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On the Geometry of Diffusion Processes in Continuized Dislocated Crystals

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Abstract

Nonequilibrium diffusion processes of point defects in continuized dislocated crystals are considered. A generalized, stochastically motivated gauge procedure to introduce the geometry of a material space describing the influence of dislocations on the free diffusion process, is used. The dependence of diffusing processes and their steady states on the curvature of the material space of edge dislocations, on the scalar density of these dislocations, and on the interaction energy between dislocations and a diffusing atom, is analysed. An equation defining the interaction energy is deduced, using statistical arguments, from the material space geometry.

1. Introduction

The diffusion can be regarded in many cases as a random motion of a particle [1, 2]. Such an approach is justified for example if in an alloy the atoms of one element are in the interstitial position of another element of the crystal lattice. In this case the diffusion has thermally activated interstitial random walk character and sequential jumps of atoms can be regarded as independent random events. Moreover, in this case, the influence of diffusing atoms on the matrix crystal lattice can be usually neglected. If an additional drift (e.g. due to the influence of the body boundary, external fields, or another crystal lattice defects) of diffusing atoms is absent, the diffusion can be regarded as a pure random phenomenon – the *free diffusion* in a homogeneous body.

We will neglect the influence of the body boundary on diffusion processes, so we will restrict our considerations to the body $\mathscr{B}$ identified with the Euclidean point space E^3 – the space of positions of diffusing particles. We will consider also the case of identical but distinguishable particles. In a consequence, if $n(X, t)$ denotes the density of the number of particles diffusing at the instant of time $t \geqq 0$, the probability $p(X, t)\, dV(X)$ of observing a diffusing particle in the volume $dV(X)$ can be assumed to be [3]

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

$$N(t) = \int_{R^3} n(X, t)\, dV(X) < \infty \tag{1.1}$$

where $X = X(Q)$ denotes coordinates of a point $Q \in E^3$ in a (Lagrange) coordinate system $X = (X^A;\ A = 1, 2, 3)$ on E^3. We will use the so-called *geometric frame references*, i.e.

dimensional coordinate systems $X=(X^A)$ such that $[X^A]=[dX^A]=[l]$, $[\partial_A=\partial/\partial X^A]=[l^{-1}]$, where $[l]=cm$ in the cgs units system. $N(t)$ is a finite but very large number of particles diffusing at the instant t and the above approximation of $p(X, t)$ is the better, the greater $N(t)$ is.

A stochastic description of the free diffusion can be reduced, under the above assumptions, to a Brownian motion in the Euclidean point space E^3 of one of the diffusing particles (arbitrary distinguished). It is well-known that the probability of localization of a Brownian particle is defined by the following Fokker-Planck equation [4]:

$$\partial_t p - W(\partial)p = 0$$
$$W(\partial) = D^{AB}\partial_A\partial_B, \qquad \partial = (\partial_A;\ A=1,2,3) \tag{1.2}$$

where $X=(X^A)$ is a Cartesian coordinate system on E^3, and (D^{AB}) is a symmetric, positive-definite matrix of constant diffusion coefficients. From (1.1) and (1.2) follows the local balance equation of the number of diffusing particles:

$$\partial_t n + \partial_A j^A = d(t)\,n \tag{1.3}$$

where $d(t)=\dot{N}(t)/N(t)$ is the rate (e.g. radiation induced) change of the total number of diffusing particles, $\boldsymbol{j}=j^A\partial_A$ is the flux of these particles caused by their "purely" chaotic Brownian motion and it has the form of the so-called Fick law:

$$j^A = -D^{AB}\partial_B n \tag{1.4}$$

stating that the direction of the free diffusion flux is opposite to the concentration gradient direction. In the case of the diffusion of atoms in a crystalline solid, such a form of the diffusion flux may be accepted with the assumption that the lattice vacancies are everywhere in local thermal equilibrium of when their concentration is small in relation to the concentration of diffusing atoms [1]. The general balance equation is defined by (1.3) and the diffusion flux $\boldsymbol{j}$ of the form:

$$j^A = n v^A$$
$$v^A = u^A + b^A, \quad n u^A = -D^{AB}\partial_B n \tag{1.5}$$

where the vector field $\boldsymbol{u}=u^A\partial_A$ is called the *diffusion velocity*, $\boldsymbol{b}=b^A\partial_A$ denotes a *drift velocity* (depending e.g. on interactions between dislocations and point defects), and $\boldsymbol{v}=v^A\partial_A$ is called the *diffusion peculiar velocity*.

If a crystal lattice is distorted by the occurrence of many dislocations, then the influence of this distortion on the diffusion process manifests itself in the variableness of diffusion coefficients and in the appearance of a drift velocity of diffusing matter. On the other hand, the influence of many dislocations on mechanical properties of a crystalline solid is described in mechanics of continua by means of the so-called geometrical theory of dislocations [5, 6]. According to this theory, though the existence of many dislocations breaks the long-range order of a crystalline solid, 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. Consequently, the short-range order of a dislocated crystalline solid can be described, in a continuous limit defining the so-called *continuized crystal* [5, 6], by means of a triple $(\Phi, G, \boldsymbol{g})$, where $\Phi=(\boldsymbol{E}_a;\ a=1,2,3)$ is a moving (vectorial) frame globally defined on the body (identified with the Euclidean point space E^3), $G\subset SO(3)$ is a group of rotations describing material symmetries of a macroscopically homogeneous crystalline solid, and $\boldsymbol{g}$ is a metric tensor with respect to which Φ is orthonormal:

$$\boldsymbol{g} = \delta_{ab} E^a \otimes E^b \tag{1.6}$$

where $\Phi^* = (E^a)$ is the moving coframe dual to Φ:

$$\boldsymbol{E}_a = \underset{a}{\mathrm{e}}^A \partial_A, \quad E^a = \overset{a}{e}_A dX^A, \quad \underset{a}{\mathrm{e}}^A \overset{b}{e}_A = \delta^b_a. \tag{1.7}$$

The vector fields $\boldsymbol{E}_a$ define, at each point of the body, a triple of local crystallographic directions and scales of a locally Euclidean *internal length measurement* along them. The metric tensor $\boldsymbol{g}$, defining this internal length measurement, represents a property of the dislocated crystalline solid that dislocations have no influence on local metric properties of a crystal structure of the body and, at the same time, this metric tensor describes the influence of point defects created by the existence of many dislocations (e.g. due to intersections of dislocation lines) on this crystal structure [6]. We assume that the influence of another appearing point defects (e.g. the diffusing ones) on the internal length measurement can be neglected. Though the existence of a symmetry group G is of no importance in the present work, nevertheless the considered distributions of dislocations may be dependent on the group G indirectly. For example, it is the case of the static gauge theory of continuous distributions of dislocations with local gauges defined by moving frames Φ and the group G considered as a structure group of this theory [5] (see also Section 4 – remarks following the equation (4.22)). It is well-known that single dislocations influence the free diffusion process in a way admitting the existence of a nonuniform equilibrium steady state of diffusing matter defined by the elastic part of the interaction energy between dislocations and a diffusing atom (e.g. [1, 7, 8]). However, in general, it is not the case of the influence of many dislocations for which steady nonequilibrium thermodynamic states of diffusing matter, caused the inelastic character of these interactions and by the existence of a plastic distortion of the dislocated crystal structure, occur. In the present work, the influence of a stationary distribution of many dislocations on the free diffusion process is described with the aid of a *generalized gauge procedure* [9, 10] based on the existence of the above defined short-range order of a continuized dislocated crystal (Section 2). This procedure constitutes a geometric version of the thermodynamic hypothesis that some properties of linear systems (e.g. that one defined by (1.2)–(1.4)) are preserved in states far from the thermodynamic equilibrium state (cf. [11]). The work introduces a broad class of geometries realizing the generalized gauge procedure (Sections 2–4) and points out the geometry defined by a semi-symmetric metric connection (considered in [10]) as the one describing the influence of edge dislocations on the free diffusion process (Section 5). This geometric model makes possible to formulate an equation defining the interaction energy between edge dislocations and a diffusing atom (Sections 5 and 6). Moreover, the plastic volumetric distortion of the dislocated crystal structure is recognized as a geometric factor responsible for the variableness of the local activation energy of the diffusion (Sections 4 and 6).

2. Generalized Gauge Procedure

The generalized gauge procedure (Section 1) is based on the assumption that dislocations have no influence on local diffusion properties of a continuized crystal. Particularly, we assume that the tensor field $\boldsymbol{D}(X)$ of diffusion coefficients is a Φ – parallel field, i.e. (see (1.7)):

$$\boldsymbol{D}(X) = D^{ab}\boldsymbol{E}_a(X) \otimes \boldsymbol{E}_b(X) = D^{AB}(X)\,\partial_A \otimes \partial_B$$
$$D^{AB}(X) = D^{ab}\, \underset{a}{\mathrm{e}}^A(X)\, \underset{b}{\mathrm{e}}^B(X)$$
$$[\boldsymbol{D}] = [t^{-1}], \quad [D^{AB}] = [D^{ab}] = [\ell^2 t^{-1}] \tag{2.1}$$

where $\Phi = (\boldsymbol{E}_a)$, $[\boldsymbol{E}_a] = [\ell^{-1}]$, is a dimensional moving frame defining the short-range order of the continuized dislocated crystalline solid (Section 1), (D^{ab}) is a symmetric, positive-definite matrix of constant diffusion coefficients of a homogeneous crystalline solid taken with respect to a Cartesian frame reference (Section 1), and $[\ell] = cm$, $[t] = sec$ in the cgs units system. This tensor defines the metric tensor $\boldsymbol{G}$:

$$\boldsymbol{D}(X) = D\,\boldsymbol{G}(X)^{-1}, \quad \boldsymbol{G}(X) = G_{ab}\,E^a(X) \otimes E^b(X)$$
$$D^{ab} = D\,G^{ab}, \quad G_{ab}G^{bc} = \delta^c_a, \quad D = \text{const.} > 0, \quad [D] = [\ell^2 t^{-1}] \tag{2.2}$$

equivalent, up to its global rescaling defined by the transformation $\Phi \rightarrow \Phi\boldsymbol{L} = (\boldsymbol{E}'_a)$:

$$\boldsymbol{E}'_a(X) = \boldsymbol{E}_b(X)\,L^b{}_a, \quad \boldsymbol{L} = (L^b{}_a) \in GL^+(3) \tag{2.3}$$

where $GL^+(3)$ denotes the group of all real 3×3 matrices with positive determinant, to the internal length measurement metric tensor defined by (1.6).

We assume also, in order to define the generalized gauge procedure explicitly, that differential relations (1.2)–(1.4), with the tensor field $\boldsymbol{D}(X)$ of diffusion coefficients replacing the constant tensor of diffusion coefficients appearing in these equations, are valid. If so, fields compensating the influence of the varying of diffusion coefficients on these relations, would be introduced. It can be realized if the partial derivative ∂ appearing in (1.2)–(1.4) is changed for the Levi-Civita covariant derivative $\nabla^G = (\Gamma^A_{BC}[\boldsymbol{G}])$ corresponding to the Riemannian metric tensor $\boldsymbol{G}$:

$$\Gamma^A_{BC}[\boldsymbol{G}] = \tfrac{1}{2}G^{AD}(\partial_C G_{BD} + \partial_B G_{CD} - \partial_D G_{BC}) \tag{2.4}$$

and if as the density $n(X, t)$ of the number of particles diffusing at the arbitrary distinguished instant t is taken a scalar. The Fick law preserves then the form (1.4), and from (1.1), (1.3), (1.4) and (2.2) with ∇^G_A replacing ∂_A, we obtain the following Riemannian counterpart of (1.2):

$$\partial_t p - W(\nabla^G)\,p = 0$$
$$W(\nabla^G) = D^{AB}(X)\,\nabla^G_A \nabla^G_B = D\Delta_G \tag{2.5}$$

where Δ_G denotes the Laplace-Beltrami operator on the Riemannian manifold $(\mathscr{B}, \boldsymbol{G})$ acting on scalars according to:

$$\Delta_G\, p = G(X)^{-\frac{1}{2}}\,\partial_A(G(X)^{\frac{1}{2}}\,G^{AB}(X)\,\partial_B\, p),$$
$$G(X) = \det(G_{AB}(X)). \tag{2.6}$$

It is known that a Brownian motion on the Riemannian manifold $(\mathscr{B}, \boldsymbol{G})$ has an infinitesimal generator of the form $W(\nabla^G)$ [12]. Moreover, the probability $P(Q_t \in M)$ that the actual (at the instant t) position Q_t of the Brownian particle is a point of the domain $M \subset \mathscr{B}(=E^3)$ is given by:

$$P(Q_t \in M) = \int_M p(X, t)\, dV(X) \tag{2.7}$$

where

$$dV(X) = G(X)^{\frac{1}{2}} d^3 X \tag{2.8}$$

is the Riemannian volume element, d^3X denotes (in a Cartesian coordinate system) the Euclidean volume element in E^3, and the Fokker-Planck equation defining the density $p(X, t)$ covers with (2.5). Since in a Cartesian coordinate system on E^3 (cf. (1.2)):

$$W(\nabla^G) = D^{AB}(X)\partial_A\partial_B + c^A(X)\partial_A$$
$$c^A = -D^{BC}\Gamma^A_{BC}[\boldsymbol{G}] \tag{2.9}$$

so the Cartesian vector field $\boldsymbol{c} \stackrel{*}{=} c^A\partial_A$ vanishes if $\boldsymbol{G}$ is an Euclidean metric tensor (i.e. for constant Cartesian diffusion coefficient), and thus $\boldsymbol{c}$ defines the mean velocity of a Riemannian Brownian motion. Note, that from (1.1) and (2.7) with $dV(X)$ given by (2.8) follows that $p(X, t)$ and $n(X, t)$ are scalars for an arbitrary distinguished instant t. The such defined diffusion process will be called *locally free diffusion* (in a dislocated body) [10].

The above formulated generalized gauge procedure can be extended to describe the influence of an additional drift velocity $\boldsymbol{b} = b^A\partial_A$ on the locally free diffusion. Namely, it can be shown [12] that for every vector field $\boldsymbol{b}$ tangent to the body, there exists a Riemann-Cartan covariant derivative $\nabla = (\Gamma^A_{BC})$ metric with respect to $\boldsymbol{G}$:

$$\nabla \boldsymbol{G} = \boldsymbol{O} \tag{2.10}$$

or, equivalently, preserving local diffusion properties of the body:

$$\nabla \boldsymbol{D} = \boldsymbol{O} \tag{2.11}$$

and fulfilling the condition:

$$b^A = D^{BC}(\Gamma^A_{BC}[\boldsymbol{G}] - \Gamma^A_{BC}). \tag{2.12}$$

The another covariant derivative $\nabla' = (\Gamma'^A_{BC})$ metric with respect to $\boldsymbol{G}$ satisfies the condition (2.12) iff

$$S'^A{}_{BC} = S^A{}_{BC} = \Gamma^A_{[BC]} \tag{2.13}$$

where $S'^A{}_{BC}$ and $S^A{}_{BC}$ are torsion tensors of ∇' and ∇, respectively. Since [12]

$$\Gamma^A_{BC} = \overset{o}{\Gamma}{}^A_{BC} + S^A{}_{BC}$$
$$\overset{o}{\Gamma}{}^A_{BC} = \Gamma^A_{BC}[\boldsymbol{G}] + K^A_{(BC)}, \quad K^A_{BC} = 2G^{AD}G_{BE}S^E{}_{DC} \tag{2.14}$$

we obtain, taking into account (2.2) and (2.12), that

$$b^A = -D^{BC}K^A_{BC} = 2DS^A$$
$$S^A = G^{AB}S_B, \quad S_A = S^B{}_{BA}. \tag{2.15}$$

The replacement of the partial derivative ∂ with the above defined Riemann-Cartan covariant derivative ∇ transforms the infinitesimal generator $W(\partial)$ of a Brownian motion in the Euclidean point space E^3 (the equation (1.2)) into a differential operator $W(\nabla)$ acting on scalars and given by (cf. (2.9)):

$$W(\nabla) = W(\nabla^G) + b^A\partial_A = D^{AB}(X)\partial_A\partial_B + B^A(X)\partial_A \tag{2.16}$$

where it was denoted:

$$B^A = -D^{BC}\Gamma^A_{BC} = b^A + c^A. \tag{2.17}$$

It can be shown that the differential operator $W(\nabla)$ can be treated as an infinitesimal generator of a diffusion Markov process on the Riemannian manifold ($\mathscr{B} = E^3$, $\boldsymbol{G}$) [12]. It follows from (2.16) that the localization probability (2.7) of this stochastic process is defined by the following Fokker-Planck equation [12]:

$$\begin{aligned} &\partial_t p + F(\nabla^G)p = 0 \\ &F(\nabla^G) = \mathrm{div}_G(\cdot\,\boldsymbol{b}) - D\Delta_G \end{aligned} \tag{2.18}$$

where Δ_G is the Laplace-Beltrami operator given by (2.6), div_G denotes the divergence operator on ($\mathscr{B}$, $\boldsymbol{G}$) defined by:

$$\mathrm{div}_G\, \boldsymbol{v} = \nabla^G_A v^A = G(X)^{-\frac{1}{2}}\,\partial_A(G(X)^{\frac{1}{2}} v^A) \tag{2.19}$$

and the drift velocity $\boldsymbol{b}$ is given by (2.12) and (2.15). The mean velocity of this diffusion process covers, in a Cartesian coordinate system, with the drift velocity $\boldsymbol{B} \stackrel{*}{=} B^A\partial_A$ defined by (2.17) and considered as a Cartesian vector field. From (2.18) follows the following continuity equation on the Riemannian manifold ($\mathscr{B}$, $\boldsymbol{G}$) (cf. (1.1) and (1.3)):

$$\partial_t p + \mathrm{div}_G \boldsymbol{j} = 0 \tag{2.20}$$

where, the flux $\boldsymbol{j} = j^A\partial_A$ is defined by (cf. (1.1) and (1.5)):

$$\begin{aligned} &j^A = p\,v^A \\ &v^A = u^A + b^A, \quad p u^A = -D^{AB}\partial_B p \end{aligned} \tag{2.21}$$

and the drift velocity $\boldsymbol{b}$ is given by (2.15). Conversely, the equation (2.18) can be obtained from (1.1), (1.3) and (1.5) with $D^{AB} = D^{AB}(X)$, and with the partial derivative ∂ changed for the Levi-Civita covariant derivative ∇^G. Moreover, we can assume, without loss of generality, the form (2.12) (and so – the form (2.15)) of the considered steady drift velocities.

We conclude, that as the fundamental expressions to describe the influence of many dislocations on the free diffusion process may be taken the Fokker-Planck equation (2.18) and a Riemann-Cartan covariant derivative satisfying the conditions (2.11) and (2.15). What we need are constraints to be imposed on solutions of (2.18) which give us the model of a Markov-type diffusion process in the form of a relation between the drift velocity $\boldsymbol{b}$ and the density of dislocations.

3. Density of Dislocations

The long-range distortion of a crystal structure due to dislocations is described, in the continuized crystal approximation (Section 1), by means of the so-called *Burgers field* $\tau_\Phi = (\tau^a)$ being a triple of 2-forms defined by [5, 6]:

$$\begin{aligned} &\tau^a = dE^a = \tfrac{1}{2}\tau^a{}_{bc}E^b \wedge E^c \\ &\tau^a{}_{bc} = -C^a_{bc}, \quad [\boldsymbol{E}_a, \boldsymbol{E}_b] = C^c_{ab}\boldsymbol{E}_c \\ &[\tau^a] = [\ell], \quad [\tau^a{}_{bc}] = [\ell^{-1}] \end{aligned} \tag{3.1}$$

where the moving coframe $\Phi^* = (E^a)$ dual to the moving frame $\Phi = (\boldsymbol{E}_a)$ is defined by (1.7), $\wedge$ denotes the exterior product, 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. If dislocations are absent (i.e. $\tau^a = 0$, $a = 1, 2, 3$), then there exists a Cartesian coordinate system $\xi = (\xi^a)$ on E^3 such that for $\xi^a = \xi^a(X)$ (cf. (1.7) and (2.2)):

$$E^a = d\xi^a, \quad \text{i.e.} \quad \underset{a}{\mathrm{e}}^A = \xi^a_{,A}$$

$$\boldsymbol{E}_a = \partial_a = \partial/\partial\xi^a, \quad \text{i.e.} \quad \underset{a}{\mathrm{e}}^A = X^A_{,a}$$

$$\boldsymbol{D} = D^{ab}\partial_a \otimes \partial_b, \quad D^{ab} = \text{const.} \tag{3.2}$$

Let us introduce a common representation of the short and long-range effect of dislocations on a crystal structure in the form of a tensor field $\boldsymbol{\tau}_\Phi$ defined by [6]:

$$\boldsymbol{\tau}_\Phi = \boldsymbol{E}_a \otimes \tau^a = \tfrac{1}{2}\tau^a{}_{bc}\boldsymbol{E}_a \otimes E^b \otimes E^c. \tag{3.3}$$

Since this representation is invariant under the global rescaling (2.3) (i.e. $\boldsymbol{\tau}_\Phi = \boldsymbol{\tau}_{\Phi L}$), the short-range order of the continuized dislocated crystal can be equivalently described by a triple $(\Phi, G_L, \boldsymbol{G})$, $G_L = \boldsymbol{L}G\boldsymbol{L}^{-1}$. This tensorial measure of the dislocation effect can be represented in the Riemannian material space $(\mathscr{B}, \boldsymbol{G})$ by the *dislocation density tensor* $\boldsymbol{\alpha}$ defined by [6]:

$$\boldsymbol{\alpha} = \alpha^{ab}\boldsymbol{E}_a \otimes \boldsymbol{E}_b$$

$$\alpha^a = *\tau^a = \alpha^{ba}E_b, \quad E_a = G_{ab}E^b \tag{3.4}$$

where $*$ denotes the Hodge operator for $(\mathscr{B}, \boldsymbol{G})$ [13], and

$$\alpha^{ab} = \tfrac{1}{2}e^{acd}\tau^b{}_{cd}, \quad e^{bcd} = G_0^{-\frac{1}{2}}\varepsilon^{bcd}$$

$$G_0 = \det(G_{ab}), \quad [\alpha^{ab}] = [\ell^{-1}] \tag{3.5}$$

where ε^{bcd} denotes the permutation symbol. Conversely, the tensor field $\boldsymbol{\tau}_\Phi$ can be expressed in terms of the dislocation density tensor:

$$\tau^a{}_{bc} = e_{bcd}\gamma^{da} - t_{[b}\delta^a_{c]}, \quad \gamma^{ab} = \alpha^{(ab)},$$

$$t_a = \tau^b{}_{ba} = e_{abc}\alpha^{bc}, \quad [\gamma^{ab}] = [t_a] = [\ell^{-1}] \tag{3.6}$$

where $e_{abc} = G_0^{\frac{1}{2}}\varepsilon_{abc}$, $\varepsilon_{abc} = \varepsilon^{abc}$.

The long-range distortion can be locally quantitatively measured by the so-called *local Burgers vector* $\boldsymbol{\beta} = \beta^a\boldsymbol{E}_a$ defined by [6]:

$$\varrho\boldsymbol{\beta} = \ell < \boldsymbol{\alpha}, \quad \text{i.e.} \quad \varrho\beta^a = \ell_b\alpha^{ba}$$

$$\ell = \ell^a\boldsymbol{E}_a, \quad \ell_a = G_{ab}\ell^b, \quad \ell_a\ell^a = 1$$

$$[\varrho] = [\ell^{-2}], \quad [\beta^a] = [\ell], \quad [\ell_a] = [1] \tag{3.7}$$

where ℓ denotes the unit vector field tangent to a dislocation line, and $\varrho > 0$ is the so-called (volume) *scalar density of dislocations* independent of the choice of ℓ and defined as the length of all dislocation lines included in the volume unit. Note, that ϱ can be replaced for the so-called *surface scalar density* of dislocations defined as the number of dislocations cutting the surface unit normal to their lines. If all the dislocation lines are parallel, the two densities are the same, but for a completely random arrangement of dislocations, the volume density is twice the surface density [8]. The volume density is more useful in the considered volume diffusion theory. A slip plane of a dislocation is defined as a plane containing both the dislocation line and Burgers vector of the dislocation [8]. So, a plane $\pi(\ell, \boldsymbol{\beta})$ containing vectors ℓ and $\boldsymbol{\beta}$ can be interpreted as a *local slip plane* [6].

A line can be interpreted as an *edge dislocation* line if [6]

$$\beta^a \ell_a = 0, \quad \boldsymbol{\beta} \neq \boldsymbol{o}. \tag{3.8}$$

For example, the Burgers field of the form

$$\tau^a = E^a \wedge S, \quad S = \tfrac{1}{2} t \tag{3.9}$$

where $t = t_a E^a$, describes a distribution of edge (and only edge) dislocations. Namely, in this case:

$$\begin{aligned} &\tau^a{}_{bc} = -t_{[b}\delta^a_{c]} \\ &\alpha^{ab} = \tfrac{1}{2} t_c e^{cab} = -\alpha^{ba}, \quad \gamma^{ab} = 0. \end{aligned} \tag{3.10}$$

The local Burgers vector is given then by

$$\varrho \beta^a = \tfrac{1}{2} t_c \ell_b e^{cba}, \quad \ell_a \ell^a = 1 \tag{3.11}$$

and it follows form (3.11) that

$$\beta^a \ell_a = 0, \quad \beta^a t_a = 0. \tag{3.12}$$

Moreover, the magnitude β_G of the local Burgers vector $\boldsymbol{\beta}$ defined by (3.11) is given by

$$\begin{aligned} &\varrho \beta_G = \tfrac{1}{2} [\mu^2 - (t^a \ell_a)^2]^{\frac{1}{2}} \\ &\beta_G^2 = \beta^a \beta_a, \quad \mu^2 = t^a t_a. \end{aligned} \tag{3.13}$$

Thus, independently of the choice of a dislocation line fulfulling the condition

$$t^a \ell_a = 0, \quad \ell_a \ell^a = 1 \tag{3.14}$$

the following relation is valid:

$$\varrho \beta_G = \kappa, \quad \kappa = \tfrac{1}{2} \mu \tag{3.15}$$

where the scalar β_G is independent of ℓ. It is a Riemannian generalization of the known relation describing the influence of dislocations on the mean normal curvature κ of a crystalline network [14]. A *screw dislocation* line is defined by the condition [6]

$$\beta^a = \eta \ell^a \tag{3.16}$$

where η is a scalar. Note, that if there exists a field $\boldsymbol{Q} = (Q^a{}_b) : \mathscr{B} \longrightarrow SO(3)$ of local rotations such that

$$\begin{aligned} &\Phi \boldsymbol{Q} = (\boldsymbol{e}_a), \quad \boldsymbol{e}_a = \boldsymbol{E}_b Q^b{}_a \\ &\Phi^* \boldsymbol{Q} = (e^a), \quad e^a = Q_b{}^a E^b \end{aligned} \tag{3.17}$$

where $(Q_a{}^b) = \boldsymbol{Q}^T$, and

$$\begin{aligned} \boldsymbol{\gamma} &= \gamma^{ab} \boldsymbol{E}_a \otimes \boldsymbol{E}_b = \gamma^a \boldsymbol{e}_a \otimes \boldsymbol{e}_a \\ t &= t_a E^a = \mu e^3, \quad [\mu] = [\gamma^a] = [\ell^{-1}] \end{aligned} \tag{3.18}$$

then in the base $(\boldsymbol{e}_a)$:

$$(\alpha^{ab}) \overset{*}{=} \begin{pmatrix} \gamma^1 & \kappa & 0 \\ -\kappa & \gamma^2 & 0 \\ 0 & 0 & \gamma^3 \end{pmatrix}, \quad \kappa = \frac{\mu}{2} \tag{3.19}$$

where diagonal elements correspond to screw dislocation lines (with their unit tangent vector fields $\ell = \boldsymbol{e}_a$, $a = 1, 2, 3$), whereas non-diagonal elements correspond to edge dislocation lines [6]. For example, in the case (3.10) we have

$$t_a = \mu \delta^3_a, \quad \gamma^a = 0. \tag{3.20}$$

A distribution of dislocations is called *uniformly dense* iff $\tau^a{}_{bc} = \text{const.}$ in (3.1) (and so $\alpha^{ab} = \text{const.}$ in (3.5)). It can be shown that then the following conditions are fulfilled [6]:

$$\begin{aligned} \boldsymbol{\gamma t} &= 0, \qquad \text{i.e. } \gamma^{ab} t_b = 0 \\ \boldsymbol{t} &= t^a \boldsymbol{E}_a, \quad t^a = G^{ab} t_b \end{aligned} \tag{3.21}$$

and

$$dt = 0 \tag{3.22}$$

that is, at least locally, should be

$$t = d\varphi \tag{3.23}$$

where φ is a scalar. In this case, up to a global rescaling (2.3), the dislocation density tensor is represented by the constant matrix (3.19) and the covector field t has the following representation:

$$t = \mu E^3, \quad dE^3 = 0, \quad \gamma^3 \mu = 0. \tag{3.24}$$

It follows from (3.12) and (3.23) that, in the case of an uniformly dense distribution of edge dislocations defined by (3.9), the local slip planes $\pi(\ell, \boldsymbol{\beta})$ for dislocation lines satisfying the condition (3.14) are tangent to the surfaces $\varphi = \text{const.}$, and thus these surfaces can be considered as geometrically distinguished *slip surfaces* [6].

4. Drift Velocity

Let us consider, in order to formulate a relation between the drift velocity $\boldsymbol{b}$ (the equation (2.15)) and the dislocation density tensor $\boldsymbol{\alpha}$ (the equation (3.4)), connection 1-forms $\omega^a{}_b$ of the Riemann-Cartan covariant derivative $\nabla = (\Gamma^A_{BC})$ (Section 2) defined by

$$\begin{aligned} \nabla \boldsymbol{E}_a &= \omega^b{}_a \otimes \boldsymbol{E}_b, \quad \omega_{ab} = -\omega_{ba} \\ \omega_{ab} &= G_{ac} \omega^c{}_b, \quad \omega^a{}_b = \omega_c{}^a{}_b E^c. \end{aligned} \tag{4.1}$$

It follows from (1.7), (2.14) and (4.1) that

$$\omega^b{}_a = \overset{b}{e}_B \, d\underset{a}{e}^B + \Gamma^b{}_a$$

$$\Gamma^b{}_a = \underset{a}{e}^A \, \overset{b}{e}_B \, \Gamma^B{}_A, \quad \Gamma^B{}_A = \Gamma^B_{CA} \, dX^C. \tag{4.2}$$

These connection 1-forms define both the curvature 2-forms $\Omega^a{}_b$:

$$\Omega^a{}_b = d\omega^a{}_b + \omega^a{}_c \wedge \omega^c{}_b = \tfrac{1}{2} R_{bcd}{}^a E^c \wedge E^d \tag{4.3}$$

and the torsion 2-forms Σ^a (cf. (2.13)):

$$\Sigma^a = \nabla E^a = \tau^a + \omega^a{}_b \wedge E^b = \tfrac{1}{2} T^a{}_{bc} E^b \wedge E^c$$

$$T^a{}_{bc} = 2 \overset{a}{e}_A \, \underset{b}{e}^B \, \underset{c}{e}^C \, S^A{}_{BC} \tag{4.4}$$

of the Riemann-Cartan covariant derivative. Particularly, since for the Levi-Civita covariant derivative $\nabla^G = (\Gamma^A_{BC}[\boldsymbol{G}]) = (\omega^a{}_b[\boldsymbol{G}])$, $\omega^a{}_b[\boldsymbol{G}] = \omega_c{}^a{}_b[\boldsymbol{G}] E^c$, defined by (2.4), should be $\Sigma^a = 0$, $a = 1, 2, 3$, (3.1) and (4.4) lead to the following condition:

$$\tau^a{}_{bc} = \omega_c{}^a{}_b[\boldsymbol{G}] - \omega_b{}^a{}_c[\boldsymbol{G}]. \tag{4.5}$$

The conditions

$$\omega^a{}_b \overset{*}{=} 0, \quad \Omega^a{}_b = 0 \tag{4.6}$$

define the so-called teleparallel covariant derivative $\nabla = \nabla^\Phi$ for which

$$\Sigma^a = \tau^a, \quad \text{i.e.} \quad T^a{}_{bc} = \tau^a{}_{bc} \tag{4.7}$$

what means that the torsion tensor of ∇^Φ covers with the tensor field $\boldsymbol{\tau}_\Phi$ defined by (3.3). Note, that the condition

$$\nabla^\Phi \boldsymbol{\tau}_\Phi = 0 \tag{4.8}$$

defines uniformly dense distributions of dislocations (Section 3). It follows from (3.1), (4.1) and (4.4) that for the general Riemann-Cartan covariant derivative

$$T^a{}_{bc} = \tau^a{}_{bc} + \omega_b{}^a{}_c - \omega_c{}^a{}_b \tag{4.9}$$

and from (2.15), (3.6), (4.1) and (4.9) we obtain:

$$b_a = \underset{a}{e}^A b_A = D T_a, \quad b_A = G_{AB} b^B$$

$$T_a = T^b{}_{ba} = t_a + \omega_a, \quad \omega_a = \omega_b{}^b{}_a. \tag{4.10}$$

Moreover, (1.7), (2.14), (2.15), (4.2) and (4.10) lead to the following identity:

$$\operatorname{div}_G \boldsymbol{E}_a = -t_a, \quad \text{i.e.} \quad \partial_A \underset{a}{e}^A = -(t_a + \Gamma_a) \tag{4.11}$$

where the divergence operator div_G is given by (2.19), and it was denoted:

$$\Gamma_a = \underset{a}{e}^A \Gamma_A, \quad G = \det(G_{AB})$$

$$\Gamma_A = \Gamma^B_{AB} = \Gamma^B_{AB}[G] = \partial_A \ln G^{\frac{1}{2}}. \tag{4.12}$$

The geometric object Γ_A can be recognized as the one responsible for dislocation lines termination within the crystal caused by its plastic volumetric distortion (appearing e.g. due to the existence of point defects created by intersections of many dislocation lines) [6]. This plastic distortion is represented by the Riemannian volume element (2.8). Since

$$\nabla_D e_{ABC} = 0, \quad e_{ABC} = G^{\frac{1}{2}} \varepsilon_{ABC} \tag{4.13}$$

where ε_{ABC} denotes the permutation symbol, this volume element can be parallely transported by means of the Riemann-Cartan covariant derivative.

It follows from (3.6) and (4.10) that in the case (4.7):

$$b_a = D t_a, \quad t_a = e_{abc} \alpha^{bc}. \tag{4.14}$$

It is e.g. the case of the teleparallel covariant derivative ∇^Φ defined by (4.6). Note, that for a distribution of edge dislocations defined by (3.9) and (3.10), the conditions (2.10) and (4.7) define the so-called semi-symmetric metric covariant derivative [15] with connection 1-forms $\omega^a{}_b$ of the form (see designations (4.1)):

$$\omega_c{}^a{}_b = \omega_c{}^a{}_b[G] + \tfrac{1}{2}(\delta^a_c t_b - G_{cb} t^a). \tag{4.15}$$

If

$$t = 0 \tag{4.16}$$

then screw dislocation lines are admitted and

$$b_a = D \omega_a \tag{4.17}$$

i.e. there exists then no direct relation between the drift velocity and the dislocation density tensor.

Let us consider the Ricci tensor R_{AB} defined by (see (4.3)):

$$R_{AB} = \overset{a}{e}_A \overset{b}{e}_B R_{ab}, \quad R_{ab} = R_{cab}{}^c. \tag{4.18}$$

It follows from (2.13)–(2.15), (4.4), (4.10), (4.13), (4.18), and from the so-called second identity for the curvature tensor [15] that

$$\begin{aligned} W_{AB} &= R_{[AB]} = \nabla_C S^C{}_{AB} - \nabla_{[A} T_{B]} - T_C S^C{}_{AB} \\ &= \nabla_C S^C{}_{AB} - \partial_{[A} T_{B]}, \\ T_A &= 2 S_A = \overset{a}{e}_A T_a. \end{aligned} \tag{4.19}$$

Particularly, in the case (4.7) we obtain:

$$\begin{aligned} W_{AB} &= w_{AB} - t_{AB}, \quad t_{AB} = \tfrac{1}{2} \partial_{[A} t_{B]} \\ w_{AB} &= \tfrac{1}{2} e_{ABC} w^C, \quad w^C = \nabla_D \gamma^{CD} - \gamma^{CD} t_D. \end{aligned} \tag{4.20}$$

If $W_{AB}=0$ then (4.20) reduces to the following condition:

$$dS = * w, \quad S = \tfrac{1}{2} t, \quad w = w_A \, dX^A$$
$$* w = w_{AB} \, dX^A \wedge dX^B, \quad w_A = G_{AB} w^B \tag{4.21}$$

where $*$ denotes the Hodge operator on $(\mathscr{B}, \boldsymbol{G})$. It is, for example, the case of vanishing curvature tensor (i.e. $\nabla = \nabla^{\Phi}$ – (4.6)), or the case of a Riemann-Cartan covariant derivative fulfilling the condition (4.7) and possessing a sectional isotropic curvature $k(X) \neq 0$, that is with the curvature tensor of the form:

$$R_{abc}{}^{d}(X) = k(X) \, (\delta_b^d G_{ac} - \delta_a^d G_{bc}). \tag{4.22}$$

If $\nabla = \nabla^{\Phi}$ and the distribution of dislocations is uniformly dense (equations (3.6), (3.21), (3.22) and (4.8)), then the condition (4.21) is an identity. We see, that the distribution of dislocations is constrained by the curvature effect of the Riemann-Cartan space. This curvature effect depends on the long-range distortion of the continuized dislocated crystal and characterizes distributions of dislocations admitting the Markov-type diffusion processes of point defects (Section 2). On the other hand, the Riemann-Cartan covariant derivative may be considered as a geometric object representing the simultaneous existence of dislocations and such additional distortion of the continuized crystal that has no influence on its local diffusion properties (the condition (2.11)) but contributes to the drift velocity $\boldsymbol{b}$ (cf. [5] and the present work – Section 1, (2.1)–(2.3), (2.10) and (2.15)). Field equations of the static gauge theory of continuous distributions of dislocations [5], describing dislocations and distortions of this type by means of a Riemann-Cartan covariant derivative, can be thus considered as those defining distributions of dislocations in a way consistent with the above constraints.

Let us assume that the line element $l(X)$ of the internal length measurement (Section 1):

$$l(X) = [G_{AB}(X) \, dX^A \, dX^B]^{\frac{1}{2}} \tag{4.23}$$

is undergone a distortion, say (for the simplicity) independent of the choice of this element:

$$\frac{\delta l(X)}{l(X)} = \varepsilon(X) \tag{4.24}$$

where $\delta = dX^A \nabla_A$ denotes the variation defined by a covariant derivative ∇, and $\varepsilon = \varepsilon_A \, dX^A$ is a 1-form. The condition (4.24) is equivalent to [9]:

$$\nabla \boldsymbol{G} = \pi \otimes \boldsymbol{G}, \quad \pi = 2\varepsilon \tag{4.25}$$

what means that ∇ is the so-called Cartan-Weyl covariant derivative. It is well-known that the condition (4.25) is invariant under the following gauge transformation:

$$\boldsymbol{G} \rightarrow \hat{\boldsymbol{G}} = f \boldsymbol{G}$$
$$\pi \rightarrow \hat{\pi} = \pi + d \ln f \tag{4.26}$$

where $f > 0$ is a dimensionless scalar, leading to

$$\nabla \hat{\boldsymbol{G}} = \hat{\pi} \otimes \hat{\boldsymbol{G}}. \tag{4.27}$$

The 1-form $\hat{\pi}$ vanishes iff

$$\pi = -d \ln f. \tag{4.28}$$

The Cartan-Weyl geometry can be reduced then to a Riemann-Cartan geometry defined by (2.10) with $\boldsymbol{G}$ replaced by $\hat{\boldsymbol{G}}$. If the gauge transformation (4.26) is generated by a transformation $\Phi^* \to \hat{\Phi}^* = (\hat{E}^a)$ defined by

$$E^a \to \hat{E}^a = f^{\frac{1}{2}} E^a \tag{4.29}$$

then Burgers field $\tau_\Phi = (\tau^a)$ (see (3.1)) transforms according to:

$$\tau^a \to \hat{\tau}^a = d\hat{E}^a = f^{\frac{1}{2}}(\tau^a - E^a \wedge d\ln f^{\frac{1}{2}}). \tag{4.30}$$

The transformed Burgers field $\hat{\tau}_\Phi = (\hat{\tau}^a)$ vanishes iff 2-forms τ^a, $a = 1, 2, 3$, have the form (3.9) and the 1-form t is given by (3.23) with $\varphi = \ln f$. The Burgers field τ_Φ of the form (3.9) transforms under the gauge transformation (4.29) according to:

$$\begin{aligned} &\tau^a \to \hat{\tau}^a = \hat{E}^a \wedge \hat{S} \\ &t \to \hat{t} = 2\hat{S} = t - d\ln f. \end{aligned} \tag{4.31}$$

A conformal change $\boldsymbol{G} \to \hat{\boldsymbol{G}}$ can be interpreted as a transformation estimating the influence of vacancies and (self-) interstitials on the internal length measurement [16]. In this case equations (4.26), (4.28) and (4.31) mean that a distribution of edge dislocations defined by (3.9) and (3.23) can be annihilated by a certain distribution of point defects. The diffusion process takes then the form of a Brownian motion on the Riemannian manifold $(\mathscr{B}, \hat{\boldsymbol{G}})$ (see Section 2). The influence of a temperature field $T = T(X)$ on the internal length measurement in a thermally isotropic continuized crystal gives another example of the gauge transformation. Namely, in this case we can assume that the infinitesimal strain ε in the condition (4.24) has the form:

$$\varepsilon = \nu(T)\, dT \tag{4.32}$$

where $\nu(T)$ is the coefficient of infinitesimal thermal expansion. Equations (4.26), (4.27) and (4.29)–(4.31) with

$$f = \exp\left(-2 \int_{T_0}^{T} \nu(s)\, ds\right) \tag{4.33}$$

define then a gauge transformation describing the influence of a temperature field on the diffusion process in an isotropic continuized dislocated crystal.

5. Influence of Edge Dislocations

We will deal with distributions of edge dislocations defined by (3.9). Their influence on the free diffusion process is described by a semi-symmetric metric connection $\nabla = (\omega_c{}^a{}_b)$ defined by (4.15) for which the conditions (4.7) (with $\tau^a{}_{bc}$ given by (3.10)) and (4.14) are satisfied. It follows from (4.20) that such distributions of dislocations are constrained by the following condition:

$$\begin{aligned} &dS = -W \\ &W = W_{AB}\, dX^A \wedge dX^B, \quad W_{AB} = R_{[AB]} \end{aligned} \tag{5.1}$$

where R_{AB} denotes the Ricci tensor of ∇. Thus, the Ricci tensor of the semi-symmetric metric connection is symmetric iff the 1-form t is closed (the condition (3.22)). For example, it can be shown [17] that if the semi-symmetric metric connection has a sectional isotropic curvature $k(X) \neq 0$ (i.e. its curvature tensor has the form (4.22)) then in the equation (3.23) should be

$$\begin{aligned} &\varphi = \ln |k_0/k| \\ &[k] = [k_0] = [\ell^{-2}], \quad k_0 = \text{const.} > 0. \end{aligned} \tag{5.2}$$

A steady state of the considered diffusion process is defined by the following equation (see (1.1), (2.6), (2.18) and (2.19)):

$$\begin{aligned} &D \Delta_G p - \operatorname{div}_G(p \boldsymbol{b}) = 0 \\ &N(t) = N_0 = \text{const.} \end{aligned} \tag{5.3}$$

which is fulfilled if e.g.

$$b = b_A dX^A = D\, d\varphi, \quad b_A = G_{AB} b^B \tag{5.4}$$

and

$$p = p_0 e^{\varphi}, \quad \int p\, dV = 1, \quad p_0 = \text{const.} \tag{5.5}$$

Particularly, in the case (5.2) the stationary probability density has the form

$$\begin{aligned} &p = \frac{k_0}{V_0} |k|^{-1} \\ &V_0 = \int |k_0/k|\, dV, \quad [V_0] = [\ell^3] \end{aligned} \tag{5.6}$$

where dV denotes the Riemannian volume element.

The Riemannian manifold $(\mathscr{B}, \boldsymbol{G})$ admits the existence of a semi-symmetric metric covariant derivative with the vanishing curvature tensor iff $(\mathscr{B}, \boldsymbol{G})$ is conformally flat [17], that is iff there exists (at least locally) a Cartesian coordinate system $X = (X^A)$ on $\mathscr{B}(= E^3)$ such that

$$G_{AB}(X) \overset{*}{=} \lambda^{-1}(X)\, \delta_{AB} \tag{5.7}$$

where λ is a positive dimensionless scalar. Therefore, in this case the diffusive properties of the continuized crystal are isotropic (cf. (2.2)):

$$D^{AB}(X) \overset{*}{=} \lambda(X)\, \delta^{AB}. \tag{5.8}$$

It follows from (5.1) that then the covector field t has (at least locally) the form (3.23), and so there exists a stationary probability density of the form (5.5). For example, if the considered distribution of edge dislocations is uniformly dense (Section 3), then the Riemannian space $(\mathscr{B}, \boldsymbol{G})$ has a constant scalar curvature K, $[K] = [\ell^{-2}]$ [6]. Thereby, it is a conformally flat Riemannian space [18] and the corresponding semi-symmetric metric connection (4.15) has the vanishing curvature tensor. Moreover, in this case the potential φ in the condition (3.23) fulfills the following equation [6]:

$$\Delta_G \varphi = 4K \tag{5.9}$$

where the Laplace-Beltrami operator Δ_G is defined by (2.6), equivalent, in a Cartesian coordinate system $X=(X^A)$ on E^3, to

$$\Delta\varphi-\tfrac{1}{2}d\ln\lambda\cdot d\varphi-\tfrac{4K}{\lambda}=0 \tag{5.10}$$

where $\Delta=\delta^{AB}\partial_A\partial_B$ is the (Euclidean) Laplacian, and it was denoted $v\cdot w=\delta^{AB}v_A w_B$. Note, that (up to a global rescaling (2.3) of Φ) we can assume that the considered uniformly dense distribution of edge dislocations is defined by a moving frame $\Phi=(\boldsymbol{E}_a)$ satisfying the following commutation rules (see (3.1), (3.10), (3.20) and (3.24)) [6]:

$$\begin{aligned}&[\boldsymbol{E}_1,\boldsymbol{E}_2]=\boldsymbol{O},\quad [\boldsymbol{E}_3,\boldsymbol{E}_2]=2\kappa\boldsymbol{E}_2,\quad [\boldsymbol{E}_3,\boldsymbol{E}_1]=2\kappa\boldsymbol{E}_1\\ &dE^3=0,\quad \kappa=\tfrac{1}{2}\mu=\text{const.}>0.\end{aligned} \tag{5.11}$$

For example, a covector base fields $\Phi^*=(E^a)$ of the form

$$E^1=ae^{-\kappa u^3}du^1,\quad E^2=ae^{-\kappa u^3}du^2,\quad E^3=du^3 \tag{5.12}$$

where $u=(u^A)$ is a coordinate system on $(\mathscr{B},\boldsymbol{G})$, satisfy the conditions (5.11) and define an internal length measurement metric tensor $\boldsymbol{g}$ of the form (cf. (1.6)):

$$\boldsymbol{g}(u)\stackrel{*}{=}a^2e^{-2\kappa u^3}(du^1\otimes du^1+du^2\otimes du^2)+du^3\otimes du^3 \tag{5.13}$$

which is a well-known form of the metric tensor of a Riemannian space of negative constant (scalar) curvature K given by [19]

$$K=-\kappa^2,\quad [\kappa]=[\ell^{-1}] \tag{5.14}$$

and (5.14) is a property of $\boldsymbol{g}$ invariant under the global rescaling (2.3) of Φ. It is known that for a Riemannian space of negative constant curvature there exists locally a coordinate system $X=(X^A)$ such that [20]

$$\begin{aligned}&\boldsymbol{g}(X)\stackrel{*}{=}a(r(X))^2\delta_{AB}dX^A\otimes dX^B\\ &a(r)=(1+\tfrac{K}{4}r^2)^{-1},\quad r^2=\delta_{AB}X^AX^B,\quad 0\leqq r<2/\kappa\end{aligned} \tag{5.15}$$

and (5.7) takes then the form:

$$\begin{aligned}&\boldsymbol{G}(X)\stackrel{*}{=}\lambda(r(X))^{-1}\delta_{AB}dX^A\otimes dX^B\\ &\lambda(r)=\lambda_0\,a(r)^{-2},\quad \lambda_0>0,\quad [\lambda_0]=[1].\end{aligned} \tag{5.16}$$

A *slip direction* is necessarily always parallel to the Burgers vector of the dislocation responsible for slip [8]. It suggests that if the local Burgers vector $\boldsymbol{\beta}$ is a local generalized translation defined by [6]

$$L_\beta\boldsymbol{E}_a=0,\quad a=1,2,3 \tag{5.17}$$

where L denotes the Lie derivative operator, then $\boldsymbol{\beta}$ can be considered as the example of a *local slip* in the continuized dislocated crystal. It can be shown [6] that if the considered distribution of edge dislocations is uniformly dense and the local Burgers vector $\boldsymbol{\beta}$ corresponds to a Φ – parallel dislocation line (i.e. $\boldsymbol{l}=l^a\boldsymbol{E}_a$, $l^a=\text{const.}$, and $t_a=\text{const.}$ in (3.11)), then the condition (5.17) reduces to

$$\varphi=2\ln(\varrho/\varrho_0) \tag{5.18}$$

where ϱ is the scalar density of edge dislocations (Section 3), and ϱ_0, $[\varrho_0]=[\ell^{-2}]$, is a positive constant. The system of equations (5.8), (5.10), (5.14) and (5.18) defines then a way the diffusion coefficients would depend on the scalar density of edge dislocations. In this case the probability density $p(X)$ defined by (5.5) can be written in the form:

$$\begin{aligned} &p=L_0\varrho^2, \quad \varrho=\varrho_0\exp(\varphi/2) \\ &L_0^{-1}=\varrho_0^2/p_0=\int\varrho^2\,dV, \quad [L_0]=[\ell] \end{aligned} \tag{5.19}$$

where the scalar φ satisfies (5.10) with K given by (5.14).

The conditions (3.9) and (5.17) lead to a generalization of the dislocation fluid model (with the fluid consisting of infinitesimal dislocation loops) that has been proposed in [9] as an approximation describing the influence of mobile dislocations on the crystal lattice plastic distortion. Namely, let us consider the static distribution of edge dislocations as the one defining a steady state of mobile dislocations corresponding to their (steady) mean velocity $\boldsymbol{v}_d=\boldsymbol{v}_d(X)$. Then, the line element (4.23) of the internal length measurement is undergone to an infinitesimal plastic strain ε (see (4.24)) due to the dislocation motion. On the other hand, the increment Δe in the time internal Δt of a plastic strain e caused by mobile dislocations with ϱ, $\boldsymbol{\beta}$ and $\boldsymbol{v}_d$ being their scalar density, mean Burgers vector and mean velocity, respectively, is given by a kinematic relation of the form [21]:

$$\begin{aligned} &\Delta e=\varepsilon(\boldsymbol{v}_d)\Delta t, \quad \varepsilon(\boldsymbol{v}_d)=\varrho\boldsymbol{\beta}\cdot\boldsymbol{v}_d \\ &[\Delta e]=[1], \quad [\varrho]=[\ell^{-2}], \quad [\boldsymbol{\beta}\cdot\boldsymbol{v}_d]=[\ell^2 t^{-1}] \end{aligned} \tag{5.20}$$

where $\boldsymbol{a}\cdot\boldsymbol{b}$ denotes the scalar product of vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ (originally it is an Euclidean scalar product – [21]). We can generalize this kinematic formula assuming that in (4.24):

$$\begin{aligned} &\varepsilon=\varrho\beta, \quad d\varepsilon\neq 0 \\ &\beta=\boldsymbol{G}\boldsymbol{\beta}=\beta_a E^a, \quad \beta_a=G_{ab}\beta^b, \quad [\beta]=[\ell^2] \end{aligned} \tag{5.21}$$

where $\boldsymbol{\beta}=\beta^a\boldsymbol{E}_a$, $[\boldsymbol{\beta}]=[1]$, is a local Burgers vector of the form (3.11). The condition (5.17) may be interpreted then as a definition of a class of mobile edge dislocations moving with their mean velocity parallel to the local Burgers vector $\boldsymbol{\beta}$, that is such that if $\boldsymbol{v}_d\neq\boldsymbol{o}$, then

$$\boldsymbol{\beta}=t_d\boldsymbol{v}_d, \quad [t_d]=[t], \quad [\boldsymbol{v}_d]=[t^{-1}] \tag{5.22}$$

where t_d is a positive scalar, and thus

$$\varepsilon=t_d\varrho v_d, \quad v_d=\boldsymbol{G}\boldsymbol{v}_d, \quad [v_d]=[\ell^2 t^{-1}]. \tag{5.23}$$

If the condition (3.14) is additionally fulfilled, then planes tangent to slip surfaces $\varphi=$ const. (Section 3) become the so-called (local) *glide planes*, that is such (local) slip planes in which (local) translational motions of dislocations (called their glide motions) occur. The surfaces $\varphi=$ const. are called then *glide surfaces*. For example, in the case of an edge dislocation loop defined by (3.11) and (3.14) with $\boldsymbol{l}$ being the unit vector field tangent to a closed circuit (a loop), the dislocation can only move along the cylindrical surface generatrix parallel to the local Burgers vector of the loop. If $t_d=$ const. is a characteristic time of the dislocation motion, then (3.9), (3.23), (4.25), (5.18) and (5.23) are governing equations of the above mentioned dislocation fluid model. Putting $\varepsilon=0$ in (4.25) and (5.23), and adding (5.4), (5.8), (5.10), (5.14) and (5.19) to these governing equations, we obtain a static counterpart of the dislocation fluid model describing the influence of edge dislocations on the free diffusion process. Note, that e.g. the irradiation of a crystal with fast neutrons produces very small circular edge dislocation loops [7]. The loops can be treated then (in the continuized crystal approximation – Section 1) as the infinitesimal ones, and the dislocation fluid can be interpreted as consisting of infinitesimal edge dislocation loops [9].

6. Geometry and Interactions

The proposed theory describes the influence of the breakage of crystalline solids material symmetries on the free diffusion phenomenon. The classical approach (e.g. [1, 2]) is based on the consideration of interactions between single dislocations and a diffusing atom. Let us consider, in order to see whether the proposed geometric theory can be formulated in terms of such interactions, the case of isotropic diffusive properties of a continuized dislocated crystal. In this case there exists (at least locally) such Cartesian geometric frame reference $X=(X^A)$ on E^3 (see Section 1) that the equation (5.8) (and thus (5.7)) is valid. Introducing an energy H of the form:

$$H=\Theta h$$
$$h=\ln(\lambda_0/\lambda), \quad \text{i.e. } \lambda=\lambda_0 e^{-h} \tag{6.1}$$

where Θ, $[\Theta]=[m\ell^2 t^{-2}]$, $[m]=g$ in the cgs units system, is a characteristic energy of the considered diffusion process, and λ_0 is a dimensionless positive constant, we can write (5.8) in the form:

$$D^{AB}(X)=D(X)\,\delta^{AB} \tag{6.2}$$

where the diffusion coefficient $D(X)$ is given by the following Arrhenius-type law:

$$D(X)=D_0\exp(-H(X)/\Theta)$$
$$D_0=\lambda_0 D=\text{const.}, \quad [D_0]=[\ell^2 t^{-1}]. \tag{6.3}$$

Thus, the energy $H(X)$ can be treated as a *local activation energy* (possibly of effective energy character) of the considered locally free diffusion process (Section 2). Assuming e.g. that $\Theta=k_B T$, where k_B is the Boltzman constant and T is the temperature of the thermostat, we can consider a nonequilibrium diffusion process (cf. Section 1) as the one thermally activated in the temperature T of the environment of the body (cf. [22]). It follows from (4.12), (5.7) and (6.1) that

$$\Gamma_A \stackrel{*}{=} \tfrac{3}{2}\partial_A h \tag{6.4}$$

what means that the activation energy variableness and the existence of a plastic volumetric distortion (Section 4) of the continuized dislocated isotropic crystalline solid are mutually related phenomena.

Assuming that the condition (5.4) is satisfied and rewriting (5.5) in the form

$$p(X)=p_0\exp(-U(X)/\Theta), \quad U=-\Theta\varphi \tag{6.5}$$

we can recognize $U(X)$ as an *own energy* of the microstate X of a diffusing particle (defined as its place X). From (2.4), (2.9), (2.17), (5.4), (5.7), (5.8), (6.1) and (6.5) we obtain that

$$c_A=G_{AB}c^B=(D/2)\,\partial_A h$$
$$B_A=G_{AB}B^B=b_A+c_A=-(D/\Theta)\,\partial_A E \tag{6.6}$$

where it was denoted:

$$E = U - \tfrac{1}{2}H. \tag{6.7}$$

If a drift of diffusing point defects is small compared with their chaotic motion, then the mean velocity $\boldsymbol{B}$ (see Section 2) and the force $\boldsymbol{F}$ acting on a diffusing point defects are related by the so-called Stokes relation [1]:

$$F^A = \zeta B^A$$
$$[F^A] = [m\ell t^{-2}], \quad [\zeta] = [mt^{-1}] \tag{6.8}$$

where ζ is a friction coefficient assumed, for the simplicity of the discussion, to be a positive constant. From (6.6)–(6.8) we obtain that

$$F_A = -\partial_A E \tag{6.9}$$

iff

$$\Theta = \zeta D. \tag{6.10}$$

Therefore, the potential energy E has a physical meaning of the *interaction energy* between dislocations and a diffusing atom.

The isotropy condition is realized, for example, in the case of an uniformly dense distribution of edge dislocations defined by (3.9) (Section 5). It follows from (5.9) and (6.5) that, in this case, the own energy U should satisfy the equation:

$$\Delta_G U = -4K\Theta \tag{6.11}$$

or, rewriting (5.10) in terms of a Cartesian coordinate system $X = (X^A)$ on E^3 and energies U and H, the equation:

$$\Delta U + \tfrac{1}{2} dU \cdot dh - \frac{4\zeta_0}{t_D} e^h = 0 \tag{6.12}$$

where it was denoted (assuming that $K \neq 0$):

$$t_D = \frac{1}{|K|D}, \quad \zeta_0 = \frac{\zeta}{\lambda_0}$$
$$[t_D] = [t], \quad [\zeta_0/t_D] = [mt^{-2}] \tag{6.13}$$

and equations (5.14), (6.1), (6.5) and (6.10) was taken into account. Since for $K \neq 0$ the diffusion coefficient D_0 (see (6.3)) can be rewritten in the form:

$$D_0 = \lambda_0 \frac{l_d^2}{t_D}, \quad l_d = \kappa^{-1}, \quad [l_d] = [l] \tag{6.14}$$

so t_D has a physical meaning of the relaxation time needed the diffusion process to reach a steady state (possibly the nonequilibrium one) characterized by the existence of its characteristic length $L_D = (D_0 t_D)^{\frac{1}{2}} = \lambda_0^{\frac{1}{2}} l_d$ depending on the distribution of dislocations (the length parameter l_d). It follows from the commentary following (3.15) that the inverse $\kappa = l_d^{-1} = \text{const.}$ of the length parameter l_d can be interpreted as a mean normal curvature of the crystalline network of the dislocated crystal. From (5.14)–(5.16), (6.7), (6.10), (6.13) and (6.14) we obtain that, in a coordinate system in which the metric tensor $\boldsymbol{G}$ takes the form (5.16), the equations (6.1) and (6.12) become respectively:

$$H = 2\Theta \ln a(r) \tag{6.15}$$

and

$$\Delta E + A(r)\boldsymbol{n} \cdot \operatorname{grad} E + B(r) = 0 \tag{6.16}$$

where $\boldsymbol{a} \cdot \boldsymbol{b} = \delta_{AB} a^A b^B$, and it was denoted:

$$A(r) = \frac{|K|}{2} r a(r), \quad B(r) = \Theta A(r) \left(2A(r) + \frac{3}{r} - \frac{8}{\lambda_0} \frac{a(r)}{r}\right)$$

$$a(r) = \left(1 - \frac{|K|}{4} r^2\right)^{-1}, \quad |K| = \zeta/\Theta t_D$$

$$\boldsymbol{n} = n^A \partial_A, \quad n^A = \delta^{AB} n_B = X^A/r, \quad n_A = \partial_A r$$

$$r^2 = \delta_{AB} X^A X^B, \quad 0 \leqq r < 2\ell_d. \tag{6.17}$$

The appearance of a time parameter in the equation (6.16) defining the interaction energy E suggests that inelastic interactions contribute to this energy.

It follows from (1.1), (5.3) and (5.4) that an uniform distribution of diffusing matter (i.e. the case $n(x) = n_0 = \text{const.}$) is admitted as a steady state of the diffusion iff

$$\Delta_G U = 0. \tag{6.18}$$

Particularly, for the uniformly dense distribution of edge dislocations, it is equivalent to the vanishing of the scalar curvature K (see (6.11)). Since $K = 0$ iff $\lambda = \lambda_0 = \text{const.}$ (see (5.16)), we obtain that then $H = 0$ and $U = E$ (see (6.1) and (6.7)). It follows from (3.19), (3.20) and (5.14) that in this case the Burgers field (3.9) vanishes, and so the drift velocity $\boldsymbol{b}$ defined by (4.14) vanishes too. Therefore, $E = \text{const.}$, $D(X) = D_0$ (cf. (6.2) and (6.3)), the equation (6.16) becomes an identity, and the Fokker-Planck equation (2.18) reduces to the well-known form (cf. (1.2)):

$$\partial_t p - D_0 \Delta p = 0 \tag{6.19}$$

describing, for $D_0 = k_B T/\zeta_0$, a chaotic thermal motion of point defects in an isotropic medium (the free diffusion process – Section 1).

We conclude that the own energy U of a diffusing atom defined by (6.5) and, for an uniformly dense distribution of edge dislocations, computed from (6.7) and (6.15)–(6.17), defines a nonequilibrium steady state of diffusing matter. This own energy is caused by interactions between dislocations and a diffusing atom (the interaction energy E) and by the influence of the plastic volumetric distortion of the crystal structure (the local activation energy H). The constant energy surfaces $U = \text{const.}$ can be considered as slip surfaces (Section 3) which may appear as glide surfaces (Section 5). If the condition (5.18) is fulfilled, then the constant energy surfaces cover with surfaces of constant scalar density of dislocations. The drift velocity $\boldsymbol{b}$ defined by (5.4) and (6.5) is normal to the surfaces $U = \text{const.}$ and can be computed from (2.9), (5.8), (5.16), (6.6), (6.16) and (6.17):

$$b_A = -\left(\frac{1}{\zeta} \partial_A E + \frac{1}{t_D} \gamma(r) n_A\right)$$

$$\gamma(r) = \tfrac{1}{2} r a(r)^4, \quad 0 < r < 2\ell_d. \tag{6.20}$$

Thus, for the uniformly dense distribution of edge dislocations defined by (3.9), the equations (2.6), (2.19), (5.16), (6.16), (6.17) and (6.20) specify (in a Cartesian coordinate system) a local form of the Fokker-Planck equation (2.18). The absolute value of the scalar curvature K of the material Riemannian space $(\mathscr{B}, \boldsymbol{G})$ turns out to be a geometric measure of the distance of such defined nonequilibrium Markov-type diffusion process from the equilibrium free diffusion process defined by (6.19).

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