International Journal of Theoretical Physics, Vol. 36, No. 1, 1997

On the Isotropy of Continuized Dislocated Crystals. II. The Isotropy of Diffusive Properties

A. Trzęsowski[1]

Received February 16, 1996

The classical theory of the influence of single immobile dislocations on the diffusion of point defects cannot be applied to the description of the influence of a finite but very large number of dislocations on this diffusion, because in this case dissipative effects (due to dislocations) cannot be neglected. In this paper these dissipative effects are described by means of a generalized gauge procedure taking advantage of the existence of the short-range order in continuized dislocated crystals. It is shown that, for uniformly dense distributions of dislocations, the existence of dissipative effects means the existence of a (nonvanishing) scalar curvature of a conformally flat configurational space of a single diffusing point defect. Equations describing the interaction energy between dislocations and a diffusing point defect are proposed, and the contribution to this energy of elastic as well as inelastic interactions is discussed.

1. INTRODUCTION

The *balance equation* of point defects diffusing in a crystalline solid has the form

$$\partial_t n + \operatorname{div}(n\boldsymbol{v}) = \sigma \tag{1}$$

where $n = n(X, t)$ is the density of the number of defects diffusing at the instant t, $\boldsymbol{v} = \boldsymbol{v}(X, t)$ is the so-called *diffusion peculiar velocity*, and $\sigma = \sigma(X, t)$ is a source term. $X = (X^A)$ denotes a Lagrange coordinate system on the body $\mathcal{B}$ considered as an open connected subset of its configurational Euclidean point space E^3, and E^3 is identified [by means of a distinguished Cartesian coordinate system $Z = (Z^A)$] with the arithmetic point space R^3 (see, e.g., Trzęsowski, 1993b). We will neglect the influence of the body boundary on the diffusion. The body $\mathcal{B}$ can be identified then with its

[1] Institute of Fundamental Technological Research, Świętokrzyska 21, 00-049 Warsaw, Poland.

0020-7748/97/0100-0193$12.50/0

configurational space $E^3 \triangleq R^3$; $\triangleq$ means that a formula is valid in a distinguished (Cartesian) coordinate system. The considered coordinate systems will be assumed to be *geometric frame references*, i.e., dimensional coordinate systems with $[X^A] = [dX^A] = \text{cm}$, $[\partial_A = \partial/\partial X^A] = \text{cm}^{-1}$ (in the cgs units system).

The simplest model of the diffusion phenomenon is based on the following assumptions. First, it is assumed that point defects are identical but distinguishable and interactions between them can be neglected. The probability $P(Q_t \in U)$ that the actual (at the instant t) position Q_t of a diffusing defect is a point of the domain $U \subset \mathcal{B}$ ($\triangleq R^3$) is then given by

$$P(Q_t \in U) = \int_U p(X, t)\, dV(X) \tag{2}$$

where we have denoted (Klimontovitch, 1982)

$$p(X, t) = \frac{n(X, t)}{N(t)} \tag{3}$$

$$N(t) = \int_{R^3} n(X, t)\, dV(X) < \infty$$

where $dV(X)$ denotes the Euclidean volume element. $N(t)$ is a finite but very large number of point defects diffusing at the instant t, and the above approximation of $p(X, t)$ is the better, the greater $N(t)$ is.

The second basic assumption is that the influence of diffusing point defects on the matrix crystal lattice can be neglected. Then, if additionally external fields or other crystal lattice defects are absent, the flux $\boldsymbol{j}$ of diffusing point defects has (in Cartesian coordinates) the form of the so-called *Fick law*:

$$j^A = nu^A \triangleq -D^{AB}\partial_B n, \qquad \text{i.e.,} \quad v^A = u^A \tag{4}$$

where the matrix (D^{AB}) of *diffusion coefficients* is a constant, symmetric, positive-definite matrix, and $\boldsymbol{u} = u^A\partial_A$ is called the *diffusion velocity*. For Fick's law to be valid, the concentration of the diffusing point defects in the background crystalline medium must be small. Consequently, the influence of external fields (or other crystal lattice defects) on the diffusion flux is described by the so-called *drift velocity* $\boldsymbol{b}$ defined as

$$\boldsymbol{b} = \boldsymbol{v} - \boldsymbol{u} \tag{5}$$

Assuming the source term σ in the form

$$\sigma = d(t)n, \qquad d(t) = \dot{N}(t)/N(t) \tag{6}$$

as it is, e.g., for radiation-induced point defects, we obtain from (1)–(6) the following diffusion equation:

$$\partial_t p + F(\partial)p = 0 \tag{7}$$

$$F(\partial) \triangleq \partial_A(\cdot b^A) - D^{AB}\partial_A\partial_B$$

If the drift velocity does not depend on the density of diffusing point defects, then this equation can be considered as a *Fokker–Planck equation* describing the localization probability of a Markov motion (with mean velocity $\boldsymbol{b}$) in the Euclidean configurational space R^3 of an arbitrary distinguished diffusing point defect. If the drift vanishes, the diffusion can be regarded as a pure random phenomenon—the *free diffusion* in a homogeneous body.

We see that the fundamental expressions to describe a Markov-type diffusion process are the balance equation of the form

$$\partial_t p + \partial_A(pv^A) = 0, \qquad v^A = u^A + b^A \tag{8}$$

where

$$pu^A = -D^{AB}\partial_B p \tag{9}$$

and a constitutive relation defining the dependence of the drift velocity on external fields or crystal lattice defects. For example, if the drift is small compared with the chaotic motion of point defects, then this constitutive relation can be assumed in the form of the so-called *Stokes relation*:

$$b^A = M^{AB}F_B, \qquad F_B = \delta_{AB}F^B \tag{10}$$

where $\boldsymbol{F} = F^A\partial_A$ denotes the force acting on a point defect, and M^{AB} are (constant) *mobility coefficients* of the defect. Since we ignore the influence of diffusing point defects on interatomic forces in the crystal lattice, the force $\boldsymbol{F}$ caused by an external field of small lattice strains ϵ_{AB} takes the form

$$F_A = \mu V^{BC}\partial_A\epsilon_{BC} \tag{11}$$

where V^{BC} are constants with the dimension of volume, and μ is a constant with the dimension of stress (Kosevitch, 1972). In the isotropy approximation

$$D^{AB} = D\delta^{AB} \tag{12}$$

$$M^{AB} = \zeta^{-1}\delta^{AB}, \qquad V^{AB} = V_0\delta^{AB}$$

where ζ is a friction coefficient, V_0 is the volume of the material "transferred" by the diffusing point defect, and μ is equal to the bulk modulus of the elastic medium. Then

$$F_A = -\partial_A E \tag{13}$$

where the (elastic) interaction energy E is given by

$$E = V_0\tau, \qquad \tau = \tfrac{1}{3}\operatorname{tr}\boldsymbol{\tau} \tag{14}$$

and τ denotes the hydrostatic pressure corresponding to the field $\boldsymbol{\tau}$ of external stresses. The force $\boldsymbol{F}$ of the form (13) and (14) is, in the linear approximation, the force with which the external field acts on a center of dilatation in the isotropic medium. It can be shown that in this approximation the point defects do not interact (Kosevitch, 1972).

It follows from (3) with $N(t) = \text{const}$, (7), (10), (12), and (13) that there exists a heterogeneous steady distribution of diffusing defects given by

$$n(X) = n_0 \exp(-E(X)/\Theta), \qquad \Theta = \zeta D \tag{15}$$

where Θ is a characteristic energy of the diffusion process. Since in the considered linear diffusion equation [and thus in the balance equation (1)] there is then no source term, we can consider $n(X)$ of (15) as the one defining a steady equilibrium state of diffusing point defects. In particular, if $\Theta = k_B T$, where k_B is Boltzmann's constant and T is the absolute temperature of the body, then it is a steady equilibrium distribution of a thermally activated diffusion process in the external elastic field. We assume that the considered diffusion process also admits a spatially uniform equilibrium distribution of diffusing point defects, i.e., that the considered diffusion equation also admits a constant solution $n(X, t) = n_0$. Then the energy E of (13) and (15) should be a harmonic function:

$$\Delta E = 0, \qquad \Delta = \delta^{AB}\partial_A\partial_B \tag{16}$$

This classical approach to the description of the diffusion phenomenon can be applied to the description of the influence of single dislocations on the diffusion. Namely, it is well known (Hull and Bacon, 1984; Orlov, 1973) that the most important contribution to the interaction between a point defect and a dislocation is usually that due to the distortion the point defect produces in the surrounding crystal. The distortion may interact with the stress field of the dislocation to raise or lower the elastic energy of the crystal. This change is the interaction energy E. Estimates of the interaction energy may be obtained by treating the crystal as a continuum elastic solid and using elasticity theory. The simplest model of a point defect is an isotropic elastic sphere inserted into a smaller or greater spherical hole in an elastic isotropic matrix with the same elastic coefficients. Oversized or undersized defects are interpreted as those modeling mass point defects (substitutional or interstitial impurities or self-interstitials) or vacancies, respectively (Hull and Bacon, 1984). The force acting on a point defect then has the form defined by (13) and (14). For example, the irradiation of a crystal with fast neutrons produces very small circular edge dislocation loops. These loops can be treated, in the continuized crystal approximation, as infinitesimal ones, and the interaction energy E can be approximated then by the following particular solution of (16) (Bullough and Newman, 1970):

$$E(r, \vartheta) = \epsilon V_0 \Theta \frac{1 - \cos^2 \vartheta}{r^3} \tag{17}$$

where spherical coordinates (r, ϑ, α), $r \geq 0$, $0 \leq \vartheta \leq \pi$, $-\pi < \alpha < \pi$, are used, r denotes the distance between the (infinitesimal) dislocation loop and a point lying on a conical surface $\vartheta = \text{const}$, and Θ and V_0 denote a characteristic energy and volume, respectively. For oversized (undersized) point defects we have $\epsilon = 1$ ($\epsilon = -1$) (Hull and Bacon, 1984). It is known that if the interaction energy $E = E(r, \vartheta, \alpha)$ is taken into account in order to define a drift term in the diffusion equations (7), (10), (12), and (13), then an estimation of this energy neglecting its angular dependence may be acceptable (Bullough and Newman, 1970). The elastic interaction energy becomes then the harmonic function

$$E(r) = \epsilon \Theta \frac{L}{r} \tag{18}$$

where L is a characteristic linear parameter. Note that $|E(L)| = \Theta$ and $|E(r)| \leq \Theta$ for $r \geq L$. Thus, for $\Theta = k_B T$, L can be interpreted as a distance over which an equilibrium distribution of point defects is "smeared" by their thermal motion (Orlov, 1973).

The occurrence of many dislocations causes an inelastic distortion of the crystal lattice, and the influence of this distortion on the diffusion process manifests itself in the variableness of diffusion coefficients and in the appearance of some dissipative effects due to the inelastic character of interactions between dislocations and a point defect diffusing in the distorted crystalline solid. Consequently, we can expect then, e.g., the existence of nonequilibrium steady states of diffusing defects. Thus, the classical approach, based on the model of the diffusion in a homogeneous, elastically distorted body, cannot be used. However, though the existence of many dislocations breaks the long-range order of a crystalline solid (and the dislocated crystalline solid becomes a heterogeneous one), nevertheless its short-range order is remarkably preserved, and the dislocated crystalline solid can be locally approximately described as a (macroscopically) small part of an ideal crystal. It leads, in a continuous limit defining the so-called continuized crystal, to the geometrical theory of dislocations (Trzęsowski, 1997; hereafter referred to as Part I) and to the gauge theory of dislocations (Trzęsowski, 1993b) describing the mechanical properties of continuized dislocated crystals. It also enables us to formulate a generalized gauge procedure (Section 2) based on the assumption that dislocations have no influence on local diffusive properties of a continuized crystal (Trzęsowski, 1989, 1993a, 1995). This procedure constitutes a geometric version of the thermodynamic hypothesis that some properties of linear systems [e.g., the one defined by (8) and (9)] are preserved in

states far from the thermodynamic equilibrium state (Glansdorff and Prigogine, 1973).

In this paper we consider distributions of dislocations admitting the isotropy of diffusive properties of a dislocated continuized crystal. In particular, this means that the considered tensor field of diffusion coefficients has the form

$$D^{AB}(Z) = D(Z)\delta^{AB} \tag{19}$$

$$D(Z) = D\lambda(Z), \qquad [D] = \text{cm}^2\,\text{sec}^{-1}$$

where D is a characteristic diffusion coefficient, λ is a positive dimensionless scalar, and $Z = (Z^A)$, $[Z^A] = \text{cm}$, is a Cartesian geometric frame reference. The diffusion coefficient tensor field can be used to define an associated Riemannian metric

$$g_{AB}(Z) = \lambda^{-1}(Z)\delta_{AB} \tag{20}$$

The considered body endowed with this metric constitutes a conformally flat material Riemannian space being, at the same time, the configurational space of a single diffusing point defect (Section 2). It turns out that the constant (sectional) scalar curvature of this configurational space is a geometric factor representing the existence of dissipative effects in the considered diffusion process as well as being a measure of the distance of a nonequilibrium Markov-type diffusion process from the equilibrium (Markov-type) one (Sections 2–4).

2. GENERALIZED GAUGE PROCEDURE

Let us consider a pair $(\Phi, \boldsymbol{g})$ defining the short-range order of the considered isotropic continuized crystal (see Part I), where $\Phi = (\boldsymbol{E}_a;\ a = 1, 2, 3)$ is a *Bravais moving frame* and $\boldsymbol{g}$ denotes the *internal length measurement* metric tensor defined by the condition that dislocations as well as the secondary point defects created by them have no influence on local metric properties of the continuized crystal, i.e., that

$$\boldsymbol{g}(X) = \delta_{ab}E^a(X) \otimes E^b(X) \tag{21}$$

where $X = (X^A)$ is a geometric frame reference (Section 1) and $\Phi^* = (E^a)$ is the moving coframe dual to Φ, i.e.,

$$\boldsymbol{E}_a(X) = \underset{a}{e}{}^A(X)\partial_A, \qquad E^a(X) = \overset{a}{e}{}_A(X)\,dX^A$$

$$\overset{a}{e}{}_A(X)\underset{b}{e}{}^A(X) = \delta^a_b \tag{22}$$

$$[E^a] = \text{cm}, \qquad [\boldsymbol{E}_a] = \text{cm}^{-1}, \qquad [\overset{a}{e}{}_A] = [\underset{a}{e}{}^A] = [1]$$

and, additionally, by the isotropy condition written as (see Part I)

$$g_{AB}(Z) \triangleq (1 + \delta(Z))^2 \delta_{AB} \tag{23}$$

where $Z = (Z^A)$ is a Cartesian frame reference and the scalar δ describes the influence of secondary point defects, created by the distribution of many dislocations, on the internal length measurement.

The assumption of the generalized gauge procedure that dislocations have no influence on local diffusive properties of a continuized crystal (Section 1) means, among other things, that the diffusion coefficient tensor field ought to have constant coefficients with respect to the Bravais moving frame, that is, for isotropic bodies one should have [cf. (19)]

$$D(X) = D^{ab} \boldsymbol{E}_a(X) \otimes \boldsymbol{E}_b(X), \qquad D^{ab} = D\delta^{ab} \tag{24}$$

where D^{ab} are diffusion coefficients of a homogeneous isotropic continuized crystal taken with respect to a Cartesian coordinate system. It follows from (21)–(24) that the conformally flat metric tensor associated with the diffusion coefficient tensor field [(19) and (20)] covers with the internal length measurement metric tensor, and [in Cartesian coordinates of (20) and (23)] should be

$$\lambda(Z) = (1 + \delta(Z))^{-2} \tag{25}$$

This means that the considered point defects are assumed to be immobile ones created by the distribution of dislocations and distorting the internal length measurement (of a continuized crystal), and the diffusing ones that influence this measurement can be neglected. This assumption can be accepted if the concentration of diffusing point defects is small in relation to the concentration of immobile ones.

The second assumption of the generalized gauge procedure states that a diffusion equation of the type (7), with the diffusion coefficients changed for spatially varying (in a smooth manner) ones, can be deduced from a balance equation of the form (8) and (9). It can be realized when fields compensating the influence of the varying diffusion coefficients on these relations are introduced. These compensating fields may be defined by changing the partial derivative appearing in (7)–(9), by the Levi-Civita covariant derivative $\nabla^{\boldsymbol{g}} = (\Gamma^A_{BC}[\boldsymbol{g}])$ associated with the internal length measurement metric tensor:

$$\Gamma^A_{BC}[\boldsymbol{g}] = \tfrac{1}{2} g^{AD}(\partial_C g_{BD} + \partial_B g_{CD} - \partial_D g_{BC}) \tag{26}$$

i.e., by a symmetric covariant derivative metric with respect to $\boldsymbol{g}$. Then

$$\nabla^{\boldsymbol{g}} \boldsymbol{D} = 0 \tag{27}$$

and the modified diffusion equation becomes (Trzęsowski, 1993a, 1995)

$$\partial_t p + F(\nabla^{\boldsymbol{g}}) p = 0, \qquad F(\nabla^{\boldsymbol{g}}) = \operatorname{div}_{\boldsymbol{g}}(\cdot \boldsymbol{b}) - D\Delta_{\boldsymbol{g}} \tag{28}$$

where the Laplace–Beltrami operator Δ_g and the divergence operator div_g act according to

$$\Delta_g p = g^{AB}\nabla^g_A\nabla^g_B p = g^{-1/2}\partial_A(g^{1/2}g^{AB}\partial_B p) \tag{29}$$
$$\mathrm{div}_g \boldsymbol{v} = \nabla^g_A v^A = g^{-1/2}\partial_A(g^{1/2}v^A)$$

and g is a scalar density (of weight 2) defined in (30). Equation (28) can be considered as an equation defining the localization probability of the stochastic motion of a point defect on the Riemannian configurational space $(R^3, \boldsymbol{g})$. This localization probability is given by (2) and (3) with Riemannian volume element $dV(X)$:

$$dV(X) = g(X)^{1/2}dV_0(X) \tag{30}$$
$$g(X) = \det(g_{AB}(X)), \qquad dV_0(X) = dX^1 \wedge dX^2 \wedge dX^3$$

where $dV_0(X)$ covers, in Cartesian coordinate systems of (20) and (25), with the Euclidean volume element. Note that a probability density p so defined is a scalar.

It can be shown that for a steady drift velocity $\boldsymbol{b}$ ($\partial_t \boldsymbol{b} = 0$), (28) is a *Fokker–Planck equation* for a diffusion Markov process on $(R^3, \boldsymbol{g})$, and the drift velocity can be taken, without loss of generality, in the following form (Ikeda and Watanabe, 1981):

$$b^A = D^{BC}(\Gamma^A_{BC}[\boldsymbol{g}] - \Gamma^A_{BC}) \tag{31}$$

where the Christoffel symbols $\Gamma^A_{BC}[\boldsymbol{g}]$ are defined by (26) and Γ^A_{BC} are connection coefficients defining a covariant derivative ∇ preserving local diffusion properties of the body, that is, $\nabla = (\Gamma^A_{BC})$ and

$$\nabla \boldsymbol{D} = 0 \tag{32}$$

Then (Trzęsowski, 1995)

$$b^A = 2DS^A, \qquad S^A = g^{AB}S_B, \qquad S_B = S^A{}_{AB}, \qquad S^A{}_{BC} = \Gamma^A_{[BC]} \tag{33}$$

and

$$T_A = \tfrac{1}{2}S_A = \overset{a}{e}_A T_a, \qquad T_a = \omega_a + t_a, \qquad t_a = C^b_{ab}, \qquad \omega_a = \omega_b{}^b{}_a \tag{34}$$

where

$$[\boldsymbol{E}_a, \boldsymbol{E}_b] = C^c_{ab}\boldsymbol{E}_c \tag{35}$$
$$\nabla \boldsymbol{E}_a = \omega^b{}_a \otimes \boldsymbol{E}_b, \qquad \omega^a{}_b = \omega_c{}^a{}_b E^c$$

and $[\boldsymbol{u}, \boldsymbol{v}] = \boldsymbol{u} \circ \boldsymbol{v} - \boldsymbol{v} \circ \boldsymbol{u}$ denotes the commutator product (bracket) of

vector fields $\boldsymbol{u}$ and $\boldsymbol{v}$ considered as first-order differential operators. Since the condition (32) means

$$\nabla \boldsymbol{g} = 0 \tag{36}$$

and such covariant derivatives are the subject of the gauge theory of static distributions of dislocations (Trzęsowski, 1993b), we can compute the drift velocity $\boldsymbol{b}$ based on this gauge theory. In Sections 3 and 4 we will show that, for uniformly dense distributions of dislocations (see Part I) satisfying the isotropy condition (23), the drift velocity can be computed in an another way.

The mean velocity of the considered diffusion Markov process is a Cartesian vector field $\boldsymbol{B} = B^A \partial_A$ defined by (Trzęsowski, 1995)

$$B^A \triangleq b^A + c^A, \qquad c^A = -D^{BC}\Gamma^A_{BC}[\boldsymbol{g}] \tag{37}$$

It follows from (19), (20), and (26) that

$$c^A = g^{AB}c_B = -(D/2)\delta^{AB}\partial_B \lambda \tag{38}$$

$$c_B = (D/2)\partial_B h, \qquad h = -\ln \lambda$$

If the drift velocity b^A vanishes, then $B^A = c^A$ is the mean velocity of a Brownian motion on the Riemannian manifold $(R^3, \boldsymbol{g})$. We will then call the diffusion process *locally free diffusion*. If additionally the metric $\boldsymbol{g}$ is flat, then $c^A = 0$ and we obtain a classical Brownian motion on the Euclidean space R^3 describing the free diffusion process (Section 1).

It follows from (5), (9) [with D^{AB} changed to $D^{AB}(Z)$], (19), and (27) that the Fokker–Plank equation (28) can be written in the form of a balance equation on the Riemannian manifold $(R^3, \boldsymbol{g})$:

$$\partial_t p + \nabla^{\boldsymbol{g}}_A (pv^A) = 0 \tag{39}$$

$$v^A = u^A + b^A, \qquad pu^A = -D^{AB}(Z)\partial_B p$$

From (3), (6), (29), and (38) we obtain that, in the Cartesian coordinate system $Z = (Z^A)$ of (19) and (20), the balance equation (39) takes the form (1) with

$$\sigma = \Sigma(Z, t)n, \qquad \Sigma(Z, t) = -\frac{3}{D} v^A(Z, t)c_A(Z) + d(t) \tag{40}$$

Since $\boldsymbol{c} = \boldsymbol{0}$ iff $\lambda = \text{const}$ [see (38)], thus (19), (39), and (40) mean that dissipative effects due to dislocations described by the generalized gauge procedure are equivalent to the appearance of a locally free diffusion in the continuized dislocated crystal. The locally free diffusion is caused in turn by the occurrence of secondary point defects created by the distribution of dislocations [see (23) and Part I].

3. INTERACTION ENERGY

The long-range distortion of a crystal structure due to the influence of many dislocations is described in the continuized crystal approximation by the *Burgers field* $\tau_\Phi = (\tau^a)$, a triple of 2-forms defined as (see Part I)

$$\tau^a = dE^a = \tfrac{1}{2}\tau^a{}_{bc} E^b \wedge E^c \tag{41}$$

$$\tau^a{}_{bc} = -C^a_{bc}, \qquad [\tau^a{}_{bc}] = \text{cm}^{-1}$$

where the moving coframe $\Phi^* = (E^a)$ dual to the Bravais moving frame $\Phi = (\boldsymbol{E}_a)$ is defined by (22), and smooth scalars C^a_{bc} constitute the object of anholonomity of Φ [see (35)]. If $C^a_{bc} = \text{const}$, then the distribution of dislocations is called *uniformly dense*, and the object of anholonomity becomes a set of structure constants of the three-dimensional real Lie algebra $\mathbf{g}_\Phi$ of vector fields tangent to the body and possessing Φ as its base (see Part I). It can be shown that there are only three types of nonisomorphic Lie algebras $\mathbf{g}_\Phi$ for which the internal length measurement metric tensor (Section 2) has a constant (sectional) scalar curvature (see Part I). Namely, edge dislocations are described by the Lie algebra denoted by $\mathbf{g}_t$, screw dislocations by the Lie algebra $\mathbf{g}_\gamma$, and mixed dislocations by a family $\{\mathbf{g}_\kappa, 0 \leq \kappa \leq 1\}$ of Lie algebras.

If the internal length measurement metric tensor $\boldsymbol{g}$ has the constant scalar curvature K, then the isotropy condition (19) [with λ given by (25)] is fulfilled, and $\boldsymbol{g}$ is a flat metric iff $K = 0$. If the scalar curvature K does not vanish, then there are two characteristic parameters associated with the generalized gauge procedure: the diffusion coefficient D, $[D] = \text{cm}^2\,\text{sec}^{-1}$, and the linear parameter $r_d = |K|^{-1/2}$, $[r_d] = \text{cm}$. Combining these parameters, we obtain a time parameter t_D:

$$t_D = \frac{1}{D|K|}, \qquad [t_D] = \text{sec} \tag{42}$$

Since the diffusion coefficient can be written as

$$D = \frac{r_d^2}{t_D}, \qquad r_d = |K|^{-1/2} \tag{43}$$

this time parameter can be interpreted as a *relaxation time* needed by the diffusion process to reach a steady state with the characteristic length r_d. Since $t_D = \infty$ for $K = 0$, the finiteness of this relaxation time means the existence of dissipative effects due to dislocations in the considered diffusion process [see (40) and the related commentary].

Let us assume that the drift velocity $\boldsymbol{b} = b^A \partial_A$ is given by

$$b = D\,du = b_A\,dZ^A, \qquad b_A = g_{AB} b^B \tag{44}$$

where $Z = (Z^A)$ is the Cartesian coordinate system of (20). A steady state

of the considered diffusion process is defined by (28), (44), and the condition $\partial_t p = 0$. In particular, the localization probability defined by

$$p(Z) = p_0 \exp(-U(Z)/\Theta) \tag{45}$$

$$U(Z) = -\Theta u(Z), \qquad [\Theta] = \text{g cm}^2 \text{ sec}^{-2}$$

where Θ is a characteristic energy of the diffusion process, fulfills these conditions. Therefore, $U(Z)$ can be recognized as the *self-energy* of the reduced microstate Z of the system of noninteracting diffusing point defects defined as a place Z of a single distinguished point defect moving on the Riemannian manifold $(R^3, \boldsymbol{g})$ in a random way (Trzęsowski and Piekarski, 1992). Taking $\Theta = k_B T$, where T is the temperature of a thermostat, we can consider a nonequilibrium diffusion process as one thermally activated at the temperature T of the environment of the body (Trzęsowski and Piekarski, 1992) and admitting a heterogeneous nonequilibrium steady distribution of diffusing defects defined by (45) [see the commentary following (15)].

The mean velocity $\boldsymbol{B} = B^A \partial_A$ of diffusing point defects [defined by (37) and (38)] can be written [in the case (44)] as

$$B_A = g_{AB} B^B = b_A + c_A = -\zeta^{-1} \partial_A E \tag{46}$$

$$E = -\Theta(u + h/2), \qquad \zeta = \Theta/D, \qquad [\zeta] = \text{g sec}^{-1}$$

where ζ is a characteristic friction coefficient of the diffusive motion of a point defect [cf. (12) and (15)]. If the drift of diffusing point defects is small with respect to their chaotic (thermal) motion, then the force $\boldsymbol{F} = F^A \partial_A$ acting on a point defect can be estimated by means of the Stokes relation (Section 1):

$$F^A = \zeta B^A \tag{47}$$

and the condition (13) is fulfilled with E given by (46). Thus, the energy E has the physical meaning of an *interaction energy* (possibly of effective energy character) between dislocations and a diffusing point defect. Comparing (44) and (46) with (33) and (34) and taking into account that (see Part I)

$$t_A = \partial_A \varphi \qquad \text{for} \quad K < 0 \tag{48}$$

$$t_A = 0 \qquad \text{for} \quad K \geq 0$$

we obtain

$$\omega_A = \overset{a}{e}_A \omega_a = \partial_A \psi, \qquad \psi = u - \varphi \tag{49}$$

and

$$E = E_e + E_p \tag{50}$$

$$E_e = -\Theta\psi, \qquad E_p = -\Theta(\varphi + \ln|1 + \delta|)$$

It can be shown (see Part I) that if $K < 0$, then the potential φ of (48) and (50) should fulfill the equation

$$\Delta_g \varphi = 4K \tag{51}$$

or, writing (51) in terms of dissipative effects due to the influence of dislocations on the diffusion [see (19), (25), and (40)], the equation

$$r_d^2 \Delta\varphi + t_D \boldsymbol{c} \cdot \operatorname{grad} \varphi + 4(1 + \delta)^2 = 0 \tag{52}$$

where Δ denotes the Euclidean Laplacian [see (16)], $\boldsymbol{u} \cdot \boldsymbol{v} = \delta^{AB} u_A v_B$ is the Euclidean scalar product, and (23), (29), (30), (38), (42), and (43) were taken into account.

Let us compute, in the limit $K \to 0$, the interaction energy limit. It needs to take into account the commutation rules defining the Lie algebras $\mathbf{g}_t$, $\mathbf{g}_\gamma$, and $\mathbf{g}_\kappa$ [see the commentary following (41)]. These are as follows (see Part I). The Lie algebra $\mathbf{g}_\gamma$ is isomorphic to the Lie algebra $so(3)$ of the group $SO(3)$ of (proper) rotations in three real dimensions:

$$[\boldsymbol{E}_a, \boldsymbol{E}_b] = 2k\epsilon_a{}^c{}_b \boldsymbol{E}_c, \qquad \epsilon_a{}^c{}_b = \delta^{dc}\epsilon_{adb} \tag{53}$$

where ϵ_{abc} denotes the permutation symbol. The Lie algebra $\mathbf{g}_t$ is defined by

$$[\boldsymbol{E}_1, \boldsymbol{E}_2] = 2k\boldsymbol{E}_2, \qquad [\boldsymbol{E}_1, \boldsymbol{E}_3] = 2k\boldsymbol{E}_3, \qquad [\boldsymbol{E}_2, \boldsymbol{E}_3] = 0 \tag{54}$$

Lie algebras $\boldsymbol{g}_\kappa$, $0 \leq \kappa \leq 1$, are defined by

$$[\boldsymbol{E}_1, \boldsymbol{E}_2] = 2k(\kappa\boldsymbol{E}_2 + \boldsymbol{E}_3), \qquad [\boldsymbol{E}_1, \boldsymbol{E}_3] = 2k(\kappa\boldsymbol{E}_3 - \boldsymbol{E}_2), \qquad [\boldsymbol{E}_2, \boldsymbol{E}_3] = 0 \tag{55}$$

Moreover, we have

$$\begin{aligned} &K = l_d^{-2}, && t_a = 0 && \text{for} \quad \mathbf{g}_\Phi = \mathbf{g}_\gamma \\ &K = -l_d^{-2}, && t_a = 4k\delta_a^1 && \text{for} \quad \mathbf{g}_\Phi = \mathbf{g}_t \\ &K = -\kappa l_d^{-2}, && t_a = 4k\kappa\delta_a^1 && \text{for} \quad \mathbf{g}_\Phi = \mathbf{g}_\kappa \\ &l_d = 1/k > 0, && [k] = \mathrm{cm}^{-1}, && [\kappa] = [1] \end{aligned} \tag{56}$$

It follows from (53)–(56) that if $k \to 0$, then $K \to 0$ and dislocations vanish. So in this limit the interaction energy E should vanish, too. Since $\varphi \to \text{const}$ [see (48)] and $\delta \to 0$ [see (25)] for $K \to 0$, the energy E_e should be taken, e.g., in the form

$$E_e(Z) = \Theta\eta(k)\chi(Z), \qquad \eta(0) = 0, \quad [\eta\chi] = [1] \tag{57}$$

Let us observe that if $\kappa \to 0$, then $K \to 0$, although $k \neq 0$. Thus, in this case dislocations do not vanish, and the interaction energy E reduces to its

part E_e defined by (57). This distribution of dislocations is described by the Lie algebra $\mathbf{g}_0$ defined by [see (55)]

$$[\boldsymbol{E}_1, \boldsymbol{E}_2] = 2k\boldsymbol{E}_3, \qquad [\boldsymbol{E}_1, \boldsymbol{E}_3] = -2k\boldsymbol{E}_2, \qquad [\boldsymbol{E}_2, \boldsymbol{E}_3] = 0 \tag{58}$$

and admitting the existence of mixed as well as screw dislocation lines (see Part I). It follows from (58) that $\mathbf{g}_0$ is isomorphic to the Lie algebra $e(2)$ of the group $E(2)$ of motions of the plane R^2.

4. CLASSICAL LIMIT

It follows from Section 3 that in the case of uniformly dense distributions of dislocations, the potential u of (44) defining the drift velocity $\boldsymbol{b}$ can be represented in the form [see (49), (50), and (57)]

$$u = \psi + \varphi, \qquad \psi = -\eta(k)\chi, \quad \eta(0) = 0 \tag{59}$$

where the potential φ is defined by (51) for $K < 0$ and reduces to a constant (say equals zero) for $K \geq 0$. In the limit $K \to 0$ we have $\lambda = 1$ [see (20)], $\varphi = 0$, the dissipative effects of the form (40) reduce to (6), and the diffusion equation (28) reduces to its classical equilibrium form (7) with

$$D^{AB} = D\delta^{AB}, \qquad b_A = \delta_{AB}b^B = -\zeta^{-1}\partial_A E_e \tag{60}$$

where E_e has the form (57). Since for Lie algebras $\mathbf{g}_t$ and $\mathbf{g}_\gamma$ the limit $K \to 0$ is equivalent to $k \to 0$ [see (56)], we obtain that (28) then reduces to the form

$$\partial_t p - D\Delta p = 0 \tag{61}$$

describing the free diffusion process (Section 1).

For the family $\mathbf{g}_\kappa$, $0 \leq \kappa \leq 1$, of Lie algebras, the limit $K \to 0$ can be considered as a consequence of the limit $\kappa \to 0$ [see (56)]. Then, for $K = 0$, the energy E_e preserves its general form (57), and the considered distributions of dislocations reduce to the one described by the Lie algebra $\mathbf{g}_0$ [see (58)]. Moreover, the assumption of the existence of a spatially uniform distribution of diffusing point defects (Section 1) needs the energy E_e to be a harmonic function [see (16)], i.e. [see (57) and (59)] it should be

$$\Delta\chi = 0 \tag{62}$$

Therefore, the energy E_e can be interpreted, at least in the case of a Lie algebra $\mathbf{g}_\kappa$, as the elastic part of the interaction energy E defined by (50). Equations (50) and (52) mean that the part E_p of the interaction energy can be considered as that to which inelastic interactions between dislocations and a diffusing point defect contribute. Since the separation (50) of the interaction energy does not depend on the choice of the Lie algebra, we can postulate an extension of the definition (57) and (62) of the elastic interaction energy

on the Lie algebras $\mathbf{g}_t$ and $\mathbf{g}_\gamma$. Then the influence of elastic and inelastic interactions on the drift velocity $\boldsymbol{b}$ is described by (44), (59), (62), and (52) for $K < 0$ or $\varphi = \text{const}$ for $K \geq 0$.

A broad class of elastic interaction energies, containing continuous counterparts of energies mentioned in Section 1 [see (17) and (18)], can be obtained by assuming the form (57) of this energy and, in spherical coordinates (Section 1), that

$$\chi(Z) = \frac{e(\xi)}{r^n}, \qquad \xi = \cos\vartheta, \qquad [\eta(k)] = \text{cm}^n \tag{63}$$

The Laplace equation (62) then reduces to

$$(1 - \xi^2)e''(\xi) - 2\xi e'(\xi) + n(n-1)e(\xi) = 0 \tag{64}$$

For $n = 1$ the general solution of (64) has the form

$$e(\xi) = \frac{1}{2}\ln\left|\frac{1+\xi}{1-\xi}\right| + c_0 \tag{65}$$

and for $\xi = 0$ and $c_0 = 1$ we obtain a counterpart of (18) with

$$\eta(k) = \epsilon L(k), \qquad \chi(Z) = \frac{1}{r}, \qquad L(0) = 0, \qquad [L(k)] = \text{cm} \tag{66}$$

If $|\xi| << 1$ and $c_0 = 0$, then

$$\chi(Z) = \frac{\cos\vartheta}{r} \tag{67}$$

For $n = 3$ the counterpart of (17) defined by

$$\eta(k) = \epsilon V_0(k), \qquad \chi(Z) = \frac{1 - 3\cos^2\vartheta}{r^3}, \qquad V_0(0) = 0, \qquad [V_0(k)] = \text{cm}^3 \tag{68}$$

is a particular solution of (64), and thus the general solution of (64) defines

$$\chi(Z) = \frac{e(\xi)}{r^3}, \qquad \xi = \cos\vartheta$$

$$e(\xi) = c_1 e_1(\xi) + c_2 e_2(\xi), \qquad e_1(\xi) = 1 - 3\xi^2 \tag{69}$$

$$e_2(\xi) = \tfrac{1}{4}(1 - 3\xi^2)[\text{artgh}\,\xi - \sqrt{3}\,\text{artgh}(\sqrt{3}\xi)] + \tfrac{3}{4}\xi$$

The elastic interaction energy of the form (57), (68) may be applied, e.g., in the case of the dislocation fluid model (based on the Lie algebra $\mathbf{g}_t$; see Part I) for a crystal irradiated with fast neutrons [see remarks preceding (17)].

5. CONCLUSIONS

It was shown (see Part I) that the existence of point defects created by a distribution of many dislocations influences, in the continuized crystal approximation, the geometry of this distribution. For example, a conformal change (even small) of the internal length measurement in a continuized crystal due to the influence of these point defects transforms glide planes onto flat umbilical surfaces. The generalized gauge procedure presented in this part of the paper leads to the conclusion that this conformal change is also a source of the appearance of dissipative effects in diffusion processes of point defects (in continuized dislocated crystals; see Section 2).

If we restrict ourselves to uniformly dense distributions of dislocations with the internal length measurement of a constant scalar curvature (see Part I), then it turns out that this curvature has a fundamental character in the description of the geometry of continuous distributions of dislocations (see Part I) as well as in the description of diffusion processes of point defects due to their interactions with dislocations. Namely, dissipative effects (due to dislocations) in such diffusion processes vanish if the scalar curvature vanishes (Sections 2 and 4), and the existence of a finite relaxation time of these diffusion processes is equivalent to the existence of a nonvanishing scalar curvature (Section 3).

If the scalar curvature vanishes, then the nonequilibrium diffusion equation obtained by means of the generalized gauge procedure reduces to the classical diffusion equation (Section 4). The analysis of this "classical limit" shows that the interaction energy between dislocations and a diffusing point defect (Section 3) can be divided into two parts: the elastic interaction energy being a harmonic function, and a part to which inelastic interactions contribute (Section 4). An equation describing this inelastic contribution can be deduced from the geometry of the distribution of dislocations (Section 3).

REFERENCES

Bullough, R., and Newman, R. (1970). *Reports on Progress in Physics,* **33**, 101.

Glansdorff, P., and Prigogine, I. (1973). *Theory of Structure, Stability and Fluctuations,* Mir, Moscow [in Russian].

Hull, D., and Bacon, D. J. (1984). *Introduction to Dislocations,* Pergamon Press, Oxford.

Ikeda, N., and Watanabe, S. (1981). *Stochastic Differential Equations and Diffusion Processes,* North-Holland, Amsterdam.

Klimontovitch, I. N. (1982). *Statistical Physics,* Nauka, Moscow [in Russian].

Kosevitch, A. M. (1972). *Foundations of Crystal Lattice Mechanics,* Nauka, Moscow [in Russian].

Orlov, A. N. (1973). *Thermally Activated Processes in Crystals,* Mir, Moscow [in Russian].

Trzęsowski, A. (1989). *International Journal of Theoretical Physics,* **5**, 545.

Trzęsowski, A. (1993a). In *Continuum Models of Discrete Systems,* K.-H. Anthony and H. I. Wagner, eds., Trans Tech, Brookfield, Vermont.
Trzęsowski, A. (1993b). *Reports on Mathematical Physics,* **1**, 71.
Trzęsowski, A. (1995). *Progress of Physics,* **43**, 1.
Trzęsowski, A. (1997). *International Journal of Theoretical Physics,* this issue.
Trzęsowski, A., and Piekarski, S. (1992). *Nuovo Cimento,* **14D**, 767.