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Thermodynamic approach to the description of dislocation mobility in quasicrystals

G N Lazareva and A S Bakai

National Science Center Kharkov Institute of Physics and Technology, 1, Akademicheskaya Street, Kharkov 61108, Ukraine

E-mail: g_lazareva@kipt.kharkov.ua

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Abstract
Dislocation mobility in quasicrystals is calculated using basic thermodynamic and hydrodynamic equations. The dependence of the dislocation mobility on viscosity, vacancies and phasons is given. It is shown that the phasonic defects make the major contribution to the inverse mobility of the free segments of dislocations.

1. Introduction

The mechanical properties of quasicrystals as well as usual materials strongly depend on the behavior of defects [1–3]. Much about the structure of the defects, particularly dislocations, in quasicrystals has been learned from experiments. Dislocations in quasicrystals move preferentially by climbing [4]. But there is still no consistent theory describing the dynamics of dislocations in quasicrystals. Previously Lubensky *et al* [5] developed a general approach and derived expressions for the dislocation mobility in quasicrystals in terms of vacancy diffusion constants. Later on Khannanov [6] noted that the hydrodynamic equations used in [5] did not explicitly treat vacancy diffusion. In [7] the dynamic equations for the interrelated elastic and phason fields derived in [6] and the description of the dislocation mobility in a quasicrystal developed in [5] were used. This approach enabled us to find the dependence of dislocation mobility on vacancy diffusion in an explicit way.

In the present work expressions for the dislocation mobility are found using a different approach based on the classical equations of thermodynamics and hydrodynamics including the viscosity. The contributions of the vacancy diffusion and phasons to the dislocation drag are derived. The obtained relations are evaluated for the most studied icosahedral quasicrystal, Al–Pd–Mn, as an example.

2. Dislocation mobility

2.1. General equations

For simplicity let us consider rectilinear dislocation with a Burgers vector of length b in a crystal or quasicrystal of linear size L under a shear stress σ. The stress generates the force acting on unit length of the dislocation, $F_{\mathrm{D}} = \sigma b$. The dislocation velocity is proportional to F_{D},

$$v_{\mathrm{D}} = M F_{\mathrm{D}}, \tag{1}$$

where coefficient M is the mobility.

In crystals the Peach–Koeler force $\mathbf{F_D}$ on a straight dislocation line is proportional to the applied stress $\hat{\sigma}$ and the Burgers vector $\mathbf{b}$ [8],

$$F_{\mathrm{D}i} = e_{ijk} b_n \sigma_{nj} l_k, \tag{2}$$

where e_{ijk} is the antisymmetric unit tensor and $\mathbf{l}$ is the unit vector along the dislocation line.

Icosahedral quasicrystals are modeled by projecting the six-dimensional (6D) cubic crystal on the three-dimensional (3D) space. For this reason equation (2), which is valid for six-dimensional space, has to be transformed by projecting on 3D space [7, 9],

$$F_{\mathrm{D}i} = e_{ijk} b_n^{6\mathrm{D}} \sigma_{nj}^{6\mathrm{D}} l_k^{6\mathrm{D}} = e_{ijk} b_n^{\parallel} \sigma_{nj} (P\hat{r}^{\parallel}\mathbf{l})_k + e_{ijk} b_n^{\perp} P_{nj} (P\hat{r}^{\perp}\mathbf{l})_k, \tag{3}$$

where $b_n^{\parallel}$, $b_n^{\perp}$ and $(P\hat{r}^{\parallel}\mathbf{l})_k$, $(P\hat{r}^{\perp}\mathbf{l})_k$ are the projections of the six-dimensional Burgers vector and the unit vector along the dislocation line on the physical and phason space, respectively.

The work done by the force $\mathbf{F_D}$ is equal to the rate of energy dissipation of a moving dislocation

$$\mathbf{F_D} \cdot \mathbf{v_D} = -\frac{\mathrm{d}}{\mathrm{d}t} \int \mathrm{d}^2 r \, E_{\mathrm{el}}, \tag{4}$$

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where $E_{\rm el}$ is the density of the elastic energy. The integral is over the two-dimensional plane orthogonal to the (presumably straight) dislocation line. The vectors $\mathbf{F_D}$ and $\mathbf{v_D}$ can be considered parallel, neglecting the effects of anisotropy [5]. Choosing the coordinate x along the direction of $\mathbf{F_D}$, we can present the equation for the inverse dislocation mobility M^{-1} in the following way:

$$M^{-1} = |\dot{E}| \cdot \mathbf{v_D}^{-2}, \tag{5}$$

where $|\dot{E}|$ is the magnitude of the elastic energy dissipation rate.

2.2. Contribution of viscous flow

There are stresses generated by a moving dislocation in a quasicrystal. These stresses and the corresponding mechanical energy relax. These energy dissipation processes can be termed (as in liquids) the internal friction or viscosity processes [10, 11]. The relaxation can be described using conventional hydrodynamic approach.

The motion of a dislocation in a quasicrystal is hindered by the lack of translational symmetry. The viscosity causes the energy dissipation of a dislocation. As is well known [12], the dissipated mechanical energy per unit time is

$$\dot{E}_{\rm mech} = -T\dot{S}, \tag{6}$$

where T is the temperature and $\dot{S}$ is the derivative of the entropy over time. Neglecting the thermal conductivity and using the general equation of heat transfer [12] we obtain

$$\rho T\left(\frac{\partial s}{\partial t} + \mathbf{v}\nabla s\right) = \sigma'_{ik}\frac{\partial v_i}{\partial x_k}, \tag{7}$$

where ρ is the density, s is the entropy per unit mass, $\mathbf{v}$ is the velocity ($\mathbf{v} \equiv \mathbf{v_D}$) and σ'_{ik} is the viscous stress tensor. Hence we derive

$$\frac{\partial}{\partial t}\int \rho s \,\mathrm{d}V = \int \frac{\sigma'_{ik}}{T}\frac{\partial v_i}{\partial x_k}\,\mathrm{d}V, \tag{8}$$

where the left-hand side of the equation corresponds to the rate of change of the total entropy per unit time. Substituting (8) in (6) we obtain:

$$\dot{E}_{\rm mech} = -\int \sigma'_{ik}\frac{\partial v_i}{\partial x_k}\,\mathrm{d}V = -\frac{1}{2}\int \sigma'_{ik}\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i}\right)\mathrm{d}V. \tag{9}$$

The latter equality follows from the symmetry of the tensor σ'_{ik}.

In the paper of Khannanov [6] the viscous stress tensor for quasicrystals is represented as follows:

$$\sigma'_{ik} = \eta_{iklm}\, v_{lm}, \tag{10}$$

where η_{iklm} is the viscosity tensor, v_{lm} is the strain rate tensor and

$$v_{ij} = \tfrac{1}{2}(\nabla_i v_j + \nabla_j v_i). \tag{11}$$

The vector of macroscopic velocity $\mathbf{v}$ is determined by the derivative of the total displacement field $\mathbf{U}$ over time,

$$\mathbf{v} = \frac{\partial \mathbf{U}}{\partial t}. \tag{12}$$

Let us consider the self-similar solution for the displacement field of a dislocation which is described by one variable $\mathbf{r} - \mathbf{v_D}t$ [5], i.e.

$$\mathbf{U}(\mathbf{r}, t) = \mathbf{U}(\mathbf{r} - \mathbf{v_D}t). \tag{13}$$

Substituting (10), (11) into (9) and considering (13) we obtain

$$\dot{E}_{\rm visc} = -\tfrac{1}{4}\eta_{iklm}\int [\nabla_i(\mathbf{v_D}\nabla)U_k + \nabla_k(\mathbf{v_D}\nabla)U_i] \times [\nabla_l(\mathbf{v_D}\nabla)U_m + \nabla_m(\mathbf{v_D}\nabla)U_l]\,\mathrm{d}^2 r. \tag{14}$$

Let us choose the coordinate system with the axis z directed along the dislocation line. Performing two-dimensional Fourier transformation in the plane (x, y) we obtain from (14)

$$\dot{E}_{\rm visc} = -\tfrac{1}{4}\eta_{iklm}\int [q_i U_k(-\mathbf{q}) + q_k U_i(-\mathbf{q})] \times [q_l U_m(\mathbf{q}) + q_m U_l(\mathbf{q})](\mathbf{v_D}\mathbf{q})^2\,\mathrm{d}^2 q. \tag{15}$$

Since the viscosity is isotropic for the icosahedral quasicrystal, the viscosity components can be presented as follows:

$$\eta_{ijkl} = \left(\eta_{\rm L} - \tfrac{4}{3}\eta_T\right)\delta_{ij}\delta_{kl} + \eta_T\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \tfrac{2}{3}\delta_{ij}\delta_{kl}\right), \tag{16}$$

where $\eta_{\rm L}$ and η_T are the longitudinal and transverse viscosities, respectively. The diagonal component of the viscosity tensor reduces to $\eta_{iiii} = 9\eta_{\rm L}$. In this case

$$\dot{E}_{\rm visc} = -9\eta_{\rm L}\int |U_i(\mathbf{q})|^2 q_i^2 (\mathbf{v_D}\mathbf{q})^2\,\mathrm{d}^2 q. \tag{17}$$

It follows from (5) and (19) that the contribution of the viscosity to the dislocation mobility is

$$M^{-1}_{\rm visc} = 9\eta_{\rm L}\int |U_i(\mathbf{q})|^2 q_i^2 q_x^2\,\mathrm{d}^2 q. \tag{18}$$

2.3. The contribution of vacancies

The lack of translational symmetry of quasicrystals manifests itself in the inherent phason defects, i.e. thermally activated transformations of the atomic structure of quasicrystals. As a result additional defects emerge, and hence it is required to account for the diffusion of vacancies when regarding the dynamics of dislocations. The growth rate of the entropy with time, allowing for the vacancies, was obtained in [12]:

$$\frac{\partial S}{\partial t} = -\int \frac{1}{T}\mathbf{j}\nabla\mu\,\mathrm{d}^2 r. \tag{19}$$

Then the energy dissipation equals

$$\dot{E}_{\rm dif} = \int \mathbf{j}\nabla\mu\,\mathrm{d}^2 r. \tag{20}$$

Let us denote by C the additional vacancy concentration (the part due to the vacant nodes), caused by the deformations [6]. In this case, the expression for the vacancy flux density is as follows:

$$\mathbf{j} = -D\frac{k_p}{p}\nabla p, \tag{21}$$

where D is the diffusion coefficient, k_pD is the coefficient of pressure diffusion, k_p is the pressure diffusion relation,

$$k_p = p\left(\frac{\partial V}{\partial C}\right)_{p,T} \Big/ \left(\frac{\partial \mu}{\partial C}\right)_{p,T}, \tag{22}$$

where V is the volume, p is the pressure, T is the temperature, μ is the chemical potential. A one-component quasicrystal is considered for simplicity. The vacancy is the dilatation center and

$$p = -\tfrac{1}{3}\sum_i \sigma_{ii}, \tag{23}$$

where σ_{ii} is the diagonal component of the elastic stress tensor σ_{ij}.

Taking into account the vacancy stress field, the relation of the total distortion $\nabla_i U_j$ to the elastic distortion β_{ij} is as follows:

$$\nabla_i U_j = \beta_{ij} + \tfrac{1}{3}\Omega C\delta_{ij}, \tag{24}$$

where $\Omega = (\frac{\partial V}{\partial C})_{p,T}$ is the vacancy dilatation volume. The quantity $\frac{1}{3}\Omega C\delta_{ij}$ is the distortion caused by the vacancies. In the absence of applied stresses, this distortion determines the dilatation of a physically small volume of a quasicrystal, which is, however, rather large compared to the atomic one, and is thus an inherent distortion. Since the vacancy concentration $C = C(\mathbf{r})$ is heterogeneous in the general case, such a distortion causes incompatibility of the sections of a quasicrystal lattice.

The chemical potential gradient depends on the concentration and pressure gradients as follows,

$$\nabla\mu = \left(\frac{\partial \mu}{\partial C}\right)_{p,T}\nabla C + \left(\frac{\partial \mu}{\partial p}\right)_{C,T}\nabla p. \tag{25}$$

Let us introduce a new constant $\gamma = k_p/p$, then

$$\left(\frac{\partial \mu}{\partial C}\right)_{p,T} = \frac{\Omega}{\gamma}. \tag{26}$$

Equation (25) reads

$$\nabla\mu = \frac{\Omega}{\gamma}\nabla C + \Omega\nabla p. \tag{27}$$

Combining (20), (21) and (25) we have

$$\dot{E}_{\rm dif} = -D\Omega\int[\gamma(\nabla p)^2 + \nabla C\nabla p]\,\mathrm{d}^2 r. \tag{28}$$

The linearized equation of momentum conservation for the quasicrystal is [6]

$$\rho\frac{\partial v_i}{\partial t} = \nabla_j\sigma_{ji} + \nabla_i\sigma'_{ij}. \tag{29}$$

At a small dislocation velocity the left side of this equation can be set equal to zero and hence it follows from (10)–(13), (30) that

$$\sigma_{ij} = \frac{1}{2}\eta_{kjlm}\frac{1}{\nabla_i}\nabla_k(\nabla_l(v_{\rm D}\nabla)U_m + \nabla_m(v_{\rm D}\nabla)U_l). \tag{30}$$

The pressure gradient can be obtained from (23) and (30),

$$\nabla p = -\frac{1}{6}\nabla\frac{\nabla_i}{\nabla_k}\eta_{iklm}(\nabla_l(v_{\rm D}\nabla)U_m + \nabla_m(v_{\rm D}\nabla)U_l). \tag{31}$$

Substituting (31) in (28) and making transformations similar to those of the formula (15) we get

$$\begin{aligned}\dot{E}_{\rm dif} = {} & -\tfrac{1}{6}D\Omega\eta_{iklm}\int(q_lU_m(\mathbf{q}) + q_mU_l(\mathbf{q}))\\ & \times\frac{q_i}{q_k}q^2C(-\mathbf{q})(\mathbf{v_D q})\,\mathrm{d}^2q\\ & -\tfrac{1}{36}D\Omega\gamma\eta_{iklm}\eta_{pfdg}\int(q_lU_m(\mathbf{q}) + q_mU_l(\mathbf{q}))\\ & \times(q_{\rm d}U_g(-\mathbf{q}) + q_gU_{\rm d}(-\mathbf{q}))\frac{q_i}{q_k}\frac{q_p}{q_f}q^2(\mathbf{v_D q})^2\,\mathrm{d}^2q.\end{aligned} \tag{32}$$

At the nonzero diagonal component of a viscous tensor the energy dissipation reduces to

$$\begin{aligned}\dot{E}_{\rm dif} = {} & -3D\Omega\eta_{\rm L}\int U_i(\mathbf{q})C(-\mathbf{q})q_iq^2(\mathbf{v_D q})\,\mathrm{d}^2q\\ & -9D\Omega\gamma\eta_{\rm L}^2\int|U_i(\mathbf{q})|^2q_i^2q^2(\mathbf{v_D q})^2\,\mathrm{d}^2q.\end{aligned} \tag{33}$$

As is seen from (5) and (33), the contribution of diffusion to the dislocation mobility is

$$\begin{aligned}M_{\rm dif}^{-1} = {} & \frac{3D\Omega\eta_{\rm L}}{|v_{\rm D}|}\int U_i(\mathbf{q})C(-\mathbf{q})q^2q_iq_x\,\mathrm{d}^2q\\ & + 9D\Omega\gamma\eta_{\rm L}^2\int|U_i(\mathbf{q})|^2q^2q_i^2q_x^2\,\mathrm{d}^2q.\end{aligned} \tag{34}$$

The first and second terms of the right-hand side of (34) describe the interaction of the elastic fields with the dilatations caused by vacancies and the higher order of influence of the elastic deformations, respectively. Thus, finally

$$\begin{aligned}M_{\rm dif}^{-1} &= M_{\rm difUC}^{-1} + M_{\rm difU}^{-1},\\ M_{\rm difUC}^{-1} &= \frac{3D\Omega\eta_{\rm L}}{|v_{\rm D}|}\int U_i(\mathbf{q})C(-\mathbf{q})q^2q_iq_x\,\mathrm{d}^2q,\\ M_{\rm difU}^{-1} &= 9D\Omega\gamma\eta_{\rm L}^2\int|U_i(\mathbf{q})|^2q^2q_i^2q_x^2\,\mathrm{d}^2q.\end{aligned} \tag{35}$$

2.4. Phason contribution

As was previously noted, quasicrystals possess so-called phason defects—local violations of the quasiperiodicity of a quasicrystal [1–3, 6]. Their presence additionally hinders the dislocation motion in a quasicrystal. Due to the lack of translational symmetry of quasicrystals, a moving dislocation necessarily leaves behind a planar defect consisting of a plane of phason defects [13]. It is considered that a so-called phason wall dissolves upon annealing. The energy dissipation due to this process can be calculated similarly to that described by equation (9). But in this case we have to substitute the phason stress tensor P_{ij} [6] for the viscous stress tensor and the phason drift velocity $\dot{\mathbf{w}}$ ($\mathbf{w}$ is the phason field) for the dislocation velocity $\mathbf{v} = \frac{\partial \mathbf{U}}{\partial t}$:

$$\dot{E}_{\rm mech} = \int P_{ik}\frac{\partial\dot{w}_i}{\partial x_k}\,\mathrm{d}V. \tag{36}$$

Just like for the field **U**, we will consider the field **w** which is described by a single variable $\mathbf{r} - \mathbf{v_D}t$ [5], $\mathbf{w}(\mathbf{r}, t) = \mathbf{w}(\mathbf{r} - \mathbf{v_D}t)$. The linearized equation of motion for the field **w** is obtained in [6],

$$\frac{\partial \mathbf{w}}{\partial t} = \Gamma_w(\nabla \cdot \hat{P}), \tag{37}$$

where Γ_w is the phason kinetic coefficient. From (37) we derive the expression for the phason stress tensor:

$$P_{ij} = -\frac{1}{\Gamma_w \nabla_i}(\mathbf{v_D} \cdot \nabla) w_j. \tag{38}$$

Substituting (38) in (36) we obtain

$$\begin{aligned}\dot{E}_{\text{phas}} &= \frac{1}{\Gamma_w}\int \frac{1}{\nabla_i}(\mathbf{v_D}\nabla) w_k \cdot \nabla_k (\mathbf{v_D}\nabla) w_i \, \mathrm{d}^2 r \\ &= -\frac{1}{\Gamma_w}\int w_k(\mathbf{q}) w_i(-\mathbf{q}) \frac{q_k}{q_i}(\mathbf{v_D}\mathbf{q})^2 \, \mathrm{d}^2 q.\end{aligned} \tag{39}$$

For the diagonal component we have

$$\dot{E}_{\text{phas}} = -\frac{1}{\Gamma_w}\int |w(\mathbf{q})|^2 (\mathbf{v_D}\mathbf{q})^2 \, \mathrm{d}^2 q. \tag{40}$$

Thus the contribution of the phason deformations to the dislocation mobility is

$$M_w^{-1} = \frac{1}{\Gamma_w}\int |w(\mathbf{q})|^2 q_x^2 \, \mathrm{d}^2 q. \tag{41}$$

Comparing the results obtained for the dislocation mobility with those obtained in [7], one can see that the term $M_w^{\text{diag},-1}$ is the same in both papers. The vacancy diffusion terms M_{difUC}^{-1} and M_{difU}^{-1} (35) in [7] differ only in numerical coefficients $\propto 1$. This difference is unimportant due to the simplifications of the models used. The viscosity term M_{visc}^{-1} has a slightly different form in [7] but its general structure remains the same.

3. Numerical estimations of dislocation mobility

In order to estimate the dislocation mobility M, the coefficients in (18), (34) and (41) are to be evaluated. The coefficients are considered in detail in the appendix.

The gradients of the elastic and phason displacement fields are roughly constant on a circle of radius r centered on the dislocation line [5]:

$$(\nabla u) r \approx b \approx (\nabla w) r. \tag{42}$$

The displacements induced by vacancies have to be considered too. Thus instead of the elastic displacement field **u** we should use the total displacement field **U**. It follows from (24) and (42) that

$$\nabla U(r) = b/r + \Omega C(r), \tag{43}$$

or

$$U(r) \approx b \ln \frac{r}{b} + \Omega \int_b^r C(r) \, \mathrm{d}r. \tag{44}$$

Substituting the vacancy concentration around a dislocation $C(r)$ calculated in appendix (A.3) into (44) gives

$$U(r) = b \ln \frac{r}{r_{\text{d}}} + \Omega C_{\text{d}}(r - r_{\text{d}}) + \Omega C_2 r\left(\ln \frac{r}{r_{\text{d}}} - 1\right), \tag{45}$$

where $C_{\text{d}} = C(r_{\text{d}})$ is the vacancy concentration in the vicinity of the dislocation core, $r_{\text{d}} \approx b$ is the radius of the dislocation core, $C_2 = (C_1 - C_{\text{d}})/\ln(R/r_{\text{d}})$, $R \sim 1/\sqrt{\rho}$ is the distance between dislocations and $C_1 = C(R)$. The Fourier transforms of the total displacement field $U(\mathbf{q})$ and the vacancy concentration $C(\mathbf{q})$ in the cylindrical coordinates read

$$U(q) \approx \frac{b}{q^2} + \frac{\Omega}{q^3}(C_{\text{d}} + C_2) - 2\pi\Omega C_{\text{d}} r_{\text{d}} \delta(q_x)\delta(q_y), \tag{46}$$

$$C(q) \approx (C_{\text{d}} - C_2 \ln r_{\text{d}}) 2\pi \delta(q_x)\delta(q_y) + \frac{C_2}{q^2}, \tag{47}$$

and the Fourier transform of the phason displacement field, as was found in [5],

$$w(q) \approx b/q^2 \tag{48}$$

can be substituted into (18), (35) and (41).

We now turn to the estimation of the summands of the inverse mobility (18), (34) and (41). The integration in these relations is in the range from $q_{\min} = 1/R$ to $q_{\max} = 1/b$. Thus from (41) subject to (48) we obtain

$$M_w^{-1} \approx \frac{b^2}{\Gamma_w} \ln\left(\frac{R}{b}\right). \tag{49}$$

Substituting the values of the parameters entering into (49) from the appendix we can estimate

$$M_w^{-1} \approx 3.3 \times 10^4 \text{ Pa s}. \tag{50}$$

For the estimate the inverse dislocation mobility considering viscosity (18) and diffusion (34) at the temperature $T = 1000$ K we have

$$\begin{aligned} M_{\text{visc}}^{-1} &\approx 0.4 \text{ Pa s}, \qquad M_{\text{difUC}}^{-1} \approx 2.5 \times 10^{-4} \text{ Pa s}, \\ M_{\text{difU}}^{-1} &\approx 10^{-9} \text{ Pa s}. \end{aligned} \tag{51}$$

Thus, the total inverse mobility reads

$$\begin{aligned} M^{-1} &= M_w^{-1} + M_{\text{visc}}^{-1} + M_{\text{difUC}}^{-1} + M_{\text{difU}}^{-1} \\ &\approx 0.4(8.3 \times 10^4 + 1 + 6.5 \times 10^{-4} + 2.5 \times 10^{-9}) \text{ Pa s}. \end{aligned} \tag{52}$$

It appears that for the chosen magnitudes of the parameters which enter into the expression for dislocation mobility in quasicrystals, the phason term makes the major contribution to the inverse mobility. The viscous flow of the vacancies cloud has much less influence on the mobility.

4. Discussion

In [5] the quantities entering the expression for the contribution of the phason deformations into the drag of a dislocation were evaluated using the dynamic characteristics of dislocations in crystals. This has led to the estimate $M_w^{-1} \approx 10^5$ Pa s.

Table 1. The dislocation mobility calculated based on the experimental data from [14] at different temperatures.

T (°C)	σ (MPa)	ρ (10^9 cm^{-2})	v (10^{-10} m s^{-1})	M^{-1} (10^8 Pa s)	F_D (N m^{-1})
695	500	9	2.2	11	52.7
730	350	6	3.3	5.3	45.2
790	150	1	20	3.75	47.4
820	100	0.5	40	1.25	44.7

Instead, in the estimation (50), we use the values of the Burgers vector, shear modulus and diffusion coefficient which are experimentally obtained for Al–Pd–Mn quasicrystals. As a result, the value of M_w^{-1} turned out to be one order smaller than that in [5], i.e. the mobility of the unpinned dislocation in [5] is overrated.

It is interesting to compare the estimations of the dislocation mobility for the alloy Al–Pd–Mn obtained in the present work with the experimentally measured values in [14] at different temperatures and dislocation densities. We assume that the plastic deformation of quasicrystals Al–Pd–Mn is of a pure dislocation nature and described by the Orowan equation [15]

$$\dot{\varepsilon}_{\text{plast}} = \rho b v \tag{53}$$

where $\dot{\varepsilon}_{\text{plast}}$ is the plastic deformation rate and v is the dislocation velocity. Thus it follows that

$$v = \dot{\varepsilon}_{\text{plast}}/b\rho. \tag{54}$$

From (1), (2) we get $F = b\sigma$ and the inverse dislocation mobility

$$M^{-1} = b\sigma/v. \tag{55}$$

The relations (54), (55) enable us to find an estimation of the mobility using the experimentally measured values of $\rho, \sigma, \dot{\varepsilon}_{\text{plast}}$ at different temperatures as shown in table 1. The drag force on dislocations in a real quasicrystal at $T = 730\,^{\circ}\text{C}$ turns out to be approximately three orders larger than the quantity calculated for free parts of dislocations (52).

The reason for this disagreement lies, firstly, in the drag of dislocations due to their mutual pinning. Assuming the density of the pinning centers to be of the order of ρ we estimate the distance between two pinning points on a dislocation as $l \propto 1/\sqrt{\rho}$ and, consequently, the force acting on a dislocation segment of length l is $F_D = \sigma l \approx \sigma/\sqrt{\rho}$. It is seen from table 1 that this quantity is weakly dependent on the temperature and is close to $F_D \approx 46$ N m^{-1}. One can conclude that the origin of the observed force is just the mutual pinning of dislocation which defines the magnitude of the drag force in a real Al–Pd–Mn quasicrystal. This means that the dislocations become mobile when the tension of the dislocation segment F_D becomes equal to the pinning force which is weakly dependent on the temperature. As can be seen from table 1, the dislocation density quickly decreases with temperature. Consequently it can be expected that the effects of pinning of dislocations are small and the drag mechanism described in this paper dominates at high temperatures close to the melting point. On the other hand, the mobility of *freely* moving dislocation segments directly measured in [4] is properly consistent with our calculations if we assume the same order of magnitude for stresses as in experimental conditions of [4] and [14].

5. Conclusions

An expression for the mobility of the free dislocation segments in quasicrystals caused by the structure of a quasicrystal and the presence of vacancies and phasons was obtained using the basic relations of thermodynamics and hydrodynamics. The expressions for the dislocation mobility in icosahedral quasicrystals subject to the vacancy emission and inelastic transformations related to the phason deformations are deduced. It shows from the numerical evaluations of the main contributions to the dislocation mobility that the phason deformations appear to have the major contribution to the drag of the free dislocations.

Similar values for the dislocation mobility in quasicrystals have been obtained in [7] while applying a different technique developed in [5]. The obtained results confirm the validity of both approaches. A minor difference in the expressions for the mobility is related to the simplifications of the models used. Due to this similarity one can conclude that both approaches give a reasonable description of the dislocation mobility in quasicrystals.

Appendix

Here we calculate some parameters used in section 3 taking into account the experimental data [4, 5, 16–18]. The dislocations in quasicrystals become mobile at a temperature of about 80% of the melting point [4]. In the examined Al–Pd–Mn quasicrystal this temperature amounts to $T = 993$ K and the dislocation velocity is $v_D \approx 2 \times 10^{-6}$ m s^{-1} [4].

The diffusion coefficient D_v can be presented in the Arrhenius form [16],

$$D_v = D_{v0} \exp\left(-\frac{E_v^m}{k_B T}\right), \tag{A.1}$$

where E_v^m is the vacancy migration energy and D_{v0} is the pre-exponential factor. At the values $E_v^m = 1.5$ eV and $D_{v0} = 10^{-4}$ m^2 s^{-1} [16] experimentally obtained for the quasicrystals we get $D = 2.7 \times 10^{-12}$ m^2 s^{-1} at $T = 993$ K.

Since the dislocation velocity in quasicrystals is small, we can consider the vacancy distribution around the moving dislocation to be roughly quasi-stationary. The expression for the vacancy concentration around a dislocation in cylindrical coordinates can be derived from the stationary diffusion equation

$$\Delta C = 0 \tag{A.2}$$

with the boundary conditions in the vicinity of a dislocation $C(r_d) = C_d$, where $r_d \approx b$ is the radius of the dislocation core and $C_1 = C(R)$ is the concentration at the mean distance R between dislocations. The solution to this equation is of the form

$$C(r) = C_d + C_2 \ln(r/r_d), \tag{A.3}$$

where $C_2 = (C_1 - C_d)/\ln(R/r_d)$. The mean distance between dislocations, R, can be estimated as follows: $R = 1/\sqrt{\rho}$, where ρ is the dislocation density. At $\rho = 10^{14}$ m^{-2} [14] we have $R \approx 10^{-7}$ m.

The relation for the vacancy concentration (A.3) can be used if the diffusion time τ_{diff} is much less than the time t_1 when a dislocation covers the distance R: $\tau_{\text{diff}} \ll t_1$. Here $\tau_{\text{diff}} = R^2/D$ and $t_1 = R/v_{\text{D}}$. Substituting the values of the parameters R, D_{v}, v_{D} we obtain that $\tau_{\text{diff}} \approx 10^{-2}$ s. Thus the value of t_1 is larger than τ_{diff} by one order, so that (A.3) turns out to be acceptable under the considered conditions.

The length of the Burgers vector is taken to be $b \approx 0.5$ nm $= 0.5 \times 10^{-9}$ m [4].

Let us evaluate the parameter C_2. For that we will regard the vacancy flux through a cylinder of radius r, surrounding the dislocation. The vacancy flux density is

$$j_{\text{v}} = -D\nabla C \tag{A.4}$$

and the vacancy flux per unit dislocation length is

$$J = j_{\text{v}} \cdot 2\pi r = \text{const.} \tag{A.5}$$

It follows from (A.3) and (A.5) that

$$\nabla C = C_2 \cdot \frac{1}{r}, \tag{A.6}$$

$$J = -2\pi D \frac{C_2}{V_{\text{a}}} L, \tag{A.7}$$

where V_{a} is the atomic volume.

On the other hand, as the dislocation of the length L is covering a distance $x = v_{\text{D}}t$ the vacancy flux is

$$J = \frac{\partial}{\partial t}\alpha \frac{L}{b}\frac{x}{b} = \frac{\partial}{\partial t}\alpha \frac{L}{b}\frac{v_{\text{D}}t}{b} = \alpha \frac{L v_{\text{D}}}{b^2}, \tag{A.8}$$

where $\alpha \cdot L/b$ is the number of vacancies emitted by the dislocation upon its displacement by one interatomic distance, $\alpha = 1$ for the edge dislocation and $\alpha = 0$ for the screw one. Assuming mixed dislocations we put $\alpha = 0.1$. The quantity x/b is the number of sites covered by a moving dislocation over a distance x. Thus $\alpha \cdot L/b \cdot x/b$ is the number of vacancies emitted by a dislocation during its displacement over a distance x and its time derivative gives (A.8).

From (A.7) and (A.8) we have

$$-2\pi D \frac{C_2}{V_{\text{a}}} L = \alpha \frac{L v_{\text{D}}}{b^2} \tag{A.9}$$

and

$$C_2 \approx -\frac{\alpha v_{\text{D}} V_{\text{a}}}{2\pi b^2 D_{\text{v}}}. \tag{A.10}$$

Substituting $V_{\text{a}} \approx b^3$ in (A.10) at $v_{\text{D}} = 2 \times 10^{-6}$ m s^{-1} [4] we have

$$C_2 \approx -\frac{\alpha v_{\text{D}} b^3}{2\pi b^2 D_{\text{v}}} = -\frac{\alpha v_{\text{D}} b}{2\pi D_{\text{v}}} \approx -4.7 \times 10^{-6}. \tag{A.11}$$

The vacancy concentration far from the dislocation, C_1, is equal to the thermally equilibrium one,

$$C_{\text{v}}^{\text{eq}} = \text{e}^{-E_{\text{v}}/k_{\text{B}}T}, \tag{A.12}$$

where k_{B} is the Boltzmann constant, E_{v} is the vacancy formation energy. Since at the melting temperature T_{m} for many metallic materials $C_{\text{v}}^{\text{eq}}(T_{\text{m}}) = 10^{-4}$ and for the icosahedral quasicrystal $Al_{72}Pd_{80}Mn_8$ $T_{\text{m}} = 1140$ K [18], we have a reasonable evaluation of the effective vacancy formation energy $E_{\text{v}} \approx 0.9$ eV. With this value the vacancy concentration reaches $C_1 = 3 \times 10^{-5}$ at $T = 1000$ K. Now we can find the vacancy concentration in the vicinity of a dislocation: $C_{\text{d}} = C_1 - C_2 \ln(R/b) \approx 5.5 \times 10^{-5}$.

The magnitude Ω determines the quasicrystal dilatation at the introduction of a vacancy and it can be estimated as $\Omega = 0.1$ like that in the usual crystal. The viscosity coefficient is $\eta = 10^{-1}$ Pa s [5]. The parameter γ depends on the dilatation Ω and the chemical potential $\mu = \mu_{\text{v}} - \mu_{\text{a}}$:

$$\gamma = \left(\frac{\partial V}{\partial C}\right)_{p,T} \Big/ \left(\frac{\partial \mu}{\partial C}\right)_{p,T} = \Omega V_{\text{a}} \Big/ \left(\frac{\partial \mu}{\partial C}\right)_{p,T}, \tag{A.13}$$

where μ_{v}, μ_{a} are the chemical potentials of the vacancy and the atom. Noting that $C_{\text{v}} + C_{\text{a}} = 1$ and $\mu = \mu_0 + \frac{k_{\text{B}}T}{v_{\text{a}}} \ln \frac{C}{C_0}$, we have

$$\left(\frac{\partial \mu}{\partial C}\right)_{p,T} = \frac{k_{\text{B}}T}{C_{\text{v}}(1 - C_{\text{v}})V_{\text{a}}}. \tag{A.14}$$

Thus at $C_{\text{v}} = C_{\text{d}}$ we get $\gamma = -5 \times 10^{-14}$ m^3 J^{-1}.

The phason kinetic coefficient was estimated in [5] as $\Gamma_w \approx D_{\text{v}}/K$, where K is the shear modulus. Substituting the diffusion coefficient D_{v} calculated above and the shear modulus $K = 70$ GPa from [17] we obtain $\Gamma_w \approx 3.8 \times 10^{-23}$ m^3 s kg^{-1}.

References

[1] Janot C 1994 *Quasicrystals: a Primer* 2nd edn (Oxford: Clarendon)
[2] Suck J B *et al* (ed) 2004 *Quasicrystals: an Introduction to Structure, Physical Properties and Applications* (Berlin: Springer)
[3] Dubois J-M 2001 *J. Phys.: Condens. Matter* **13** 7753–62
[4] Mompiou F, Caillard D and Feuerbacher M 2004 *Phil. Mag.* **84** 2777–92
[5] Lubensky T C and Ramaswamy S 1986 *Phys. Rev.* B **33** 7715
[6] Khannanov Sh Kh 2002 *Phys. Met. Metall.* **93** 397
[7] Bakai A S and Lazareva G N 2008 *Metallofiz. Noveish. Tekhnol.* **30** 1681–700 (in Russian)
[8] Peach M and Koehler J S 1950 *Phys. Rev.* **80** 436
[9] Li X-F and Fan T-Y 1999 *Phys. Status Solidi* b **212** 19–26
[10] Martin P C, Parodi O and Pershan P S 1972 *Phys. Rev.* A **6** 2401–20
[11] Landau L D and Lifshitz E M 1986 *Theory of Elasticity* 3rd edn (Oxford: Pergamon)
[12] Landau L D and Lifshitz E M 1982 *Fluid Mechanics* 2nd edn (Oxford: Pergamon)
[13] Feuerbacher M, Haggen M and Urban K 2004 *Mater. Sci. Eng.* A **375–377** 84
[14] Shall P *et al* 1999 *Phil. Mag. Lett.* **79** 785
[15] Kocks U F, Argon A S and Ashby M F 1975 *Prog. Mater. Sci.* **19** 1
[16] Blüher R, Scharwaechter P, Frank W and Kronmüller H 1998 *Phys. Rev. Lett.* **80** 1014
[17] Feuerbacher M, Weller M, Diehl J and Urban K 1996 *Phil. Mag. Lett.* **74** 81
[18] Okada J T *et al* 2006 *J. Phys.: Condens. Matter* **18** L613–8