Eur. Phys. J. B 1, 429–437 (1998)

THE EUROPEAN PHYSICAL JOURNAL B

Special interaction between quasiperiodic grain boundaries and lattice dislocations in crystalline solids

M.Yu. Gutkin[a] and I.A. Ovid'ko

Institute of Machine Science Problems, Russian Academy of Sciences, Bolshoj 61, Vas.Ostrov, St.Petersburg 199178, Russia

Received: 29 October 1996 / Revised: 22 August 1997 / Accepted: 13 November 1997

Abstract. A theoretical model is suggested which describes phason imperfections (specific excitations) in a quasiperiodic grain boundary in a polycrystalline solid as dilatation flexes. In the framework of the model, an elastic stress field of the quasiperiodic grain boundary is calculated as a stress field created by an ensemble of dilatation flexes (phason imperfections) located in the boundary. It is shown that there is a special elastic interaction between crystal lattice defects and quasiperiodic grain boundaries comprising phason imperfections. The strengthening effect in plastically deformed polycrystalline solids is quantitatively described which is related to the special elastic interaction between lattice dislocations and quasiperiodic grain boundaries.

PACS. 62.20.Fe Deformation and plasticity (including yield, ductility, and superplasticity) – 68.35.Ct Interface structure and roughness – 68.35.Dv Composition; defects and impurities

1 Introduction

Periodic grain boundaries in polycrystalline solids represent the traditional subject of intensive theoretical and experimental studies in materials science and solid state physics [1,2]. Periodic boundaries are well-known to essentially influence physical and mechanical properties of polycrystalline solids. In the general situation, polycrystals contain not only periodic but also quasiperiodic boundaries [3–10]. At present, features of polycrystals with quasiperiodic boundaries are little-known; their study is just at the starting point.

The structure and properties of quasiperiodic grain boundaries characterized by irrational disorientation parameters are different from those of "standard" periodic boundaries [3–10]. However, presently available experimental methods are weekly effective in the direct indication of the difference between periodic and quasiperiodic boundaries [4]. In other words, the presently available experimental methods, in fact, do not allow to directly and definitely recognize quasiperiodic boundaries in polycrystals. In these circumstances, of utmost interest are theoretical models which describe the features of polycrystals with quasiperiodic boundaries. Such models allow to theoretically reveal the contributions of quasiperiodic boundaries to the macroscopic properties of polycrystalline solids, in which case the models can serve as a basis for indirect experiments (related to the measurements of values characterizing the macroscopic properties of polycrystals) capable of recognizing quasiperiodic boundaries in polycrystals. In this context, recently, the special contribution of quasiperiodic boundaries to intergrain sliding processes in nanostructured polycrystals has been theoretically revealed [8,9]. Results of the studies [8,9] serve as an indirect confirmation of both existence and the specific role of quasiperiodic boundaries in nanostructured polycrystals (in particular, in quasinanocrystalline solids being nanostructured solids of a new type).

The main aim of this paper is to suggest a theoretical model which describes the elastic interaction between crystal lattice dislocations and quasiperiodic boundaries in polycrystals. In the framework of the suggested model, a contribution to the strengthening of plastically deformed polycrystals is calculated which is related to the above interaction.

2 Features of quasiperiodic boundaries in polycrystals

The notion of quasiperiodic grain boundaries is not widespread. Therefore, in the first part of this section we, following to [3–10], briefly discuss the basic features of quasiperiodic grain boundaries. In spirit of the general theory of quasiperiodic systems [11–13], a quasiperiodic grain boundary in a crystal is defined as a translationally ordered grain boundary having a reciprocal lattice with rank (number of independent basic vectors[1]) larger than

[a] e-mail: gutkin@pgpt.ioffe.rssi.ru

[1] Vectors $Y_1, \dots, Y_p$ are called independent, provided the expression $r_1 Y_1 + \cdots + r_p Y_p = 0$ (with r_j being rational) is valid for only case $r_1 = \cdots = r_p = 0$.

the dimension of this grain boundary. It means that diffraction pattern of a n-dimensional quasiperiodic boundary consists of sharp peaks, each is unambiguously indexed by m integers, where $m > n$. (Please let us remind that any n-dimensional periodically ordered grain boundary has diffraction pattern consisting of sharp peaks unambiguously indexed by $m = n$ integers.) So, according to the above definition, quasiperiodic grain boundaries, as with periodic boundaries, have a long-range translational order; it is reflected in the fact that diffraction patterns of both quasiperiodic and periodic boundaries consist of sharp peaks. However, the translational order of a quasiperiodic boundary is characterized by relationship ($n < m$) between dimensions of a boundary (n) and its reciprocal lattice (m), which is different from the corresponding relationship ($n = m$) inherent to periodic boundaries. In this context, quasiperiodic grain boundaries form the specific (new) class of translationally ordered boundaries, being different from the (standard) class of periodic grain boundaries, see, for details, [3,4,8]. (In general, quasiperiodic grain boundaries too belong to the general class of quasiperiodic systems such as quasicrystals [11–13] and quasiperiodic grain boundaries in quasicrystals [14]. In doing so, n-dimensional systems with m-dimensional ($m > n$) patterns are traditionally termed "quasiperiodic" in mathematics [15].)

As to geometry and conditions of formation of quasiperiodic grain boundaries, they are formed when there is an irrational misorientation (characterized by irrational Euler angles) between adjacent grains and/or boundary plane is irrationally oriented relative to adjacent grains, see, for details, [3,4]. Generally speaking, quasiperiodic boundaries can be plane or curved.

In spirit of structural-unit model [16], quasiperiodic boundaries can be represented as quasiperiodically ordered ensembles of structural units. So, quasiperiodic tilt boundaries are effectively modeled as quasiperiodic sequences of structural units of two types[2], A and B (Figs. 1a and b) [4,10].

Quasiperiodic grain boundaries (as with other quasiperiodic systems [11–14]) have not only standard translational degrees of freedom but also so-called phason degrees of freedom [3,4,8]. In terms of structural-unit model of quasiperiodic boundaries, the phason degrees of freedom of a quasiperiodic boundary are associated with those rearrangements of structural units (for instance, A $\leftrightarrow$ B interchanges) which do not change diffraction pattern of this boundary [2,4,8]. On the other hand, these (phason-type) rearrangements transform the initial quasiperiodic boundary structure to a new quasiperiodic boundary structure being locally indistinguished from the initial structure or, in other terms, being locally isomorphic [8–10] to the initial structure.

[2] The term "quasiperiodic sequence of structural units" is used here in the following sense: 1-dimensional sequence (lattice) of δ-functions — nodes of segments, A and B, which model structural units — is quasiperiodic; its Fourier image is a reciprocal lattice generated by two relatively irrational basic vectors.

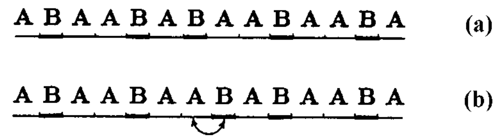

Fig. 1. Quasiperiodic tilt boundaries (structural unit representation). (a) A perfect quasiperiodic tilt boundary is modelled as a quasiperiodic consequence of A and B structural units. One cannot find any periodically repeated finite-length motif (a finit-length "word" made out of an alphabet of letters A and B) in the boundary. (b) A new perfect quasiperiodic tilt boundary resulted from the initial boundary (shown in Fig. 1a) in which an interchange A $\leftrightarrow$ B occurs. The initial and new boundaries are locally indistinguished. It means that any finite-length fragment of the new boundary (Fig. 1b) can be found in the initial boundary (Fig. 1a).

Two (infinite) quasiperiodic systems Z_1 and Z_2 are defined as locally isomorphic (locally indistinguished), if any finite fragment of the system Z_1 can be found in the system Z_2 and *vice versa* [11–13]. In this event, the system Z_1 as a whole, generally speaking, is different from the system Z_2; the system Z_1 can not be obtained as a result of some translation of the system Z_2. For instance, the phason degrees of freedom of a quasiperiodic tilt boundary, represented as a quasiperiodic consequence of A and B structural units, are associated with A $\leftrightarrow$ B interchanges which transform the quasiperiodic boundary to a new boundary being locally indistinguished from the initial boundary (Figs. 1a and b).

Phason-type rearrangements of structural units of a (infinite-length) quasiperiodic boundary leave its free energy as invariant [8]. However, in general, there are too rearrangements of structural units of a quasiperiodic boundary which increase its free energy. Such rearrangements result in formation of the so-called phason imperfections being specific excitations of quasiperiodic boundaries (see next section).

3 Phason imperfections as dilatation flexes

As noted in previous section, quasiperiodic boundaries can contain specific (inherent to only quasiperiodic systems) excitations, the so-called phason imperfections [4,7]. The phason imperfections in a quasiperiodic boundary are associated with special boundary fragments being locally distinguished from perfect boundary structures. In the general situation, by direct analogy with phason imperfections in quasicrystals [11–13,17], we characterize phason imperfections in quasiperiodic boundaries as follows [7]. Phason imperfections in a quasiperiodic boundary represent flexes comprising point excitations (Fig. 2). Each such excitation is a point where the ideal (low-energy) packing of structural units of the boundary is broken; "wrong" packing is realized in the point excitation which, therefore, creates a short-range stress field and is specified by some excess energy. In other words, a phason imperfection in a quasiperiodic grain boundary, in many respects, looks like a flex of grain boundary impurities (Fig. 2).

Fig. 2. Representation of a phason imperfection as a flex comprising point excitations (whose properties are close to those of grain boundary impurities).

The exact structure of the point excitations being consistent of phason imperfections can vary rather widely, depending on the structure of a quasiperiodic boundary. For definiteness, we restrict our consideration to only vacancy-like and intersite-like excitations with the properties of vacancy-like impurities and intersite-like impurities, respectively. We do it, since vacancy-like and intersite-like impurities are typical grain boundary excitations (related to wrong packings of boundary structural units) and are most powerful sources of stresses as compared with grain boundary impurities of other types.

Then, in the framework of the suggested model, phason imperfections are treated as chains of either vacancy-like excitations or intersite-like ones. Elastic stress fields of such chains can be effectively modelled as those of dilatation flexes. In this case, a dilatation flex represents a strained cylinder with proper elastic deformation being a pure dilatation (pure expansion or pure compression), located in an elastic medium. A fibre composite material, whose fibres have the thermal expansion coefficient being different from that of matrix, serves as the characteristic example of a material with dilatation flexes. In context of the suggested model, the two following types of dilatation flexes are present in a quasiperiodic boundary: vacancy-type dilatation flexes (corresponding to phason imperfections comprising vacancy-like point excitations) and intersite-like dilatation flexes (corresponding to phason imperfections comprising intersite-like excitations).

4 General features of special interaction between quasiperiodic boundaries and lattice defects

In previous section we have constructed a model representation of phason imperfections in a quasiperiodic grain boundary as dilatation flexes. In this context, the dilatation flexes are boundary excitations characterized by elastic stress fields which determine the elastic stress field of the quasiperiodic boundary. As a corollary, the quasiperiodic boundary containing dilatation flexes (phason imperfections) is capable of elastically interacting with crystal lattice defects (dislocations and disclinations) located near the boundary.

The elastic interaction between lattice defects and a quasiperiodic boundary, described as the interaction between lattice defects and an ensemble of dilatation flexes (phason imperfections) in the boundary, is rather special. This interaction is inherent to only quasiperiodic grain boundaries and has not analogue for periodic boundaries, since phason imperfections are inherent to only quasiperiodic boundaries.

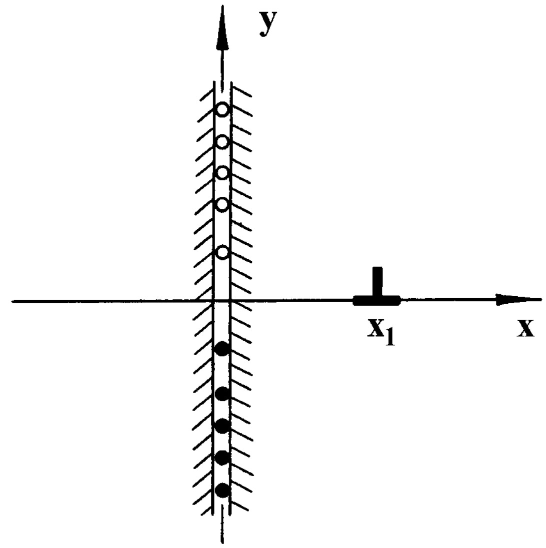

Fig. 3. An edge dislocation is located near a quasiperiodic grain boundary (shown as layer with thickness $2r_0$) comprising vacancy-type and intersite-type dilatation flexes (shown as open and full circles with radius r_0, respectively). The dislocation coordinates are $(x = x_1, y = 0)$.

A quantitative description of the special elastic interaction allows to (indirectly) recognize some specific features of quasiperiodic grain boundaries, which differ quasiperiodic boundaries from periodic ones. Below we quantitatively describe the special interaction between quasiperiodic boundaries and lattice dislocations. In doing so, the particular attention is paid to the strengthening effect, related to the special interaction, in plastically deformed polycrystalline solids.

Let us consider a quasiperiodic grain boundary comprising dilatation flexes (phason imperfections) under thermally equilibrium conditions. Spatial distribution of dilatation flexes in the boundary depends on temperature, geometric characteristics of the boundary and an external stress field. In following sections we shall examine the particular situation in which the external stress field is created by a lattice edge dislocation located near the quasiperiodic boundary. A quantitative description of this situation consists of three basic stages. First, we shall calculate the stress field of one dilatation flex (Sect. 5). Second, we shall calculate the stress field of the quasiperiodic boundary as a sum of the stress fields of dilatation flexes located in the boundary (Sect. 6). Finally, we shall calculate the shear stress acting on dislocation (Fig. 3) due to the special elastic interaction between the dislocation and the quasiperiodic boundary (Sect. 7).

It should be noted that lattice dislocations located near a quasiperiodic boundary not only elastically interact with the boundary but also can create new phason imperfections in the boundary [7]. Occurrence and contribution of this effect to the strengthening of a plastically deformed polycrystalline solid depend on the structure and properties of the quasiperiodic boundary. For instance, the effect in question does not occur in quasiperiodic tilt boundaries

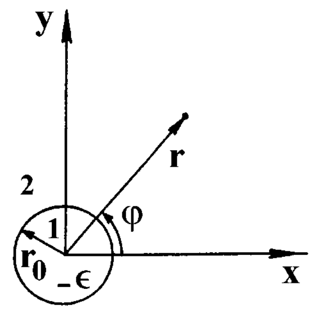

Fig. 4. A dilatation flex (shown as circle with radius r_0) in an elastic medium. $-\epsilon$ is the dilatation eigenstrain of the flex.

and is insignificant in quasiperiodic boundaries comprising high-density ensembles of "standard" phason imperfections (which are not related to presence of lattice dislocations near quasiperiodic boundaries). In this paper we restrict our consideration to the situations in which the dislocation-induced generation of new phason imperfections are not essential.

5 Elastic stress field of dilatation flex (phason imperfection)

Consider a dilatation flex serving as a model for a phason imperfection in a quasiperiodic grain boundary. Elastic stress field of the dilatation flex can be calculated in the same standard way as thermally induced elastic stresses when two elastic solids contact, having different coefficients of thermal expansion [18,19].

In doing so, let us consider a deformed cylinder with the radius r_0 and the length L ($L \gg r_0$), which is located in an elastic medium being free from other sources of stresses (Fig. 4). Let G and ν be respectively the shear modulus and the Poisson ratio for both the cylinder and the elastic medium. Let the eigenstrain of the cylinder be pure dilatation $\epsilon^*_{ij} = -\epsilon\delta_{ij}$, where δ_{ij} is the Croneker function ($\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$). Then the total resulting strain fields are as follows,

$$\varepsilon^{(1)}_{ij} = e^{(1)}_{ij} + \epsilon^*_{ij} = e^{(1)}_{ij} - \epsilon\delta_{ij} \ , \quad (1)$$

$$\varepsilon^{(2)}_{ij} = e^{(2)}_{ij} \ , \quad (2)$$

where $e^{(k)}_{ij}$ is the elastic part of the strain field which acts in kth area, $k = 1, 2$ (Fig. 4).

Due to the central symmetry of the problem, the shear components of the elastic strain field are equal to zero in the cylindrical co-ordinate system and we have the following set of normal strain components:

$$\varepsilon^{(1)}_{rr} = e^{(1)}_{rr} - \epsilon \ , \quad \varepsilon^{(1)}_{\varphi\varphi} = e^{(1)}_{\varphi\varphi} - \epsilon \ , \quad \varepsilon^{(1)}_{zz} = e^{(1)}_{zz} - \epsilon \ , \quad (3)$$

$$\varepsilon^{(2)}_{rr} = e^{(2)}_{rr} \ , \quad \varepsilon^{(2)}_{\varphi\varphi} = e^{(2)}_{\varphi\varphi} \ , \quad \varepsilon^{(2)}_{zz} = e^{(2)}_{zz} \ . \quad (4)$$

The tensor of total strains is by definition $\varepsilon^{(k)}_{ij} = [\mathrm{grad}\, u^{(k)}_{\mathrm{i}}]^{\mathrm{s}}$, where $u^{(k)}_{\mathrm{i}}$ is the vector of total displacements in kth area and the symbol $[\ldots]^{\mathrm{s}}$ means the symmetric part. It gives in our case

$$\varepsilon^{(k)}_{rr} = \frac{\partial u^{(k)}_r}{\partial r} \ , \quad \varepsilon^{(k)}_{\varphi\varphi} = \frac{u^{(k)}_r}{r} \ , \quad \varepsilon^{(k)}_{zz} = \frac{\partial u^{(k)}_z}{\partial z} \equiv 0 \ . \quad (5)$$

The elastic stress tensor is

$$\sigma^{(k)}_{ij} = 2G\left(e^{(k)}_{ij} + \frac{\nu}{1-2\nu}\, e^{(k)}\right) \quad (6)$$

with $e^{(k)} = e^{(k)}_{ii}$; it may be presented as

$$\sigma^{(1)}_{rr} = 2G\left(\varepsilon^{(1)}_{rr} + \frac{\nu}{1-2\nu}\,\varepsilon^{(1)} + \frac{1+\nu}{1-2\nu}\,\epsilon\right) \ , \quad (7)$$

$$\sigma^{(1)}_{\varphi\varphi} = 2G\left(\varepsilon^{(1)}_{\varphi\varphi} + \frac{\nu}{1-2\nu}\,\varepsilon^{(1)} + \frac{1+\nu}{1-2\nu}\,\epsilon\right) \ , \quad (8)$$

$$\sigma^{(1)}_{zz} = 2G\,\frac{\nu\varepsilon^{(1)} + (1+\nu)\epsilon}{1-2\nu} \ , \quad (9)$$

$$\sigma^{(2)}_{ij} = 2G\left(\varepsilon^{(2)}_{ij} + \frac{\nu}{1-2\nu}\,\varepsilon^{(2)}\right) \ , \quad (10)$$

where $\varepsilon^{(k)} = \varepsilon^{(k)}_{ii}$.

Introducing equations (7–10) into the standard equilibrium equation [18]

$$\frac{\partial\sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\varphi\varphi}}{r} = 0 \quad (11)$$

and taking into account equations (5), one can find the following equilibrium equation for displacements

$$\frac{\mathrm{d}^2 u^{(i)}_r}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}u^{(i)}_r}{\mathrm{d}r} - \frac{u^{(i)}_r}{r^2} = 0 \ . \quad (12)$$

It is very simply to show, using the differential chain rule, that this equation have a solution in the form

$$u^{(k)}_r = A_k\, r + \frac{B_k}{r} \ , \quad (13)$$

where A_k and B_k are constants which should be obtained from the boundary conditions of our problem. These ones are as follows

$$u^{(1)}_r(r=0) \quad \text{is limited,} \quad (14)$$

$$u^{(2)}_r(r=\infty) \quad \text{is limited,} \quad (15)$$

$$u^{(1)}_r(r=r_0) = u^{(2)}_r(r=r_0) \ , \quad (16)$$

$$\sigma^{(1)}_{rr}(r=r_0) = \sigma^{(2)}_{rr}(r=r_0) \ . \quad (17)$$

As a result,

$$A_1 = -\frac{1+\nu}{1-\nu}\,\frac{\epsilon}{2} \ , \quad A_2 = 0 \ , \quad B_1 = 0 \ ,$$
$$B_2 = -\frac{1+\nu}{1-\nu}\,\frac{\epsilon}{2}\, r_{\mathrm{o}}^2 \ , \quad (18)$$

and we find through (5) and (7–10) the required solution $\sigma_{ij}(r)$ which is equal to $\sigma_{ij}^{(1)}$ when $r < r_0$ and to $\sigma_{ij}^{(2)}$ when $r > r_0$, in the following form:

$$\sigma_{rr}(r) = \sigma^* \begin{cases} 1, & 0 \le r < r_0, \\ r_0^2/r^2, & r > r_0, \end{cases} \tag{19}$$

$$\sigma_{\varphi\varphi}(r) = \sigma^* \begin{cases} 1, & 0 \le r < r_0, \\ -r_0^2/r^2, & r > r_0, \end{cases} \tag{20}$$

$$\sigma_{zz}(r) = \sigma^* \begin{cases} 2, & 0 \le r < r_0, \\ 0, & r > r_0, \end{cases} \tag{21}$$

where $\sigma^* = G\epsilon\frac{1-\nu}{1+\nu}$. The cases $\epsilon > 0$ and $\epsilon < 0$ correspond to vacancy-type and intersite-type dilatation flexes, respectively.

From (19–21), for $r_0 \approx a$ (with a being the crystal lattice parameter) and $r > r_0$, we find the stress field components σ_{xx}, σ_{yy} and σ_{xy} in Cartesian coordinates (x, y, z) to be as follows:

$$\sigma_{xx} = -\sigma_{yy} = \sigma^* r_0^2 (x^2 - y^2)/r^4,$$
$$\sigma_{xy} = \sigma^* r_0^2 2xy/r^4. \tag{22}$$

The other components of the dilatation flex stress tensor in Cartesian coordinates are equal to zero.

6 Continuum model of quasiperiodic grain boundary

Let us consider a quasiperiodic grain boundary which contains both vacancy-type and intersite-type phason imperfections. In the framework of the suggested model, the boundary is thought of as a three-dimensional flat layer with the thickness $2r_0$, the vacancy-type and intersite-type phason imperfections are viewed as vacancy-type and intersite-type dilatation flexes, respectively (Fig. 3). In the continuum representation, an ensemble of the dilatation flexes in the boundary is characterized by the flex distribution densities $\rho_k(y)$ being continuous functions of the boundary coordinate y, where $k = v, i$ is the index showing the vacancy-type (v) or intersite-type (i), of the dilatation flexes.

We consider the quasiperiodic boundary under thermally equilibrium conditions, in which case the densities $\rho_k(y)$ are "equilibrium" ones; they correspond to the minimum free energy of the solid. In a three-dimensional quasicrystal [20], the number of flexes n_k of kth type transecting a flat unit square surface which is normal to their axes, is equal to

$$n_k = N \exp\left(-\frac{E_k^{\mathrm{el}}}{kT}\right), \tag{23}$$

where N is the number of atomic positions at the surface, E_k^{el} the elastic energy of a flex per its segment with the length b, k the Boltzmann constant and T the absolute temperature.

The elastic energy E_k^{el} may be found using the well-known expression for an inclusion with uniform dilatation eigenstrain ϵ [19], in which case

$$E_k^{\mathrm{el}} = \frac{\pi G}{2}\,\frac{1+\nu}{1-\nu}\,\epsilon_k^2\, b^3 \,. \tag{24}$$

In the case when the dilatation flexes are distributed within a three-dimensional flat layer (a grain boundary model) which is placed in a stress field of an edge dislocation, the densities (per a unit square) C_{v} and C_{i} of vacancy- and intersite-type flexes may be written, in the first approximation, as follows

$$C_{\mathrm{v}}(x=0, y>0) = C_{\mathrm{v}0}\, \exp\left(\frac{\sigma^{(\mathrm{d})}(y)\,\Delta V_{\mathrm{v}}}{kT}\right), \tag{25}$$

$$C_{\mathrm{i}}(x=0, y<0) = C_{\mathrm{i}0}\, \exp\left(\frac{\sigma^{(\mathrm{d})}(y)\,\Delta V_{\mathrm{i}}}{kT}\right), \tag{26}$$

where $C_{\mathrm{v}0}$ and $C_{\mathrm{i}0}$ are respectively the densities of vacancy- and intersite-type flexes in the situation when the dislocation stress field is absent, $C_{k0} = n_k/(Nb^2)$; ΔV_k denotes the change in the volume of the solid, related to the formation of a unit length flex, $\Delta V_k \approx -\frac{3}{4}\pi\epsilon_k\, b^3$ ($\Delta V_{\mathrm{v}} < 0$, $\Delta V_{\mathrm{i}} > 0$); $\sigma^{(\mathrm{d})} = \sigma^{(\mathrm{d})}(y)$ is the hydrostatic component of the dislocation stress field in the plane $x = 0$ (Fig. 3). This component can be written as [21]:

$$\sigma^{(\mathrm{d})}(x=0, y) = -\frac{Gb}{3\pi}\,\frac{1+\nu}{1-\nu}\,\frac{y}{x_1^2 + y^2}\,. \tag{27}$$

Here b denotes the dislocation Burgers vector, x_1 the dislocation coordinate on axis $0x$ (Fig. 3). Formulae (25, 26), in particular, reflect the fact that the dislocation stress field causes vacancy-type flexes (intersite-type flexes, respectively) to be located in the region $y > 0$ ($y < 0$, respectively) where the hydrostatic component (27) of the dislocation stress field is negative (positive, respectively).

Then the linear density of flex distribution along the grain boundary may be naturally approximated as $\rho_k = 2r_0\, C_k(x=0, y)$. As a result, one can represent the elastic stress field of the quasiperiodic boundary as $\sigma_{mn}^{\Sigma} = \sigma_{mn}^{\Sigma(\mathrm{v})} + \sigma_{mn}^{\Sigma(\mathrm{i})}$, where the sum stress field of vacancy-type dilatation flexes is

$$\sigma_{mn}^{\Sigma(\mathrm{v})}(x, y) = 2\,r_0 \int_{\delta}^{+\infty} C_{\mathrm{v}}(y')\,\sigma_{mn}^{(\mathrm{v})}(x, y-y')\,\mathrm{d}y', \tag{28}$$

while the sum stress field of intersite-type dilatation flexes is

$$\sigma_{mn}^{\Sigma(\mathrm{i})}(x, y) = 2\,r_0 \int_{-\infty}^{-\delta} C_{\mathrm{i}}(y')\,\sigma_{mn}^{(\mathrm{i})}(x, y-y')\,\mathrm{d}y'. \tag{29}$$

The parameter δ is introduced here to avoid the stress and flex density singularities at the point ($x = 0$, $y = 0$) when the dislocation is localized there. It may be estimated from the condition $b\rho_k = b^2 C_k(x_1, y) \leq 1$ which means that no more than only one flex may occupy an atomic position along the grain boundary. A simple calculation shows that δ must satisfy to the inequality $\delta^2 + x_1^2 \geq \delta b/|2\pi\epsilon_k|$, where x_1 is the dislocation position. Assuming $|\epsilon_k| \geq 0.05$, we can find $\delta \approx b$ as a good estimate when $x_1 \geq b$ for any value of temperature T.

7 Force acting on dislocation

The elastic force, acting on a unit-length edge dislocation located near a quasiperiodic grain boundary (Fig. 3), can be expressed as follows:

$$F(x_1) = b\sigma_{xy}^{\Sigma}(x = x_1, y = 0), \qquad (30)$$

where the stress field σ_{xy}^{Σ} of the boundary is determined by formulae (22, 25–29).

In the approximation in which distribution of vacancy-type and intersite-type dilatation flexes is symmetric relative to axis $0x$ (the approximation corresponds to a rather realistic situation in which changes in the volume of the solid, related to formation of vacancy-like and intersite-like excitations, are close: $\Delta V_{\rm v} \approx -\Delta V_{\rm i}$; this approximation does not essentially influence final results of our calculations but, at the same time, allows us to carry out the calculations in a compact form), formula (30) can be rewritten as:

$$F(x_1) = 2b\sigma_{xy}^{\Sigma({\rm v})}(x = x_1, y = 0), \qquad (31)$$

where

$$\sigma_{xy}^{\Sigma({\rm v})}(x_1) = -4\sigma^* r_0^3\, x_1 C_{v0} \int\limits_{\delta}^{+\infty} \frac{y'}{(x_1^2 + y'^2)^2} \times \exp\left(\frac{Dy'}{x_1^2 + y'^2}\right) {\rm d}y', \qquad (32)$$

and $D = -\frac{Gb\Delta V_{\rm v}}{3\pi kT}\frac{1+\nu}{1-\nu} > 0$. With formulae (31, 32) and the above estimate for δ taken into account, the force F can be expressed as follows:

$$F(\xi) = -8\sigma^* r_0^3\, C_{v0}\, \xi \int\limits_{1}^{+\infty} \frac{\eta}{(\eta^2 + \xi^2)^2} \times \exp\left(\frac{q\eta}{\eta^2 + \xi^2}\right) {\rm d}\eta, \qquad (33)$$

where new dimensionless parameters $\xi = x_1/b$, $\eta = y'/b$ and $q = D/b$ are used.

For vacancy-type dilatation flexes, $\sigma^* > 0$ and integral on the r.h.s. of (33) is evidently positive. In this case, the force $F(\xi) \leq 0$ for any $\xi \geq 0$. It means that the quasiperiodic boundary attracts the dislocation due to the special elastic interaction between them.

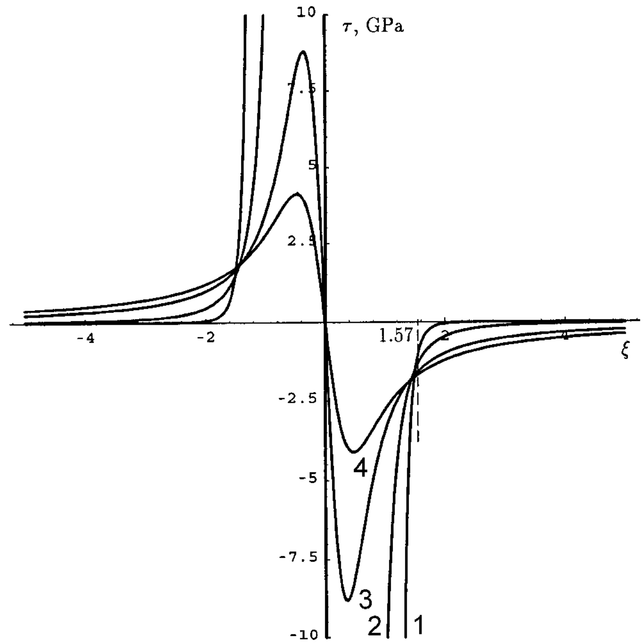

Fig. 5. Dependence of the stress τ, GPa, which acts on an edge dislocation due to the special elastic interaction between the dislocation and a quasiperiodic grain boundary, on the dislocation position $\xi = x_1/b$ for the values of temperature T = 100 (*1*), 300 (*2*), 800 (*3*) and 1300 K (*4*). The value $\xi = 1.57$ denotes the boundary of the region $|\xi| \geq 1.57$ where our model is correct.

Function $F(\xi)$ is antisymmetric, and $F(\xi=0)=F(\xi=\pm\infty) = 0$. Integral on the r.h.s. of (33), which determines value of the force $F(\xi)$, can be calculated only numerically. It is worth noting that two parameters figuring in formula (33), C_{v0} and q, depend strongly on the temperature T.

To represent our results in more convenient form, let us consider the effective shear stress $\tau(\xi, T) = F(\xi, T)/b$ acting on the dislocation from the quasiperiodic grain boundary. For characteristic values of G = 90 GPa, ν = 0.3, $\epsilon_{\rm v} \approx 0.05$ and $2r_0 = b = 3$ Å, we obtain the following expression for $\tau(\xi, T)$,

$$\tau(\xi, T) = -8.357 \exp\left(-\frac{1304.350}{T}\right) \xi \times \int\limits_{1}^{+\infty} \frac{\eta}{(\eta^2 + \xi^2)^2} \exp\left(\frac{4087.733}{T}\frac{\eta}{\eta^2 + \xi^2}\right) {\rm d}\eta\,, \qquad (34)$$

given in GPa.

Results of numerical calculations are presented in Figure 5 for T = 100, 300, 800 and 1300 K. They are indicative of the facts that the stress $\tau(\xi, T)$ has two extreme values for the dislocation positions near the boundary ($0 < |\xi| < 1$) and that the increase of T leads to the abrupt decrease of $\tau(\xi, T)$ when $|\xi| < 1.5$, and to its increase when $|\xi| > 1.5$. However, there is no sense to consider the region $|\xi| < 1.57$ because our continuum model does not work there (the condition $\rho_k b \leq 1$ is satisfied only for $|\xi| \geq 1.57$ for any temperature). Such a temperature

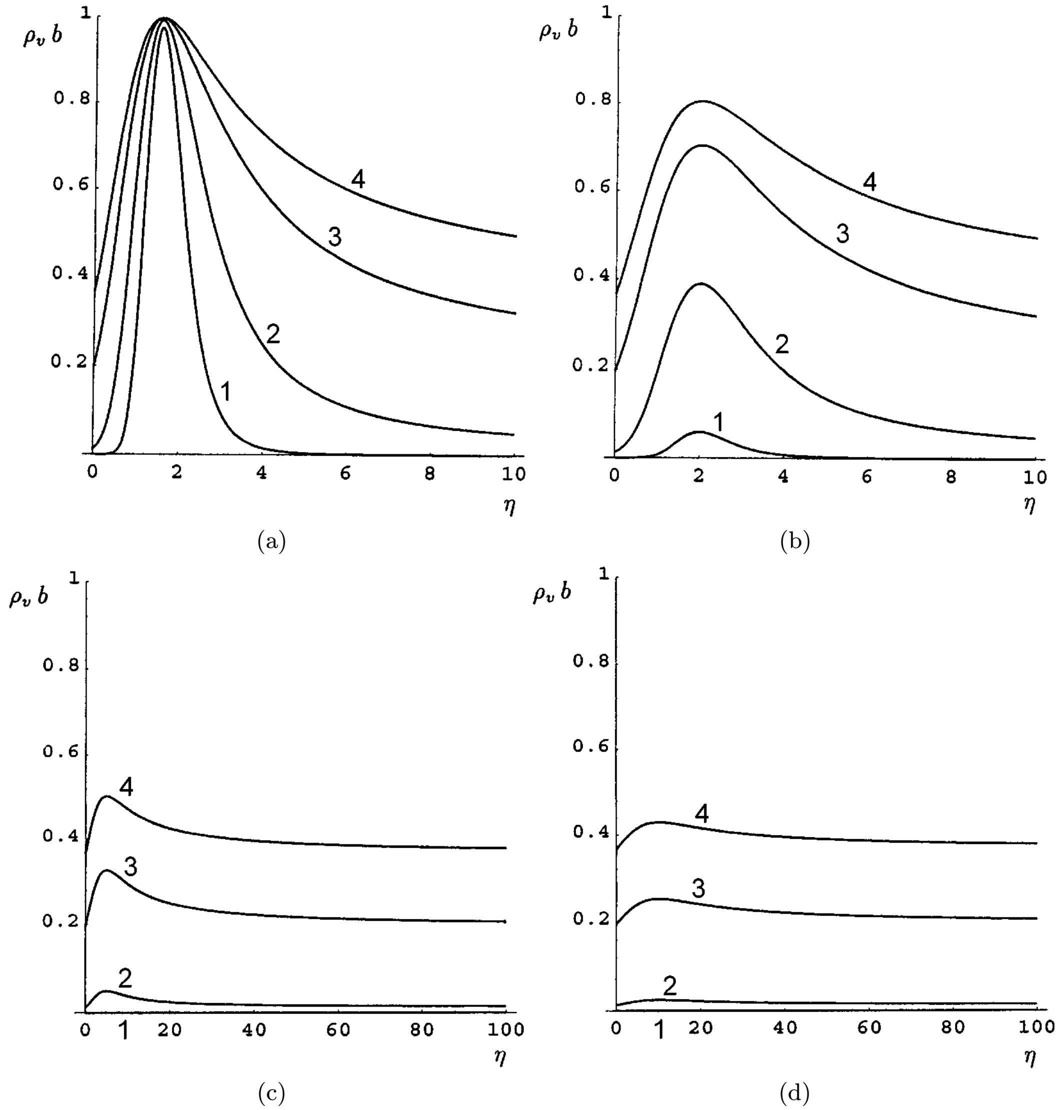

Fig. 6. Distribution of vacancy-like dilatation flexes along the quasiperiodic boundary for the values of temperature $T = 100$ (1), 300 (2), 800 (3) and 1300 K (4), and for different dislocation positions: $\xi = 1.57$ (a), 2 (b), 5 (c) and 10 (d).

dependence of $\tau(\xi, T)$ is explained by a very strong exponential dependence of dilatation flex density ρ_k on T. It is seen from the curves in Figure 6 where the distribution of vacancy-like dilatation flexes along the axes $\eta = y/b$ is shown for the dislocation positions $\xi = 1.57$, 2, 5 and 10, and temperatures $T = 100$, 300, 800 and 1300 K.

The above results of our calculations of the stress $\tau(\xi, T)$ allow us to describe the behaviour of a lattice dislocation which moves under an external shear stress $\tau_{\rm ex}$ action. The two stresses act on the dislocation which are the constant stress $\tau_{\rm ex}$ and the ξ-dependent stress $\tau(\xi) = \tau(\xi, T = 300$ K) (Fig. 7). In general, there are four following situations with the dislocation, depending on its position ξ as well as on direction and value of the stress $\tau_{\rm ex}$:

(i) The situation: $\xi < 0$, $\tau_{\rm ex}$ acts on the dislocation in direction to the quasiperiodic boundary. Both the stresses $\tau(\xi)$ and $\tau_{\rm ex}$ act in one direction (Fig. 7), causing the dislocation to move in this direction to the quasiperiodic boundary.

(ii) The situation: $\xi > 0$, the force $\tau_{\rm ex}$ acts in direction being opposite to the quasiperiodic boundary, $\tau_{\rm ex} = \tau_{\rm ex1} < |\tau_{\rm max}| = |\tau(\xi = 1.57)|$. In this situation, the stresses $\tau(\xi)$ and $\tau_{\rm ex1}$ act in opposite directions, causing the existence of two equilibrium positions, stable position $\xi_{\rm eq}^{\rm st}$ and unstable one $\xi_{\rm eq}^{\rm unst}$, of the dislocation. The stable position is fixed, $\xi_{\rm eq}^{\rm st} = 0$, while the unstable one is obtained through the condition $\tau(\xi_{\rm eq}^{\rm unst}) = -\tau_{\rm ex1}$ (Fig. 7). The position $\xi_{\rm eq}^{\rm st} = 0$ is stable relative to small displacements ($\pm\zeta$) of the dislocation in any direction, since $\tau(\xi - \zeta < 0) + \tau_{\rm ex1} > 0$ and $\tau(\xi + \zeta > 0) + \tau_{\rm ex1} < 0$. The dislocation located in the stable equilibrium position can "jump" with the help of thermal fluctuations into the unstable position, if value of $\tau_{\rm ex1}$ is slightly smaller than of $|\tau_{\rm max}|$ and if the distance d between the stable and unstable

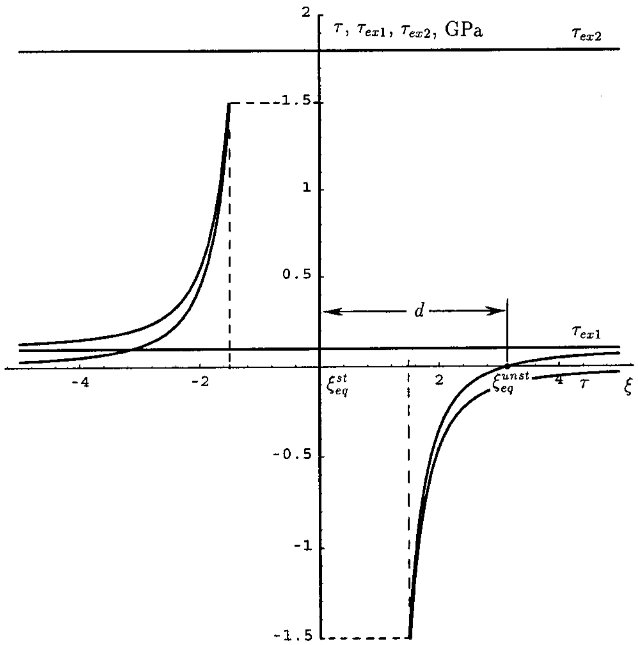

Fig. 7. Scheme illustrating the cooperative action of either the stress $\tau(\xi)$ and $\tau_{\rm ex1}$ or the stresses $\tau(\xi)$ and $\tau_{\rm ex2}$ on a lattice dislocation. Curve $\tau(\xi)$ is shown for the temperature $T = 300$ K. $\tau_{\rm ex1}$ and $\tau_{\rm ex2}$ are the external constant stresses. $\xi_{\rm eq}^{\rm st} = 0$ and $\xi_{\rm eq}^{\rm unst}$ are the stable and unstable equilibrium positions of the lattice dislocation, respectively. The dashed lines denote the extreme values of $\tau(\xi)$ which are achieved in the model and correspond to the dislocation positions $\xi \approx \pm 1.57$.

positions (Fig. 7) is small ($\approx$ several lattice parameters). If the above conditions are invalid, the dislocation is "firmly locked" in the stable equilibrium position at the quasiperiodic boundary.

(iii) The situation: $\xi > 0$, the stress $\tau_{\rm ex}$ acts in direction being opposite to the quasiperiodic boundary, $\tau_{\rm ex} = \tau_{\rm ex2} > |\tau_{\rm max}| = |\tau(\xi = 1.57)|$. In this situation, the dislocation moves in the direction being opposite to the quasiperiodic boundary. The stress $\tau_{\rm ex2}$ serves as the driving force for the dislocation motion. The stress $\tau(\xi)$ hampers the dislocation motion, contributing to the strengthening of a plastically deformed polycrystal.

(iv) The trivial situation: $\tau_{\rm ex} = 0$. The dislocation under action of the stress $\tau(\xi)$ moves to the quasiperiodic boundary for any ξ.

The situations (i) and (ii) are indicative of the non-standard features of lattice dislocations moving near quasiperiodic boundaries. Actually, when the external stress $\tau_{\rm ex} = \tau_{\rm ex1} < |\tau_{\rm max}|$ (situations (i) and (ii)), lattice dislocations easily move in one grain adjacent to a quasiperiodic boundary, while lattice dislocations in another grain adjacent to the boundary are stopped in the stable equilibrium position at the boundary. These non-standard features of lattice dislocations near quasiperiodic boundaries can be used in experiments concerning an indirect detection of quasiperiodic boundaries in polycrystalline solids.

In the situations (ii) and (iii) quasiperiodic boundaries serve as strengthening elements. Let us estimate the shear stress $\tau_{\rm s}$ characterizing the strengthening effect due to quasiperiodic boundaries, that is, the strengthening effect related to the special elastic interaction between lattice dislocations and quasiperiodic boundaries. This stress by definition is $\tau_{\rm s} = -\tau(\xi, T)$. From (34), for characteristic values of $G = 90$ GPa, $\nu = 0.3$, $\epsilon_{\rm v} \approx 0.05$ and $2r_0 = b = 3$ Å, we find for the dislocation position $\xi = 1.57$ and temperatures $T = 100$, 300, 800 and 1300 K that $\tau(\xi = 1.57) \approx -0.53$, -0.77, -0.97 and -1.05 GPa, accordingly. Thus, for mean temperatures, we can estimate $\tau_{\rm s} \approx 1$ GPa $= G/90$.

The value of $M|\tau_{\rm s}| \approx G/45$ (where $M \approx 2$ is the standard orientational factor) is much higher than the flow stress $\sigma \approx G/300 - G/120$ which usually specifies first stages of plastic deformation in metallic polycrystalline solids. This is indicative of the fact that the presence of quasiperiodic boundaries in polycrystalline solids can cause the non-standard strengthening of such solids. The above fact can be used in experiments concerning the indirect detection of quasiperiodic grain boundaries in polycrystals.

8 Concluding remarks

In this study it has been shown that there is a special elastic interaction between crystal lattice dislocations and quasiperiodic grain boundaries in polycrystalline solids. The special interaction is related to the presence of phason imperfections (specific excitations), which create elastic stress fields, at quasiperiodic grain boundaries and causes lattice dislocations to be attracted to such boundaries. This interaction is inherent to only quasiperiodic boundaries and has not analogue for periodic ones, since phason imperfections are present in only quasiperiodic boundaries.

For the calculation of elastic stress fields of phason imperfections, the model has been suggested which describes phason imperfections in a quasiperiodic boundary as dilatation flexes. In the framework of the model, exact formulae have been obtained for the elastic stress field of the quasiperiodic boundary as well as for the attraction force F and stress τ acting on an edge dislocation located near the quasiperiodic boundary. On the basis of these formulae, we have estimated the shear stress $\tau_{\rm s}$ which characterizes the strengthening effect in polycrystals due to quasiperiodic boundaries: $\tau_{\rm s}$ is about $G/90$ (where G is the shear modulus). This value is indicative of the fact that quasiperiodic boundaries serve as special strengthening elements capable of essentially contributing to the strengthening of plastically deformed polycrystalline solids.

Results of theoretical studies presented here, together with results of studies [8,9] devoted to a theoretical description of quasiperiodic boundaries in nanostructured polycrystals, can be effectively used in planning of experiments related to identification of quasiperiodic grain boundaries and their contributions to physical and mechanical properties of polycrystalline solids (see discussion in Sect. 7).

This work was supported, in part, by Grant 96-02-16807-A from the Russian Foundation of Basic Researches, and by Grant 97-3006 from the Russian Research Council "Physics of Solid Nanostructures".

References

1. H. Gleiter, Mater. Sci. Eng. **52**, 91 (1982).
2. O.K. Kaibyshev, R.Z. Valiev, *Grain Boundaries and Properties of Metals* (Moscow: Metallurgiya, 1987) in Russian.
3. D. Gratias, A. Thalal, Philos. Mag. Lett. **57**, 63 (1988).
4. A.P. Sutton, Acta Metall. **36**, 1291 (1988).
5. N. Rivier, A.J. Lawrence, Physica **B150**, 190 (1988).
6. N. Rivier, Number Theory and Physics, edited by J.M. Luck, P. Moussa, M. Waldschmidt (Berlin: Springer, 1989), p. 63.
7. I.A. Ovid'ko, Mater. Sci. Eng. **A188**, 37 (1994).
8. I.A. Ovid'ko, Phys. Solid State **39**, 268 (1997).
9. I.A. Ovid'ko, Nanostruct. Mater. **8**, 149 (1997).
10. K.N. Mikaelyan, I.A. Ovid'ko, A.E. Romanov, In: *Modern Problems of Physics and Mechanics of Materials* (St. Petersburg: St. Petersburg State University, 1997), p. 186.
11. J.E.S. Socolar, T.C. Lubensky, P.J. Steinhardt, Phys. Rev. **B34**, 3345 (1986).
12. T.C. Lubensky, Introduction to Quasicrystals, edited by M.V. Jaric (Boston: Academic Press, 1988), p. 199.
13. I.A. Ovid'ko, *Defects in Condensed Media: Glasses, Crystals, Quasicrystals, Liquid Crystals, Magnetics, Superfluids* (Leningrad: Znanie, 1991) in Russian.
14. I.A. Ovid'ko, Zeit. Phys. B **95**, 321 (1994).
15. H. Bohr, Acta Math. **45**, 29 (1924); **46**, 101 (1925).
16. A.P. Sutton, V. Vitek, Phil. Trans. Roy. Soc. London A **309**, 1 (1983).
17. I.A. Ovid'ko, Mater. Sci. Eng. **A163**, 67 (1993).
18. S.P. Timoshenko, J.N. Goodier, *Theory of Elasticity* (New York: McGraw-Hill, 1970).
19. T. Mura, *Micromechanics of Defects in Solids* (Dordrecht/Boston/Lancaster: Martinus Nijhoff Publishers, 1987).
20. M.Yu. Gutkin, I.A. Ovid'ko, Phys. Solid State **39**, 1791 (1997).
21. A.M. Kosevich, *Dislocations in Solids*, edited by F.R.N. Nabarro (Amsterdam: North-Holland Publ. Co., 1979), Vol. 1, p. 33.