Locally Equilibrium Diffusion Processes. II. Generalized Stochastic Mechanics and Plastic Yielding

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The locally equilibrium diffusion process is considered in which two mean velocities of the diffusing particles appear: the mean arrival velocity to the point and the mean starting velocity from the point. It is shown that such a diffusion process can be described by generalized Nelson stochastic mechanics. Equations describing the coupling of the diffusion process with the plastic yielding process are formulated. It is shown that the increments of the plastic strains caused by the dislocation motion can be described by a Weyl gauge field.

1. INTRODUCTION

Diffusion theories usually ignore the possibility that the mean arrival velocity of the diffusing particle to a point may differ from the mean starting velocity of the particle from the point. In fact, in these theories only the mean starting velocity is taken into account (Trzęsowski, 1989). The formulation of the diffusion description on the basis of the Markovian diffusion processes theory shows that (in the case of constant diffusion coefficients) the mean starting velocity field **b** is connected with the mean arriving velocity field \mathbf{b}_{\star} in the following way (Trzęsowski, 1989):

$$\mathbf{b} = \mathbf{b}_* - 2\mathbf{u} \tag{1}$$

where \mathbf{u} is the diffusion velocity field (Section 2), vanishing only when the distribution of the diffusing matter is homogeneous. The distinction of the mean starting velocity in the classical diffusion theory is connected with basing this theory on the so-called Stokes relation:

$$\mathbf{F}_{\text{ext}} = \zeta \mathbf{b} \tag{2}$$

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where \mathbf{F}_{ext} is the force with which the external field acts on the diffusing particle and ζ is the friction coefficient describing (together with the diffusion coefficients) the interaction of the medium on the diffusing particles. Basing this on the Stokes relation means that the classical diffusion theory is adapted to the description of diffusion processes for which the stationary distributions of the diffusing matter appear only in the thermodynamic equilibrium state of a body with diffusion (Trzęsowski, 1989).

So, if we do not treat any of the mean (starting or arriving) velocities as physically distinguished, and if we want to obtain the possibility of description of the stationary nonequilibrium distributions of the diffusing matter, we have to give up the Stokes relation. Trzęsowski and Kotowski (1985) proposed, in the case of constant diffusion coefficients, to replace that relation by the so-called Nelson relation (Nelson, 1967) of the form

$$m\mathbf{a} = \mathbf{K} \tag{3}$$

where \mathbf{a} is the appropriately defined mean acceleration of the Markovian diffusion process, m is the diffusing particle mass, and \mathbf{K} is the force acting on that particle. If one additionally takes that the force \mathbf{K} is of the form

$$\mathbf{K} = \mathbf{F}_{\text{ext}} - \zeta \mathbf{b} \tag{4}$$

and takes into account that $\tau = m/\zeta$ has the sense of the so-called kinetic relaxation time in statistical physics, and that in the limit $\tau \to 0$ ($\zeta = \text{const}$), (3) and (4) reduce to (2), then the classical diffusion theory becomes the limiting case of a more general theory, valid for arbitrary relaxation times τ (Trzęsowski and Kotowski, 1985). If **b** and \mathbf{F}_{ext} are the potential functions, then the so-called stochastic quantization method (Nelson, 1967), applied in the case when the force **K** is of the form (4), allows describing the diffusion process by a nonlinear equation of Schrödinger type.

If, however, the mean starting velocity **b** is not treated as physically distinguished, then taking the force **K** of the form (4) in equation (3) cannot be taken as the basis of the diffusion theory. Also, the assumption of the constancy of the diffusion coefficients is too great a simplification if we want to consider the stationary nonequilibrium distribution of diffusing matter. In Part I (Trzęsowski, 1989) it was shown that the case of nonconstant diffusion coefficients (in a locally homogeneous body) and locally equilibrium processes can be described as diffusion in the Riemannian space $M = (R^3, G)$, defined by

$$\mathbf{D}(\mathbf{X}) = D\mathbf{G}(\mathbf{X})^{-1}$$

= $D^{AB}(X) \partial_A \otimes \partial_B$
 $D^{AB}(X) = DG^{AB}(X)$
[G] = $[l^2], \quad [\mathbf{D}] = [t^{-1}], \quad [D] = [l^2 t^{-1}]$ (5)

where D(X), $X \in R^3$, is the diffusion coefficient tensor; $X = (X^A)$ is the designation of an arbitrary coordinate system on R^3 , as well as the designation of coordinates of the standard point $X \in R^3$ in the considered coordinate system; [A] denotes the absolute dimension of tensor A; and [l] = cm, [t] = sec in the cgs unit system. The covariant Levi-Civita derivative ∇ corresponding to the metric tensor G fulfills the following localization condition for the diffusion process in the locally homogeneous body (Trzęsowski, 1989, Sections 1 and 4):

$$\nabla \mathbf{D}(\mathbf{X}) = \mathbf{0} \tag{6}$$

For Markovian diffusion processes with values in Riemannian space, the method proposed in Nelson (1967) of defining the mean acceleration **a** fails and attempts at its generalization (e.g., Dankel, 1971, Dohrn and Guerra, 1978) do not lead to satisfactory results. The Nelson relation (3) should be modified if we want to apply the stochastic quantization method to describe locally equilibrium diffusion processes. The first part of this modification has in fact been realized in Part I (Trzęsowski, 1989) and it consisted in the consideration of the arriving Markovian diffusion process in the place of the time-reversed Markovian diffusion process. Further modification can be made with the help of a method proposed in Collins (1977) of Schrödinger equation derivation (generally nonlinear) from the continuity equation for the probability density function (Section 3). This is equivalent, with the appropriate definition of the force **K**, to generalization of the Nelson relation consisting in replacing the mean acceleration by the effective acceleration of the form

$$\mathbf{a} = \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} + \nabla \varphi_D \tag{7}$$

where v is the diffusion peculiar velocity (Trzęsowski, 1989) and φ_D is the diffusion counterpart of the so-called Bohm potential, considered in the hydrodynamic formalism of quantum mechanics. If the diffusion coefficients are constant, then the acceleration (7) equals the Nelsonian mean acceleration. In this paper the equations obtained in this way are applied to the description of the coupling of the diffusion process with the plastic yielding process caused by the motion of dislocations in the body (Sections 4 and 5).

2. MATERIAL SPACE OF BODY WITH DIFFUSION

Let \mathscr{B} be the three-dimensional, simply-connected, smooth and orientable differentiable manifold and $\varkappa : \mathscr{B} \to R^3$ the smooth diffeomorphism onto a certain simply-connected open set $\mathscr{B}_{\varkappa} = \varkappa(\mathscr{B})$. In continuum mechanics such a differentiable manifold is called the body, and is considered the geometrical model of a material body ignoring the influence of the boundary layer on its material properties. The deformation of the body, as well as some kinds of defects of its material structure, can be described by giving additional geometrical structure to it (Trzęsowski, 1987). The existence of the global diffeomorphism \varkappa makes it possible to identify the body \mathscr{B} with its image \mathscr{B}_{\varkappa} at that mapping and then these additional geometrical structures can be introduced on the set \mathscr{B}_{\varkappa} .

In Part I (Trzęsowski, 1989) it was shown that if we ignore the influence of the body boundary on the locally equilibrium diffusion process in a locally homogeneous body, then this process can be described as a Markovian diffusion process with values in the Riemannian manifold M = (R^3, G) discussed in the Introduction. In this case the assumption that $\mathscr{B}_x = R^3$ is a model element for the diffusion process, whereas the metric tensor G describes "diffusive" properties of the material structure of the body. The manifold M will be called the *material space* of the (locally homogeneous) body with (unlimited) diffusion (Trzęsowski, 1989, Section 4). In Part I it was also shown that the diffusion peculiar velocity v and the diffusion velocity u are connected with the concentration $p = p(\mathbf{X}, t)$ of the diffusing matter through the equations

$$\partial_t p + \nabla_A (pv^A) = 0 \qquad \text{in } M \times I \tag{8}$$

and [considering the localization condition (6)]

$$u^{A} = -\frac{1}{p} D^{AB}(X) \nabla_{B} p$$

= $G^{AB}(X) u_{B}$ (9)
 $u_{A} = -2D \partial_{A} R, \qquad R = \ln(p/p_{0})^{1/2}$

where $I \subset R_+$ is a time interval, ∇_A is the Levi-Civita covariant derivative corresponding to the metric tensor G, p_0 is an arbitrary homogeneous concentration, and where it was taken into account that p is a scalar (Trzęsowski, 1989, Section 4).

In the case of a diffusion process concentrated in the regular domain \mathscr{B}_{\varkappa} with the boundary $\partial \mathscr{B}_{\varkappa}$, the material space of the body with diffusion is a submanifold $M | \mathscr{B}_{\varkappa} = (\mathscr{B}_{\varkappa}, \mathbf{G})$ of the manifold M, and equations (8) and (9) should be completed by the condition that the concentration p vanishes on the boundary $\in \mathscr{B}_{\varkappa}$ (Trzęsowski, 1989, Section 6). The cases when the diffusing matter can penetrate the body boundary or concentrate in its boundary layer are not considered in this paper. I will not discuss the boundary problems for the diffusion process in the set \mathscr{B}_{\varkappa} either, and because of that I will restrict the considerations to the manifold M.

3. GENERALIZED STOCHASTIC MECHANICS

Let $p: \mathscr{B}_{\kappa} \times I \to R_+$, $I \subset R_+$ a certain time interval, be a differentiable concentration function. Because this function is nonnegative, it should fulfill the following condition (Collins, 1977):

$$\exists \mathbf{X}_0 \in \mathcal{B}_{\varkappa} \quad \forall t \in I \quad p(\mathbf{X}_0, t) = 0 \Longrightarrow \forall t \in I \quad \partial_t p(\mathbf{X}_0, t) = 0$$
(10)

Condition (10) is fulfilled by, e.g., the so-called Born representation:

$$p(\mathbf{X}, t) = p_0 \psi(\mathbf{X}, t) \psi^*(\mathbf{X}, t) = p_0 |\psi(\mathbf{X}, t)|^2$$
(11)

where $\psi: \mathscr{B}_{\kappa} \times I \to C$ is a differentiable function with complex values, p_0 is an arbitrary constant with the dimension of p, and the asterisk denotes the (complex) conjugate operation. The Born representation is not the only representation of p ensuring fulfillment of the condition (10). For example, if the function ψ in the formula (11) takes quaternion values, then (10) is also fulfilled. This paper assumes, as is in the stochastic quantization method, the Born representation.

Collins (1977) showed that in the case of Euclidean space, the nonlinear Schrödinger equation can be derived from the continuity equation (8) and from the representation (11). This result can be generalized for an arbitrary Riemannian manifold. To that purpose, it is convenient to pass to the language of differential forms, the exterior derivative d, and the codifferential δ . If v is a tangent vector to M, representing, e.g., the velocity vector, then v will denote the covector canonically assigned to it, i.e.,

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$$\mathbf{v} = v^{A} \partial_{A} \Leftrightarrow v = \mathbf{G} \mathbf{v} = v_{A} \, dX^{A}$$

$$v_{A} = G_{AB} v^{B}$$

$$[\mathbf{v}] = [t^{-1}] \Longrightarrow [v] = [l^{2} t^{-1}]$$
(12)

We will also use the formulas (Choquet-Bruhat, 1977)

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$$dv = \partial_A v_B \, dX^A \wedge dX^B = \nabla_A v_B \, dX^A \wedge dX^B$$

$$= \frac{1}{2} (\nabla_A v_B - \nabla_B v_A) \, dX^A \wedge dX^B$$

$$div \, \mathbf{v} = \nabla_A v^A = G^{-1/2} \partial_A (G^{1/2} v^A), \qquad G = \det \|G_{AB}\|$$

$$\delta f = 0 \quad \text{for} \quad f \in C^{\infty}(M)$$

$$\delta v = -\operatorname{div} \mathbf{v}$$

$$\delta(fv) = -v \cdot df + (\delta v)f, \qquad v \cdot df = v^A \partial_A f$$
(13)

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and apply the Laplace-Beltrami operator $\Delta \stackrel{\text{df}}{=} -(\delta_d + d\delta)$, which acts according to the rule (Choquet-Bruhat, 1977)

$$\Delta f = -\delta \, df = G^{AB} \nabla_A \nabla_B f$$

= $G^{-1/2} \partial_A (G^{1/2} G^{AB} \partial_B f)$
 $\Delta v = (G^{AB} \nabla_A \nabla_B v_C - R_{BC} v^B) \, dX^C$
 $R_{BC} = R^A_{ABC} = R_{CB}$ (14)

where R_{AB} is the Ricci tensor and R_{ABC}^{D} is the curvature tensor for the Levi-Civita derivative ∇ (Schouten, 1954).

In these designations equation (8) takes the form

$$\partial_t p - \delta(pv) = 0 \tag{15}$$

and the diffusion velocity vector \mathbf{u} [equation (9)] is represented by the diffusion velocity covector u of the form

$$u = -2D \, dR \tag{16}$$

Denoting

$$\psi = e^{R+iS}$$
 ([R]=[S]=[1]) (17)

we obtain from (11) and (17) that

$$Q = e^{R} = (p/p_0)^{1/2}$$
(18)

Let us define the 1-form (covector) κ by the condition that

$$dS = (1/2D)v + \kappa \tag{19}$$

where v is the diffusion peculiar velocity covector [defined by the diffusion peculiar velocity vector v according to (12)] and S is the phase appearing in (17). The covector κ is defined with exactness by the transformation

$$\kappa \to \hat{\kappa} = \kappa + d\chi \tag{20}$$

corresponding to the phase transformation $S \rightarrow \hat{S} = S + \chi$. From (16)-(19) it follows that

$$u = -Dd \ln|\psi|^2$$

$$(p/p_0)v = -Di(\psi^*d\psi - \psi d\psi^*) - 2D|\psi|^2\kappa$$
(21)

From (11), (13) and (21) it follows that equation (15) is equivalent to the following condition:

$$\forall \psi \quad F(\psi)\psi^* = F(\psi)^*\psi \tag{22}$$

where

$$F(\psi) = i \partial_t \psi - D(\delta d\psi - i\psi \delta \kappa + 2i\kappa \cdot d\psi)$$
(23)

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The condition (22) is fulfilled iff there exists a function $f: M \times I \rightarrow R$ (dependent perhaps on ψ , ψ^* and κ), such that

$$\forall \psi \quad F(\psi)\psi^* = f\psi\psi^* \tag{24}$$

Finally, we obtain that the function ψ should satisfy an equation of the form

$$F(\psi) = f\psi \tag{25}$$

Denoting

$$V_{\kappa} = -D\kappa^2 + f, \qquad \kappa^2 = G^{AB}\kappa_A \kappa_B \tag{26}$$

we can write equation (25) in the following form:

$$i\partial_t \psi = D(\delta + i\kappa)(d - i\kappa)\psi + V_{\kappa}\psi$$
(27)

or, equivalently, in the form

$$i\partial_t \psi = -D(\nabla - i\kappa)^2 \psi + V_\kappa \psi$$
(28)

where $\kappa = \kappa^A \partial_A$, $\kappa^A = G^{AB} \kappa_B$, and the formulas (13) and (14) are used.

Equation (27) can be written, with the help of (17)-(19), in the form of the following system of equations:

$$\partial_t R = D(-2dR \cdot dS + \delta dS + 2\kappa \cdot dR - \delta\kappa)$$

$$\partial_t S = D[-\delta dR + (dR)^2 - (dS)^2 + 2\kappa \cdot dS - \kappa^2] - V_{\kappa}$$
(29)

Acting with the exterior derivative d operator on both sides of equations (29), using (16), (19) and the formulas

$$\Delta u = -d\delta u$$

$$(1/2)dv^{2} = v \cdot dv + (v \cdot d)v$$

$$(1/2)du^{2} = (u \cdot d)u$$

$$[(v \cdot d)w]_{A} = v^{B}\nabla_{B}w_{A}, \quad (v \cdot dw)_{A} = v^{B}\nabla_{A}w_{B}$$
(30)

we obtain that the equation

$$\partial_t u = -d(u \cdot v) - Dd\delta v \tag{31}$$

should be satisfied, where $u \cdot v = G^{AB}u_Av_A$, and as well as the equation

$$a = -2D(dV_{\kappa} + \partial_t \kappa - v \cdot d\kappa)$$
(32)

where

$$a = \partial_t v + (v \cdot d)v - (u \cdot d)u + D\Delta u$$

[a] = [l² t⁻²] (33)

From (16), (18) and (30) it follows that the covector a can be written in the following form:

$$a = \dot{v} + d\varphi_D$$

$$\dot{v} = \partial_v v + (v \cdot d)v$$
(34)

where \dot{v} is the so-called material time derivative (Marsden and Hughes, 1978) and where

$$\varphi_D = -2D^2 (\Delta Q/Q)$$

= $D^2 [\frac{1}{2} (dp/p)^2 - \Delta p/p]$ (35)

The potential φ_D , called *the diffusion potential*, is the diffusive counterpart of the so-called Bohm potential, considered in the hydrodynamic formalism of quantum mechanics (Takabyasi, 1983). If $M = (R^3, G)$ is a Euclidean space, then there exists a Cartesian coordinate system $X = (X^A)$ on R^3 such that $G_{AB}(X) \leq G_{AB} = \text{const}$ and the vector **a** [see (12)] can be identified with the Nelsonian mean acceleration vector of the Markovian diffusion process with constant diffusion coefficients $D^{AB} \geq DG^{AB}$ (Nelson, 1967). In the case of Markovian diffusion process with values in the Riemannian manifold, one can modify the definition of the Nelsonian mean acceleration in such a way that the formula (33) also has such an additional interpretation (Dohrn and Guerra, 1978).

Let us assume additionally that diffusing (identical) particles have mass. Let us denote by \hbar a constant with the dimension of action ($[\hbar] = g \text{ cm}^2 \sec^{-1}$ in the cgs unit system), defined by

$$\hbar = 2mD \tag{36}$$

where *m* is a diffusing particle mass (possibly of effective mass character) and *D* is a characteristic constant [appearing in (5)] with the dimension of diffusion coefficient. Let *E* be a covector with the absolute dimension $[E] = [t^{-1}]$ and φ a scalar with the energy dimension $([\varphi] = [ml^2 t^{-2}])$ such that

$$\partial_t \kappa + E = -\frac{1}{\hbar} \, d\varphi \tag{37}$$

Denoting by F a covector with the absolute dimension of force $([F] = [ml^2t^{-2}])$ defined by

$$F = \hbar (E + v \cdot \Omega)$$

$$\Omega = d\kappa, \qquad (v \cdot \Omega)_A = v^B \Omega_{AB}$$
(38)

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one can write equation (32) in the form of the covectorial equivalent of equation (3):

$$ma = K$$

$$K = F - dV$$
(39)

where

$$\hbar V_{\kappa} = V + \varphi, \qquad [V] = [ml^2 t^{-2}] \tag{40}$$

If we assume that equations (37)-(39) describe the influence of a certain external field on the locally equilibrium diffusion process, and we take the potential V as known, then equation (39) can be treated as the generalization of the Nelson relation (3) in the case of a diffusion process in a Riemannian manifold. This generalization, though not connecting the covector a with any averaging procedure, does not change the basic physical sense of the Nelson relation. Namely, this relation is a kind of constraint imposed on the mean (arriving and starting) velocities of the Markovian diffusion process. So, the forces appearing in that relation do not have exactly the sense of the cause of the motion, but of the restriction of too broad (from the physical point of view) a class of trajectories admissible by the Markovian diffusion process model. With such an understanding of these forces, the covector a has the sense of the effective acceleration and the additional interpretation of this acceleration (e.g., as the Nelsonian mean in its primary or modified sense) is not indispensable. Equation (27) can be now derived (as in the stochastic quantization method) from equations (15)-(19) and (36)-(40) (Dankel, 1971; Nelson, 1967).

The potential V appearing in equation (39) is generally dependent on the function ψ . In such a case the basic equation of the theory is equation (27) [or, equivalently, equation (28)] completed by the conditions (36) and (40) and by the external field equation (37). The problem is open of the way in which V should depend on ψ in the locally equilibrium diffusion processes. For example, if $\kappa = 0$, then the potential V of the form

$$V(\psi; X, t) = U(X, t) + (\hbar/2\tau) [\ln|\psi|^2 + i \ln(\psi^*/\psi)]$$
(41)

where $\tau = m/\zeta$ [see Introduction, the commentary after equation (4)], describes the force **K** of the form (4) with $\mathbf{F}_{\text{ext}} = -\nabla U$ (Trzęsowski and Kotowski, 1985).

The influence of the external field on the diffusion process defined by equations (37)-(39) is similar to the influence of the electromagnetic field on a particle with electric charge (Nelson, 1967). A field similar to the electromagnetic one can appear, e.g., in the case when the potential field of the diffusion peculiar velocity (Trzęsowski, 1989, Section 3) is disturbed by a certain vortex field (Julia and Toulouse, 1979). Further on I will show

that the influence of the crystal plastic yielding on the diffusion process can be described by such a type of field.

4. PLASTIC YIELDING IN BODY WITH DIFFUSION

Let us consider the *diffusive volume* of a (locally homogeneous) body with diffusion, i.e., a volume element $dV(\mathbf{X})$ in the material space M of that body:

$$dV(\mathbf{X}) = G(X)^{1/2} d^{3}X$$

$$G(X) = \det \|G_{AB}(X)\|, \qquad d^{3}X = dX^{1} dX^{2} dX^{3}$$
(42)

interpreted as the volume of the physically infinitesimal neighborhood of the point $\mathbf{X} \in M$ in the (local) equilibrium thermodynamic state (Trzęsowski, 1989, Sections 1 and 4). The *diffusive line element* $l = l(\mathbf{X})$

$$l(\mathbf{X}) = [G_A \hat{B}(X) \, dX^A \, dX^B]^{1/2} \tag{43}$$

can be interpreted as the (infinitesimal) characteristic length connected with the local thermodynamic equilibrium states in the neighborhood of the point X with the volume dV(X). Let us denote by l_0 a certain distinguished diffusion characteristic length [e.g., $l_0 = l(X_0)$], by $\lambda = \lambda(X)$ the deformation of this characteristic length at the point X,

$$\lambda = l/l_0 \tag{44}$$

and by e its so-called natural (or true) strain:

$$e = \ln \lambda \tag{45}$$

or, equivalently,

$$\lambda = \exp(e) \tag{46}$$

where e is the solution of the equation

$$de = dl/l, \qquad l(\mathbf{X}_0) = l_0 \tag{47}$$

It is known that the distortion of the crystal lattice by its defects manifests itself in the plastic strain of the body (Trzęsowski, 1987, Part I). In particular, the increment of the plastic strain is defined by the moving dislocations: the dislocations which do not move do not participate in the plastic strain increment. This is described by a kinematic relation of the form (Follansbee *et al.*, 1985)

$$\Delta e = (b/M) \rho_d V_d \Delta t \tag{48}$$

where Δe is the plastic strain increment in time Δt caused by the dislocations with the mean velocity modulus V_d ($[V_d] = [lt^{-1}]$) and Burgers vector

modulus b ([b] = [l]); ρ_d is the scalar density of mobile dislocations, i.e., the length of all dislocation lines included in the volume unit which can move ("nonanchored"), and M is a dimensionless coefficient (the so-called Taylor coefficient). So, if we want to consider the influence of the dislocation motion on the deformation of the diffusion characteristic length $l(\mathbf{X})$, then we can assume that there exists a certain covector

$$\varepsilon(\mathbf{X}, t) = \varepsilon_A(X, t) \, dX^A \qquad [\varepsilon] = [1] \tag{49}$$

independent of this characteristic length and such that along an arbitrary curve $\gamma: I \to M$, $\gamma(t_0) = X_0$, equation (47) is fulfilled, in which

$$de(t) = \gamma^*(de)(t)$$

= $\varepsilon(\gamma(t), t)(\dot{\gamma}(t)) = \varepsilon_A(\gamma(t), t)\dot{\gamma}^A(t) dt$ (50)

Then the plastic deformation of the diffusion characteristic length has the form (44), (46), where

$$e = e(\gamma; t) = \int_{\gamma_t} \varepsilon = \int_{t_0}^t \varepsilon(\gamma(s), s)(\dot{\gamma}(s)) \, ds \tag{51}$$

where $\gamma_t = \gamma | [t_0, t]$. This is equivalent to the transport of the metric tensor G along that curve according to the formula

$$G(\gamma(t)) = \lambda(\gamma; t)^2 G(\gamma(t_0))$$

$$\lambda(\gamma; t)^2 = \exp[2e(\gamma; t)]$$
(52)

Hence, it follows that if we define the covariant derivative $\overline{\nabla}^t$, $t \in I$, by the rule

$$\overline{\delta}^{t} l(\mathbf{X}) / l(\mathbf{X}) = \varepsilon(\mathbf{X}, t)$$

$$\overline{\delta}^{t} = d\mathbf{X}^{A} \overline{\nabla}^{t}_{A}$$
(53)

then $\overline{\nabla}^t$ defines the so-called Cartan-Weyl geometry according to

$$\overline{\nabla}_{C}^{t} G_{AB}(X) = \kappa_{C}(X, t) G_{AB}(X)$$
(54)

where

$$\kappa(\mathbf{X}, t) = 2\varepsilon(\mathbf{X}, t) \tag{55}$$

Let us consider the one-parameter Cartan-Weyl space family $M[\mathbf{G}, \kappa] = \{(R^3, \overline{\nabla}^t), t \in I\}$ defined by (54) as the evolution in time of Cartan-Weyl geometry of the general material space of a crystal body with lattice defects (Trzęsowski, 1987, Part II). Then, the following conclusion results from the definition of the covector κ :

Conclusion. Cartan–Weyl geometry describes the distortion of the lattice of a (locally homogeneous) crystalline solid with diffusion which is accompanied by the natural plastic strain of (infinitesimal) characteristic lengths of the local thermodynamic equilibrium states of that body.

The connection $\overline{\Gamma} = (\overline{\Gamma}_{BC}^{A})$ corresponding to the covariant derivative $\overline{\nabla}$ (I omit the index t because this is a parameter only in the geometrical formulas) is of the form (Schouten, 1954)

$$\bar{\Gamma}_{BC}^{A} = \Gamma_{BC}^{A}(\mathbf{G}, D) - G^{AE} P_{BEC}(\bar{\Gamma}, \mathbf{G})$$
(56)

where $\Gamma_{BC}^{A}(\mathbf{G}, D)$ are the coefficients of the symmetric connection fulfilling the condition (54) (the so-called Weyl connection):

$$\Gamma_{BC}^{A}(\mathbf{G}, D) = \frac{1}{2} G^{AE} (D_C G_{EB} + D_B G_{EC} - D_E G_{BC})$$

$$D_A = \partial_A - \kappa_A$$
(57)

and $P_{BEC}(\overline{\Gamma}, \mathbf{G})$ is the so-called contortion tensor:

$$P_{BEC}(\Gamma, \mathbf{G}) = S_{BEC} - S_{ECB} + S_{CBE}$$

$$S_{ABC} = G_{CE} S_{AB}^{E}(\bar{\Gamma}), \qquad S_{AB}^{E}(\bar{\Gamma}) = \bar{\Gamma}_{[AB]}^{E}$$
(58)

The contortion tensor describes the distortion of the crystal lattice of crystal elements with the volume $dV(\mathbf{X})$ [equation (42)] by dislocations with (tensor) density α^{AB} of the form (Trzęsowski, 1987)

$$\alpha^{AE} = S^{A}_{BC}(\bar{\Gamma})e^{BCE}$$

$$e^{BCE} = G^{-1/2}\varepsilon^{BCE}, \qquad \varepsilon^{BCE} = \varepsilon_{BCE}$$
(59)

where ε_{ABC} is a permutation symbol. Here the description of the dislocation distribution has been related to the material space M of a body with diffusion. In the literature, the description of the dislocation distribution is usually related to a body with no lattice defects (e.g., Kröner, 1960; Bilby, 1960). In Trzęsowski (1987) this description was related to the material space of a body with dislocations.

Let us denote by $R^{D}_{ABC}(\bar{\Gamma})$ the curvature tensor of the connection (56) (Schouten, 1954) and introduce the tensor Θ by

$$\Theta = \Theta_{CD} \, dX^C \otimes dX^D$$
$$\Theta_{CD} = R_{AB(CD)}(\bar{\Gamma}, \mathbf{G}) \, dX^A \wedge dX^B \tag{60}$$
$$R_{ABCD}(\bar{\Gamma}, \mathbf{G}) = G_{DE} R^E_{ABC}(\bar{\Gamma})$$

Since (Schouten, 1954)

$$R_{AB(CD)}(\bar{\Gamma}, \mathbf{G}) = -[\bar{\nabla}_{[A}\kappa_{B]} + S^{E}_{AB}(\bar{\Gamma})\kappa_{E}]G_{CD}$$
(61)

then the tensor Θ is of the form

$$\mathbf{\Theta} = -\mathbf{\Omega} \otimes \mathbf{G} \tag{62a}$$

$$\Omega = d\kappa \tag{62b}$$

The 2-form Ω appearing in the formula (62) is called the *curvature length*. The tensor Θ defines the so-called *geometrical interactions* between point defects and dislocations (Trzęsowski, 1987). The physical sense of the geometrical interactions has not yet been fully recognized. Usually, they are connected with the creation and annihilation of point defects in a body with dislocations (Trzęsowski, 1987; Kroner, 1985).

From (55) and (32b) it follows that the curvature length Ω is defined by the infinitesimal plastic strain ε . Observe that Ω is independent of the dislocation density tensor α^{AB} , which is connected with the so-called translational plasticity, appearing in the slip phenomenon (e.g., Hull and Bacon, 1984; Panin et al., 1985). This means that Ω can be connected with the influence of the dislocations (and point defects) on other kinds of elementary acts of plasticity. Such an elementary act of plasticity is, e.g., the so-called rotational plasticity connected with the phenomenon of crystal fragmentation in the pastic yielding process (Panin et al., 1985). Though the diffusive motion of point defects and the local slips belong to mechanisms leading to the creation of plastic rotation, all these phenomena are elementary acts of plasticity on different structural levels (Panin et al., 1985). For example, in the case of point defects of 10^{-18} cm size, the elementary act of plasticity connected with the diffusive mass transport is related to the volume 10^{-21} -10⁻²² cm³. In the case of translational ("strictly dislocational") plasticity, larger structural elements take part in the elementary act of plasticity. Because as an approximation the effective width of dislocation is 10^{-7} cm and the length of its displacing part is 10^{-6} - 10^{-3} cm, the elementary act of plasticity is related here to the volume 10^{-20} - 10^{-16} cm³. In the case of crystal fragmentation, taking 10^{-5} - 10^{-2} cm as the characteristic size of the fragment or the grain, the elementary act of plasticity occurs in a volume of approximately 10^{-15} - 10^{-6} cm³. So, the crystal fragmentation should be treated as a separate act of rotational plasticity connected with the mesoscale of the deformation process (i.e., a scale intermediate between atomic and macroscopic scales) (Panin et al., 1985).

The crystal fragmentation is also connected with the existence of superficial distributions of dislocations which cause a change of relative orientation between neighboring parts of the crystal. Such a distortion of the crystal structure manifests itself in the crystal lattice bend, but is not accompanied (in the absence of external field) by a macroscopic stress field. It is accompanied by a macroscopic field of so-called couple-stresses (Kröner, 1960). As a result, a body with such a distribution of dislocations behaves like a body with internal rotational degrees of freedom (Trzęsowski, 1987, Part II, Section 4). If the crystal plastic yielding is considered as a state intermediate between crystal and fluid (the so-called dislocation fluid), then the couple-stresses field causes disturbances in that fluid, and as a consequence its flow acquires a vortical character. The consequence of this is the formation of substructures in the crystal in the form of crystal fragmentation as well as in the form of cellular dislocation structures (Panin *et al.*, 1985). These substructures are in fact dissipative structures, and can preserve themselves for a long time after the stopping of the deformation process, because a long relaxation time is a specific property of dissipative structures in crystals (Panin *et al.*, 1985).

The above remarks suggest that if one restricts oneself to the description of the plastic strain increments de(t) [equation (50)] in the dislocation fluid approximation [i.e., in the approximation of relation (48)], then [according to (55) and (62b)] the curvature length Ω should depend on the vortex field in that fluid. So, first of all, let us describe that fluid. Let us consider the case when dislocations constitute the system of (closed) dislocation loops [such a situation can occur, e.g., in the case of crystal irradiation with fast neutrons (Bullough and Newman, 1970). The dislocation loops can be described in the following way. The interpretation of the tensor α^{AB} [equation (59)] as the dislocation density tensor is connected with the interpretation of the system $\tau = (\tau^A)$ 2-forms of the form

$$\tau^{A} = S^{A}_{BC}(\bar{\Gamma}) \, dX^{B} \wedge dX^{C}$$

[S^{C}_{AB}] = [l^{-1}], [dX^{A}] = [l], [τ^{A}] = [l] (63)

as the infinitesimal counterpart of the Burgers vector (Bilby, 1960). Such a Burgers vector is connected with the dislocation density by

$$\tau^{A} = \alpha^{AB} dS_{B}$$

$$dS_{B} = \frac{1}{2} e_{BCD} dS^{CD}$$

$$dS^{CD} = dX^{C} \wedge dX^{D}$$

$$[\alpha^{AB}] = [l^{-1}], \qquad [dS_{B}] = [dS^{BC}] = [l^{2}]$$
(64)

where the 2-form dS_B is interpreted as representing the surface element dS with the unit normal n_B :

$$dS_B = dSn_B$$

$$[dS] = [l^2], \qquad [n_B] = [1]$$
(65)

which is cut by dislocation lines with the density α^{AB} . If an infinitesimal loop is identified with an infinitesimal bivector (Schouten, 1954), then the

considered dislocations will constitute a dislocation loop system if the Burgers vector $\tau = (\tau^A)$ fulfills the condition

$$\tau^{A} = d^{A}_{\tau}, \qquad \stackrel{A}{\tau} = \stackrel{A}{\tau_{B}} dX^{B}$$

$$[\stackrel{A}{\tau}] = [l], \qquad [\stackrel{A}{\tau_{B}}] = [1]$$
(66)

which is equivalent to the assumption (Kosevitch, 1972)

$$S_{BC}^{A}(\bar{\Gamma}) = \frac{1}{2} (\partial_{B} \tau_{C} - \partial_{C} \tau_{B}^{A})$$
(67)

If the dislocations are sufficiently distant one from one another that phenomena connected with their cutting can be ignored and the loops are flat (they are in their slip planes), then their distribution can be approximated, assuming that

$${}^{A}_{\tau_{B}} = b^{2} \rho_{d} \delta^{A}_{B}$$

$$[b] = [l], \qquad [\rho_{d}] = [l^{-2}]$$
(68)

where b is the characteristic length of the Burgers vector and $\rho_d = \rho_d(\mathbf{X}, t)$ is the scalar density of dislocation [see the commentary after equation (48)] related to the diffusive volume (42) [see the commentary after equation (59)]. From (66) and (68) it follows that

$$\tau^{A} = N \wedge \tilde{\tau}, \qquad N = d\xi_{d}$$

$$\tilde{\tau} = b^{2} \rho_{d} dX^{A}, \qquad \xi_{d} = \ln(b^{2} \rho_{d})$$
(69)

If the covector N is interpreted as a certain class of pairs of parallel planes with equal distances (Schouten, 1954), then (69) means that the infinitesimal loops, as well as the infinitesimal Burgers vector $\mathbf{\tau} = (\tau^A)$, "lie" in parallel planes defined by N. This means that each plane belonging to the family of planes defined by N can be considered as a (local) slip plane, i.e., a plane in which there lies a line as well as a Burgers vector of the moving dislocation. Also possible are different configurations of the dislocation loop, consistent with the condition (69). One such configuration is the so-called double cross slip (Hull and Bacon, 1984), for which the Burgers vector lies in the slip plane, but the dislocation loop is bent in such a way that one part lies on the slip plane and the other on the plane parallel to it.

The scalar density of dislocations ρ_d introduced by (68) includes in general the mobile as well as the stationary (anchored) dislocations. The influence of the crystal lattice distortion via the stationary (anchored) dislocations on the diffusion process is taken into account in the proposed

theory only through the influence of this distortion on the diffusion coefficients. It corresponds to the approximation in which the influence of the lattice distortion via the dislocation fluid on the diffusion process is described with the assumption that ρ_d is the mobile dislocation density related to the diffusive volume of the body [dependent on the stationary dislocation distribution—see (5) and (42)]. In that approximation, one can generalize the relation (48), assuming that the dislocation fluid defines the plastic strain increments de(t), according to the formula (50), in which the infinitesimal plastic strain ε is of the following form:

$$\varepsilon = \tau_d \rho_d v_d$$

$$v_d = \mathbf{G} \mathbf{v}_d, \qquad [v_d] = [l^2 t^{-1}], \qquad [\tau_d] = [t]$$
(70)

where τ_d is a certain characteristic time for the dislocation motion in a body with diffusion (see Section 5) and \mathbf{v}_d is the mobile dislocation velocity (i.e., the flow velocity of the dislocation fluid). From (55), (62b) and (70) it follows that

$$\Omega = 2\tau_d \rho_d (\Omega_d + \Sigma_d)$$

$$\Omega_d = dv_d, \qquad \Sigma_d = N \wedge v_d$$
(71)

where the covector N is defined by (69) and Ω_d is interpreted as the density of vortices in the dislocation fluid, i.e.

$$\Omega_d = \omega_d^A \, dS_A$$

$$\omega_d^C = \Omega_{dAB} \, e^{ABC}, \qquad \Omega_{dAB} = \partial_{[A} v_{dB]}$$
(72)

The vector $\mathbf{\omega}_d = (\omega_d^A)$ is here interpreted as a vortex vector (vortices in the cylinder tube with section dS_A). The 2-form Ω_d describes then the contribution of the *rotational plasticity* to the geometrical interactions. Since from (67)–(69) it follows that [cf. (61)]

$$\kappa_C \tau^C = \kappa_C S^C_{AB}(\bar{\Gamma}) \, dX^A \wedge dX^B = 2\tau_d (b\rho_d)^2 \Sigma_d \tag{73}$$

then the 2-form Σ_d describes the contribution of the *translational plasticity* to the geometrical interactions; in general, this contribution is connected with the *local slips* in the crystal. If in the plastic yielding process the effect of the translational plasticity dominates (i.e., $\Omega_d = 0$), then the dislocation fluid flow becomes potential, and crystal plastic yielding is possible with the character of the laminar flow of that fluid (Panin *et al.*, 1985). In this case, the local slips can develop into macroscopic slip in the crystal. If the geometrical interactions vanish, i.e.,

$$\Omega = 0 \tag{74}$$

then the strain ε is not the plastic strain, because from (74) the following representation is possible:

$$\kappa_t = d\zeta_t, \qquad \zeta_t \in C^{\infty}(M)$$

$$\kappa_t(\mathbf{X}) = \kappa(\mathbf{X}, t)$$
(75)

In this case, Cartan-Weyl geometry can be reduced to Cartan geometry because from (54) and (75) it follows that

$$\bar{\nabla}_C^t(\alpha_i G_{AB}) = 0, \qquad \alpha_i = e^{-\zeta_i} \tag{76}$$

and the dislocation fluid is reduced to the disclination loop fluid, because

$$\Sigma_d = -\Omega_d \tag{77}$$

In the case when in the plastic yielding process the effect of the rotational plasticity dominates (i.e., when $\Sigma_d = 0$), the crystal lattice distortion can be described by Weyl geometry, defined by the symmetric connection of the form (57).

If the dislocation loops do not change their sizes in time, then the equation of the dislocation fluid flow is reduced to the equation of its continuity (Kosevitch, 1978). Let us generalize that model of dynamics, assuming that the space in which the dislocation fluid flow takes place is the material space of a body with diffusion [see the commentary before equation (70)]. Then the equation of dislocation fluid flow takes the following form:

$$\partial_t \rho_d - \delta(\rho_d v_d) = 0 \tag{78}$$

Equation (78) can be written in the form [Trzęsowski, 1989, equation (70)]

$$\partial_{t}\rho_{d} + \partial_{A}(\rho_{d}v_{d}^{A}) = -\frac{1}{\tau_{d}}\gamma\cdot\varepsilon$$

$$\gamma = dG^{1/2}$$
(79)

where (70) is taken into account and where $\gamma \cdot \varepsilon = G^{AB} \gamma_A \varepsilon_B$. From the form of equation (79) it follows that the considered model of mobile dislocation dynamics includes their creation (or annihilation) in the plastic yielding process.

5. INFLUENCE OF PLASTIC YIELDING ON DIFFUSION

Let us consider the locally equilibrium diffusion process of point defects possessing mass (e.g., interstitial atoms) in a (locally homogeneous) crystalline solid in which there occurs plastic yielding. If the plastic yielding process is accompanied by crystal fragmentation, then such a process is 582

connected with elementary acts of plasticity on the mesoscale level (Section 4). In Section 4 it was shown that the curvature length Ω [equation (62)] is a geometrical object which describes such a plastic yielding process. As a consequence, Ω can be treated as a geometrical object connected with the mesoscale of the considered material structure. Because the diffusion process is connected with the atomic scale of that structure, Ω can be treated as an external field in the presence of which the diffusion process occurs. Such a curvature length defines the infinitesimal plastic strain ε [or, equivalently the covector κ ; see (55) and (62b)] with exactness by the gauge transformation (20). This, and the way in which κ appears in equations (28) and (57), suggest the assumption that the covector κ defined by (19) and representing a certain external field [see the commentary after equation (40)] is connected with the infinitesimal strain ε by equation (55). Then from (19), (36) and (62b) it follows that the curvature length Ω is of the form

$$\Omega = -\frac{m}{\hbar} \, dv \tag{80}$$

Let us observe that formula (80) is consistent with the hypothesis connecting the geometrical interactions [equation (62)] with the creation and annihilation of point defects [Trzęsowski, 1989, equation (70)].

Acting with the codifferential operator δ on both sides of equation (37), we obtain

$$\partial_t \delta \kappa + \delta E = \frac{1}{\hbar} \Delta \varphi \tag{81}$$

Let us write, using equations (55) and (70), the continuity equation (78) of the dislocation fluid in the form

$$\partial_t \rho_d = \frac{1}{2\tau_d} \,\delta\kappa \tag{82}$$

Multiplying both sides of equation (82) by the characteristic constant D and introducing designations

$$\varphi = \frac{\hbar^2}{m} \rho_d$$

$$c_d^2 = \frac{D}{\tau_d}, \quad [c_d] = [l t^{-1}], \quad [\varphi] = [m l^2 t^{-2}]$$
(83)

where \hbar is of the form (36), we can write equation (82) in the form

$$c_d^2 \delta \kappa = \frac{1}{\hbar} \partial_i \varphi \tag{84}$$

If the scalar φ in equation (81) is of the form (83), then equation (84), considered together with equation (81) and the gauge transformation (20), is the counterpart of the so-called Lorentz gauge condition for the electromagnetic field. Here, however, unlike in the electromagnetic field theory, this condition is physically distinguished by the equivalence of equations (78) and (84). From (81), (83) and (84) we obtain the following wave equation with sources:

$$\Delta \rho_d - \frac{1}{c_d^2} \frac{\partial^2 \rho_d}{\partial t^2} = \varkappa_d \tag{85a}$$

$$\varkappa_d = \frac{m}{\hbar} \delta E \tag{85b}$$

Equation (85) shows that the constant c_d has the sense of the propagation velocity of a density wave in the dislocation fluid. This means that c_d should be quantity of the order of the acoustic wave velocity in the crystal (Follansbee *et al.*, 1985).

Acting with the exterior derivative operator d on both sides of equation (37), we obtain

$$\partial_t \Omega + dE = 0$$

$$d\Omega = 0$$
(86)

Let us consider the field (E, Ω) as an external field in the presence of which the diffusion process occurs, and whose physical carrier is the dislocation fluid. This field acts on the diffusion atom according to equation (39), with the force F of the form (38). The influence of a field (E, Ω) on a diffusing atom is similar to the influence of the electromagnetic field on a particle with electric charge. Equation (37) denotes that the pair (φ, κ) plays in this analogy the role of the electromagnetic field potential. The field (E, Ω) is not fully determined, because of the lack of an equation defining E. For example, if we know from somewhere else the mechanical "Lorentzian" force F, then (38) becomes the constitutive equation defining the field E. Also, an additional condition, defining the form of the sources \varkappa_d in equation (85), can be used for defining the field E. Leaving the problem of the formulation of equations defining the field of E open, we restrict ourselves to the discussion of the case in which the proposed theory has a closed character.

In special conditions connected with the kind of crystal material, as well as the degree of advancement of the plastic yielding process, the contribution of the rotational plasticity to this process may become dominating (Panin *et al.*, 1985). Because the rotational plasticity does not cause stresses in the body, but is only the cause of the appearing of the couplestresses in it (Section 4), so one can expect that in this case the Lorentzian force should vanish:

$$E + v \cdot \Omega = 0 \tag{87}$$

Then E becomes a covector proportional to the current of vortices in the diffusing matter [see equation (80)], and equation (86) takes the following form:

$$\partial_t \Omega - d(v \cdot \Omega = 0$$

$$d\Omega = 0$$
(88)

The scalar \varkappa_d in equation (85) is here of the form

$$\varkappa_d = -\frac{m}{\hbar}\delta(v\cdot\Omega) \tag{89}$$

and Ω is proportional to the density of vortices Ω_d in the dislocation fluid [cf. equation (71)]:

$$\Omega = 2\tau_d \rho_d \Omega_d$$

$$\Omega_d = dv_d$$
(90)

Equations (78), (80), (85a), (89) and (90) describe the dislocation fluid in a body with diffusion. Equations (11), (21), (27), (36), (40), (55), (70) and (83) describe diffusion in a body with (rotational) plastic yielding defined by this dislocation fluid.

Finally, let us observe that from the analysis of the properties of the statistical entropy of the locally equilibrium diffusion process (Trzęsowski, 1989, Section 7), it follows that the thermodynamic openness of the system and the tendency to create the dissipative structures in it (see Section 4) will take place when the diffusion peculiar velocity \mathbf{v} fulfills almost everywhere the condition

$$-\delta v = \operatorname{div} \mathbf{v} < 0 \tag{91}$$

6. CONCLUSIONS AND REMARKS

Part I of this work (Trzęsowski, 1989) considered the locally equilibrium diffusion process in which there appear two mean velocities of the diffusing particle: the arrival velocity to the point and the starting velocity from the point. It was shown that the geometrization of the notion of local thermodynamic equilibrium leads to the description of that diffusion process as diffusion in a certain Riemannian manifold—the material space of a (locally homogeneous) body with diffusion (Section 2).

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In the present part of this work it was shown that the results of the first part and (the modified) Nelson stochastic mechanics (Section 3), considered in the material space of a body with diffusion allow the description of the coupling of the diffusion process with the plastic yielding process (Section 5). The proposed description of the coupling of these two processes is based on treating the geometrical interactions (Section 4) as an external field acting on the diffusion particles. These geometrical interactions were defined on the basis of identifying the Weyl relative change of the length scale with the increment of the plastic strain caused by the motion of the dislocations (Section 4). As a consequence, the geometrical interactions are connected with the increment of the plastic strain in an analogous way as in the Weyl theory the electromagnetic field is connected with the change of the scale, and the influence of the plastic yielding on the diffusing particle is similar to the influence of the electromagnetic field on particle with electric charge (Sections 3 and 5).

The proposed theory also includes a "relativistic effect" consisting in the existence of a dislocation limit velocity (Section 5). An effect of this kind has frequently been discussed within the framework of different models of the motion of dislocations (e.g., Kosevitch, 1972; Seeger, 1981; Günther, 1981) as well as in the analysis of experimental data (e.g., Follansbee *et al.*, 1985). Here, this effect is connected with the wave equation (85) for the dislocation fluid density. This wave equation is generally nonlinear because a source term appears in it coupling the motion of dislocations with the diffusive motion of point defects. Then, one can expect the existence of solutions of equation (85) describing soliton waves in the dislocation fluid (deWitt, 1985).

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