 b_2}{2\pi(1-\nu)}\ln\left(\frac{R}{d}\right) \quad (5)$$

with R being the screening length for elastic fields of the partial dislocations in the quasi-crystal.

Let us now consider $F^{\mathrm{el\text{-}el}}$, the fourth component of ΔF. In accordance with the theory of distortions in quasi-crystals [4, 6–8], one has

$$F^{\mathrm{el\text{-}ph}}\sim\int_S \boldsymbol{\nabla} u_{\mathrm{m}}(\boldsymbol{r})\cdot\boldsymbol{\nabla}\omega_{\mathrm{i}}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \quad (6)$$

Here $u_{\mathrm{m}}(\boldsymbol{r})$ denotes the elastic field of the mobile partial dislocation, $\omega_{\mathrm{i}}(\boldsymbol{r})$ the phason field of the immovable partial dislocation, $\boldsymbol{r}$ the two-vector in the plane perpendicular to the defect lines and $S(\approx R^2)$ the area of this plane. Following ref. 7, $|\boldsymbol{\nabla}u_{\mathrm{m}}(\boldsymbol{r})|\propto b/r$ and $|\boldsymbol{\nabla}\omega_{\mathrm{i}}(\boldsymbol{r})\propto\beta/r$. In this event, eqn. (6) is structurally like the well-known (see for instance ref. 16) formula for the energy of elastic interaction betwen two parallel dislocations in a conventional crystal. This allows us to use the results of the standard theory of dislocations in crystals in order to find the concrete structure of $F^{\mathrm{el\text{-}ph}}$. In doing this, with the aid of the above-mentioned results one obtains

$$F^{\mathrm{el\text{-}ph}}\approx\kappa C b_2\beta\ln\left(\frac{R}{d}\right) \quad (7)$$

where C is a constant (the renormalized constant of the elastic–phason interaction); $\kappa=\pm1$, depending on the orientations of the vectors $\boldsymbol{b}_2$ and $\boldsymbol{\beta}$.

From (2)–(5) and (7), one finds the following approximate formula for ΔF:

$$\Delta F\approx\frac{\mu}{4\pi(1-\nu)}(b_1^{\,2}+b_2^{\,2}-b^2)+\gamma d + \frac{\mu b_1 b_2}{2\pi(1-\nu)}\ln\left(\frac{R}{d}\right)+\kappa C b_2\beta\ln\left(\frac{R}{d}\right) \quad (8)$$

If we do not take into account the last term on the right-hand side of eqn. (8), this equation becomes identical with that describing the energetics of the decay of a perfect topological dislocation with a Burgers vector $\boldsymbol{b}$ into two partial dislocations with Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ ($b = b_1 + b_2$) in a crystal. In this event we conclude that the basic impeding force for the perfect-dislocation decay in a quasi-crystal, as in crystals [16], is related to the formation of stacking fault; this impeding force is described by the term γd in eqn. (8).

The elastic–phason interaction between the partial dislocations, which is described by the last term on the right-hand side of eqn. (8), can support (if $\kappa = -1$) or impede (if $\kappa = 1$) the decay process in a quasi-crystal. To the present author's knowledge, at present the constant C of elastic–phason interaction has not been defined experimentally or theoretically. Therefore one cannot estimate the quantitative contribution of the elastic–phason interaction to energetics of the decay process. Nevertheless, by assuming that values of μ, ν, γ and R in quasi-crystals are close to typical values in crystals one finds that the energy criterion ($\Delta F < 0$) for perfect-dislocation decay in a quasi-crystal when $\kappa = -1$ is "softer" than the criterion for dislocation decay in a crystal. As a corollary, the perfect-dislocation decay in a quasi-crystal (Fig. 1), like crystals, represents an energetically permissible process, provided that the specific energy γ of the stacking fault (which defines the basic impeding force for the decay) is small.

When the perfect-dislocation decay occurs in a quasi-crystal, the "equilibrium" distance d_0 between partial dislocations (Fig. 1) is defined via the condition $\partial(\Delta F)/\partial d|_{d=d_0} = 0$, giving

$$d_0 \approx \left(\frac{\mu b_1 b_2}{2\pi(1-\nu)} + \kappa C b_2 \beta\right) \gamma^{-1} \tag{9}$$

Thus the results in the present section allow one to conclude that perfect dislocations can decay into partial dislocations, both mobile and immovable (Fig. 1), in quasi-crystals.

3. Partial dislocations and plastic deformation in quasi-crystals

Let us now discuss the micromechanisms for plastic deformation in quasi-crystals. The mobility of perfect dislocations in quasi-crystalline alloys is very low, since the motion of perfect dislocations is associated with essential changes in "quenched" phason distortion fields [7]. Under these circumstances, the motion of the partial dislocations with "pure" translational Burgers vectors can be naturally thought of as the basic micromechanism for plastic flow in quasi-crystals. In fact, a transfer of such partial dislocations, unlike perfect dislocations, is not related to any changes in phason fields. Therefore the mobility of the partial dislocations with pure translational Burgers vectors, generally speaking, is essentially higher than that of perfect dislocations, in which case the mobile partial dislocations serve as basic carriers of plastic deformation in quasi-crystals.

Let us now consider the features of motion of mobile partial dislocations in deformed quasi-crystals with the assumption that such dislocations are formed during the decay of perfect dislocations (Fig. 1). For geometric reasons a stacking fault is formed behind each moving partial dislocation (Fig. 1). The stacking fault formation defines the basic impeding force for motion of the mobile partial dislocation, which accompanies the perfect-dislocation decay (see Section 2). All the impeding and driving forces for motion of the mobile partial dislocations—elements of decayed dislocations—in an unloaded quasi-crystal are described by the components of ΔF (see Section 2). A mechanical load induces an additional driving force τb_2 (where τ is the shear stress) which acts upon the mobile partial dislocation with a Burgers vector $\boldsymbol{b}_2$ in the quasi-crystal. This force causes each mobile partial dislocation to transfer from its initial "equilibrium" position (conditioned by $\partial(\Delta F)/\partial d = 0$; see Section 2) to a new position (Fig. 2). In this event the distance between the partial dislocations, immovable and mobile elements of a decayed dislocation, changes as $d_0 \to d'$, in which case d' is defined by the condition

$$\left.\frac{\partial(\Delta F - \tau\beta_2 d)}{\partial d}\right|_{d=d'} = 0 \tag{10}$$

This condition, which is related to the balance between the impeding and driving forces for motion of the mobile partial dislocations in a mechanically loaded quasi-crystal, gives

$$d' = \frac{D}{\gamma - \tau b_2} \tag{11}$$

where

$$D = \frac{\mu b_1 b_2}{2\pi(1-\nu)} + \kappa C b_2 \beta \tag{12}$$

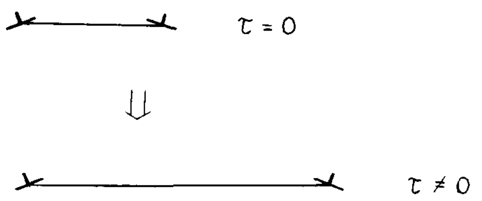

Fig. 2. Evolution of the structure of a decayed dislocation in a quasi-crystal under a mechanical load.

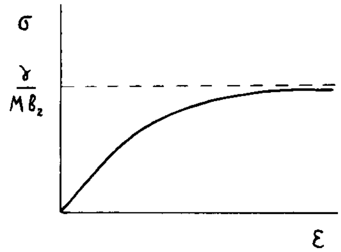

Fig. 3. The σ–ε dependence (schematic) for the quasi-crystalline sample under active loading. By basic carriers of plastic flow we mean the mobile partial dislocations which are elements of decayed dislocations.

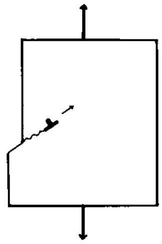

Fig. 4. The mobile partial dislocation "enters" the interior of the quasi-crystalline sample from the surface under a mechanical load. The stacking fault (~~~) is formed behind the moving dislocation.

Let us define the "flow stress σ – plastic deformation degree ε" dependence for a quasi-crystal under active loading (deformation regime $\dot{\varepsilon}$ = constant) on the assumption that (a) plastic flow occurs mainly by moving partial dislocations which are elements of decayed dislocations and (b) the parameters of all the mobile dislocations which take part in the plastic deformation are approximately identical. In this situation the Orowan formula

$$\varepsilon \approx \rho b_2(d' - d_0) \tag{13}$$

gives the relationship between ε, b_2, the density ρ of mobile partial dislocations and the mechanical-load-induced path $d' - d_0$ of each mobile partial dislocation.* From (9) and (11)–(13), one obtains

$$\sigma = \frac{\tau}{M} \approx \frac{\varepsilon\gamma^2}{M(\rho D b_2^2 + \varepsilon\gamma b_2)} \tag{14}$$

with M being the standard orientational factor (Fig. 3). For small values of ε ($\varepsilon \ll \rho D b_2/\gamma$), eqn. (14) approximately shows that the flow stress σ runs parallel to ε:

$$\sigma \approx \frac{\gamma^2}{M\rho D b_2^2}\,\varepsilon \tag{15}$$

For large values of ε, according to (14), the flow stress σ asymptotically approaches the value γ/Mb_2 (Fig. 3).

Together with the mobile partial dislocations which are elements of decayed dislocations, the mobile partial dislocations which "enter" the quasi-crystalline sample from its surface (Fig. 4) can also take part in plastic deformation. We now discuss the situation in which plastic flow is mainly provided by the motion of the partial dislocations entering the interior of a loaded quasi-crystalline sample from the surface. For motion of such dislocations the balance between the impeding and driving forces is as follows:

$$\tau b_2 \approx \gamma \tag{16}$$

in which case one finds the flow stress

$$\sigma \approx \frac{\gamma}{Mb_2} \tag{17}$$

(Fig. 5).

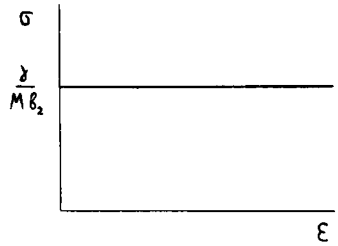

Fig. 5. The σ–ε dependence for the quasi-crystalline sample under active loading. By basic carriers of plastic flow we mean the mobile partial dislocations "entering" the interior of the loaded quasi-crystalline sample from the surface.

The σ–ε dependences that we have obtained previously, of course, are rather approximate. In revealing these σ–ε dependences (see eqns. (14) and (17)), we have assumed that all the mobile partial dislocations have approximately identical constant parameters (Burgers vectors etc.)*; interactions between dislocations (carriers of plastic flow) as well as the viscosity of the dislocation motion are not taken into account, the free-surface influence upon the dislocation motion is neglected etc. Nevertheless, we think that the suggested model correctly defines the basic micromechanism for plastic flow in quasi-crystals and takes into account the

*In the general situation (when assumption (b) is invalid) the Orowan formula contains the mean values $\langle\rho\rangle$, $\langle b_2\rangle$ and $\langle d' - d_0\rangle$.

*In real quasi-crystals, of course, Burgers vectors of different dislocations differ. Furthermore, generally speaking, the mobile partial dislocations in quasi-crystals, as with dislocations in metallic glasses [5, 17, 18], can have variable (in time and along the dislocation line) Burgers vectors.

basic factors which influence the plastic properties of quasi-crystals. This leads us to treat the proposed model as a basis for future studies of microscopic aspects of plastic deformation in quasi-crystalline alloys.

Quasi-crystals usually represent rather brittle solids (see for instance refs. 1, 4 and 7). Within the framework of the suggested model this can be naturally explained as follows. Real quasi-crystalline alloys are characterized by high values of the specific energy γ for stacking faults and contain few perfect dislocations which are internal sources of mobile partial dislocations. In this situation the "visible" plastic deformation of a loaded quasi-crystalline sample can occur as a result only of motion of mobile partial dislocations entering the sample from its surface (Fig. 4). Such a deformation is characterized by a large (at high values of γ) constant flow stress $\sigma \approx \gamma / M b_2$ (Fig. 5) and therefore cannot effectively compete with failure processes in quasi-crystals. As a corollary, quasi-crystalline alloys are brittle solids.

If the above explanation is valid, to improve the plastic properties of quasi-crystals one has to increase the density of the perfect dislocations and/or chemically (by special impurities) decrease the value of γ.

4. Conclusion

Thus perfect dislocations can decay into partial dislocations in quasi-crystals. The perfect-dislocation decay occurs by transfer of a mobile partial dislocation with a pure translational Burgers vector and is accompanied by the formation of a stacking fault (Fig. 1). The mechanical-load-induced motion of the mobile partial dislocations represents an effective micromechanism for plastic flow in quasi-crystals.

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