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Geometry of Crystal Structure with Defects. I. Euclidean Picture

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Continuously distributed defects of crystal structure are considered. The starting point is the Euclidean geometry of the ideal crystal lattice and the topological description of the distortion of the crystal structure. It is shown how the non-Euclidean geometry of distorted crystal structure, as well as the basic assumptions of the phenomenological plasticity theory concerning the deformation of a continuum, are related to those theories. A form for an affine connection describing continuously distributed dislocations is proposed.

1. INTRODUCTION

There exist many material structures for which the geometry of moving frames (triads, tetrads, etc.) is an especially convenient method of description. These include, e.g., crystalline solids with a three-dimensional crystal lattice, as well as those formed from layers with a flat crystal lattice (so-called lamellar structures, e.g., graphite). Some liquid crystals can be also described in such a formalism (e.g., cholesterics and smectics, especially smectics B). The advantages of such a description become clearer when the ideal material structure is distorted by the occurrence of various defects (point-line, linear, superficial, or volumetric).

Let us consider a crystalline solid whose crystal structure is a three-dimensional monoatomic Bravais lattice, that is, a lattice uniquely determined by giving one of its points and three lattice base vectors (Section 2). In the local theory of elastic response of such a material body, this response depends only on the actual configuration of atoms in the macroscopically small ("physically infinitesimal") neighborhood of each point of the crystal. In such a neighborhood the deformed lattice may be considered as

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homogeneously deformed. In this way the continuous description of an elastically deformed crystalline solid may be reduced (in the case of a monoatomic Bravais lattice) to the consideration of the basic element of description of its discrete structure geometry, that is, the triad of base vectors of the lattice. The existence of defects of the crystal lattice—pointline (e.g., inserted atoms) or linear (e.g., dislocations)—disturbs the continuity of distribution of these base bectors (we deal with the deformed crystal continuum).

Usually in the physically infinitesimal neighborhood of each crystalline body point, there are sufficiently many such defects in order to justify the assumption of a macroscopically continuous distribution in the body. In this case, the (macrsoscopic) continuity of distribution of the lattice base vectors is preserved, but it remains nonintegrable.

The main purpose of this paper is to establish the relations between symmetries and metric parameters of the ideal crystal lattice and the regularities of disturbances of them by continuous distributions of defects of this lattice.

From the formal point of view, the geometrical methods used in this paper are closely related to those used in the space-time theory of tetrad frames (e.g., Rumer, 1956; Sławianoski, 1985; Weyl, 1929). The fact that Lorentz three-dimensional rotations appear in this paper as one of the objects describing symmetries in the distribution of dislocations illustrate that relationship. Conversely, the notion of geometrical interactions understood in the sense attributed to it in the continuous theory of defects (Günther and Żórawski, 1985) has turned out to be useful in our analysis of properties of so-called spinor connections (Srivastava, 1983).

This work consists of two parts. In this paper (Part I) we construct the relations mentioned above, using the language of geometry of Euclidean space (i.e., the space in which both the lattice and the solid figure of the body are embedded). This is the language of description of experiment. In Part II we formulate the basic results of Part I in the language of non-Euclidean geometry, and in that language we continue their further analysis. This is the language of description of the material structure of the body. The basic results of this work are included in Part II. The Appendix to the present paper includes the designations and mathematical theorems concerning the point Euclidean space and the formulation of the Euclidean interpretation of Lorentz three-dimensional rotations.

2. THE GEOMETRY OF THE CRYSTAL LATTICE

Let $\mathbf{E}$ denote three-dimensional real Euclidean vector space. A *lattice group* is a nontrivial discrete subgroup T of the additive group $(\mathbf{E}, +)$. T

is a three-dimensional lattice group if and only if there exist linearly independent vectors $\underline{E}_a$, $a = 1, 2, 3$, such that

$$T = \{\underline{t} = n^a \underline{E}_a, \qquad n^a \in Z\}$$

where Z denotes the set of integers. The vectors $\underline{E}_a$ are called *basic vector* of the lattice group T. They are not uniquely determined, because every other set of vectors $\{\underline{E}'_a, a = 1, 2, 3\}$ is a set of basic vectors if and only if the following condition is fulfilled:

$$\underline{E}'_a = \gamma^b{}_a \underline{E}_b, \qquad \underline{\gamma} = \| \gamma^a{}_b \| \in GL(Z^3), \qquad |\det \underline{\gamma}| = 1 \tag{1}$$

where $GL(Z^3) \subset GL(R^3)$ is the group of nonsingular matrices of integer coefficients. A *primitive cell* is the parallelepiped $K(E_T)$ determined by the set of basic vectors $E_T = (\underline{E}_a)$, i.e.,

$$K(E_T) = \{\underline{x} = x^a \underline{E}_a,\ 0 \le x^a \le 1\}$$

The volume of this primitive cell

$$V_T = \mathrm{vol}\, K(E_T) \tag{2}$$

is an invariant of the choice of the lattice group basic vectors. Let E denote the point Euclidean space on $\mathbf{E}$ (see Appendix). The *lattice* (three-dimensional) S denotes a set $S \subset E$ such that (see Appendix)

$$T(S) = \{\underline{a} \in \mathbf{E}\colon\ \tau_{\underline{a}}(S) = S\}$$

is a certain three-dimensional lattice group. Further on we will not distinguish vectors $\underline{a}$ from the lattice group $T(S)$ from the translations $\tau_{\underline{a}} \in T(E)$ (see Appendix) and we will consider only three-dimensional lattice groups. Vectors $\underline{a} \in T(S)$ are called *lattice vectors* and the basic vectors $\underline{E}_a$ are called *base vectors* of the lattice. The lattice S on which its lattice group $T(S)$ acts transitively is called the *Bravais lattice.* Bravais lattices have the form

$$S = T(S)P$$

where $P \in S$ is an arbitrarily chosen point of the lattice. In this paper we will consider only Bravais lattices. The *lattice line* (of a Bravais lattice) is a straight line crossing a point of the Bravais lattice and parallel to a base vector of this lattice.

The *symmetry group* of the lattice (or the crystallographic group) is a maximal subgroup $G(S)$ of Euclidean group $E(\mathbf{E})$, such that

$$\exists O \in S \qquad G(S) = \{(\underline{a}, \underline{A}) \in E(\mathbf{E});\ \Phi_{(\underline{a},\underline{A})}(S) = S\}$$

where $\Phi = \{\Phi_{(\underline{a},\underline{A})}\}$ is the action of the group $E(\mathbf{E})$ in E, defined by the localization at the point $O \in S$ (see Appendix).

The *point group* of the lattice (or the crystallographic point group) $P = P(T)$ of the lattice S with the lattice group $T = T(S)$, is a subgroup of the orthogonal group $O(\mathbf{E})$ defined by

$$P(T) = \{\underset{\sim}{Q} \in O(\mathbf{E}): (\underset{\sim}{o}, \underset{\sim}{Q}) \in G(S)\}$$

The symmetry group $G(S)$ of the Bravais lattice S with the point group $P(T)$ has the decomposition in the form

$$G(S) = T(S)P(T(S))$$

and has the structure of the semidirect product of groups T and $P(T)$ (see Appendix):

$$G(S) \cong G(P, T) = T \,\square\, P(T) \subset \mathbf{E} \,\square\, E(\mathbf{E})$$

Let us denote by T the lattice group of the lattice S. If the basic vectors of the lattice group $E_T = (\underset{\sim}{E}_a)$ are identified with base vectors of $\mathbf{E}$, we obtain a co-ordinate system on $\mathbf{E}$, which will be denoted by ξ_T; such a system ξ_T is called the *proper system* of the lattice S (with the lattice group T) (Morzymas, 1977). The symmetrical matrix $\underset{\sim}{g}_T \in GL^+(R^3)$ defined as

$$\underset{\sim}{g}_T = \| g_{ab} \|, \qquad g_{ab} = \underset{\sim}{E}_a \cdot \underset{\sim}{E}_b \tag{3}$$

is called a lattice *metric matrix* associated with its proper system ξ_T. With the change of the proper system ξ_T for ξ'_T, the metric matrix $\underset{\sim}{g}_T$ is transformed according to the rule

$$\underset{\sim}{g}_T = \underset{\sim}{\gamma}^t \underset{\sim}{g}_T \underset{\sim}{\gamma}, \qquad (\det \underset{\sim}{g}'_T)^{1/2} = (\det \underset{\sim}{g}_T)^{1/2} = V_T \tag{4}$$

where $\underset{\sim}{\gamma} \in GL(Z^3)$ is a matrix by equation (1), t denotes the transposition, and V_T is the volume of the primitive cell defined by (2).

Orientation of the lattice means that all proper systems (of that lattice) under consideration are oriented in the same manner. For the oriented lattice

$$V_T = \underset{\sim}{E}_1 \cdot (\underset{\sim}{E}_2 \times \underset{\sim}{E}_3) > 0 \tag{5}$$

where $\underset{\sim}{a} \times \underset{\sim}{b}$ denotes the vector product.

Let us denote by $R^3(\xi^a)$ the space R^3, whose points are by standard denoted by $\xi = (\xi^a)$, and denote by $R^3_g(\xi^a)$ the space $R^3(\xi^a)$ with the metric form g defined by

$$\begin{gathered} g(\underset{1}{\xi}, \underset{2}{\xi}) = g_{ab} \underset{1}{\xi^a} \underset{2}{\xi^b} \\ \underset{\sim}{g} = \| g_{ab} \| = \underset{\sim}{g}^t, \qquad \det \underset{\sim}{g} > 0 \end{gathered} \tag{6}$$

The space $R^3_g(\xi^a)$ whose metric form g is defined by the metric matrix $\underset{\sim}{g}_T$ of the oriented lattice S with the lattice group T will be denoted by $R^3_T(\xi^a)$

and called *proper metric space* of the (oriented) lattice S (associated with the proper system ξ_T). This definition implies that the space $R^3_T(\xi^a)$ satisfies, independent of the choice of the proper system ξ_T of the (oriented) lattice S, the following condition:

$$(\det \underset{\sim}{g})^{1/2} = V_T \tag{7}$$

where V_T is the volume of the primitive cell [formulas (2) and (5)]. This means that the nonmetric properties of the oriented lattice can be described by the unimodular space $R^3(\xi^a)$, i.e., the vector space with the fundamental group $SL(R^3)$. Therefore, the distinction of the class of the proper metric spaces can be connected with the distinction of the group $H(T)$ of the *unimodular point symmetries* of the lattice:

$$H(T) = \{\underset{\sim}{A} \in SL(\mathbf{E})\colon \Phi_{\underset{\sim}{a},\underset{\sim}{A})}(S) = S\}$$

where $T = T(S)$ denotes the lattice group of the considered lattice S and $SL(\mathbf{E})$ is the special linear group (see Appendix). The semidirect product of groups T and H (see Appendix)

$$G(H, T) = T \,\square\, H(T)$$

we will call the group *equiaffinic symmetries* of the lattice.

Let us denote

$$O_g(R^3) = \{\underset{\sim}{L} \in GL(R^3)\colon \underset{\sim}{L}^t \underset{\sim}{g} \underset{\sim}{L} = \underset{\sim}{g}\} \tag{8}$$

$$\underset{\sim}{g} = \underset{\sim}{g}^t, \qquad \det \underset{\sim}{g} > 0$$

The matrix $\underset{\sim}{S}_T \in GL(R^3)$ such that

$$\underset{\sim}{g} = \underset{\sim}{g}_T = \underset{\sim}{S}^t_T \underset{\sim}{S}_T \tag{9}$$

is called the *Lamé metric matrix* (Rumer, 1956). From (8) and (9) it follows that

$$O_g(R^3) = \underset{\sim}{S}_T^{-1} O(R^3) \underset{\sim}{S}_T \tag{10}$$

i.e., $O_g(R^3)$ is conjugate to $O(R^3)$ in $GL(R^3)$. It is easy to see that if $\underset{\sim}{e}_a$, $a = 1, 2, 3$, is a base of $\mathbf{E}$ such that

$$\begin{aligned} &\underset{\sim}{E}_a = \underset{\sim}{S}_T \underset{\sim}{e}_a, \qquad \underset{\sim}{S}_T = S^a{}_b \underset{\sim}{e}_a \otimes \underset{\sim}{e}^b \in GL(\mathbf{E}) \\ &\underset{\sim}{e}_a \cdot \underset{\sim}{e}_b = \delta_{ab}, \qquad \underset{\sim}{e}_a \cdot \underset{\sim}{e}^b = \delta^b_a \end{aligned} \tag{11}$$

then the matrix $\| S^a{}_b \|$ is the Lamé metric matrix. So, the basis $(\underset{\sim}{e}_a)$ can be treated as the one defining the universal lattice of reference, which allows one to describe an arbitrary lattice in terms of the Euclideam geometry of space R^3.

The proper system ξ_T induces the following group isomorphisms:

$$
\begin{gathered}
T \cong Z^3 \\
R(T) \cong O(Z^3) = O(R^3) \cap GL(Z^3) \\
H(T) \cong SL(Z^3) = SL(R^3) \cap GL(Z^3) \\
G(P, T) \cong Z^3 \,\square\, O(Z^3), \qquad G(H, T) \cong Z^3 \,\square\, SL(Z^3)
\end{gathered} \tag{12}
$$

From the Iwasawa decomposition of the group $SL(R^3)$ [see Appendix, (A3)] it follows that

$$
\begin{gathered}
SL(Z^3) = K(Z^3)\, W(Z^3) \\
K(Z^3) \cap W(Z^3) = \{\underline{I}\}
\end{gathered} \tag{13}
$$

where $\underline{I}$ is the unit matrix, and

$$
\begin{gathered}
K(Z^3) = SO(R^3) \cap SL(Z^3) \\
W(Z^3) = W(R^3) \cap SL(Z^3)
\end{gathered} \tag{14}
$$

and it has been taken into consideration that $D(R^3) \cap SL(Z^3) \subset K(Z^3)$.

Isomorphisms (12) and formulas (9)-(11)) allow us to define the following representation of the point groups $P(T)$ and $H(T)$ in the space $R^3_T(\xi^a)$:

$$
\begin{gathered}
P_g(T) = \underline{S}_T^{-1} O(Z^3) \underline{S}_T \subset O_g(R^3) \\
H_g(T) = \underline{S}_T^{-1} SL(Z^3) \underline{S}_T \subset SL(R^3)
\end{gathered} \tag{15}
$$

From that and from the decomposition (13) it follows that

$$
\begin{gathered}
H_g(T) = SP_g(T)\, W_g(T) \\
W_g(T) = \underline{S}_T^{-1} W(Z^3) \underline{S}_T, \qquad SP_g(T) = P_g(T) \cap SL(Z^3) \\
SP_g(T) \cap W_g(T) = \{\underline{I}\}
\end{gathered} \tag{16}
$$

with [Appendix, (A6)]

$$
\begin{gathered}
\forall \underline{A} \in SP_g(T), \qquad \chi(\underline{A}) = \operatorname{tr} \underline{A} = 1 + 2\cos\theta \in Z \\
-1 \leq \chi(\underline{A}) < 3 \qquad \text{for} \qquad \theta \in (0, 2\pi) \\
\chi(\underline{I}) = 3 \qquad \text{for} \quad \theta = 2\pi
\end{gathered} \tag{17}
$$

and

$$
\forall \underline{A} \in W_g(T), \qquad \chi(\underline{A}) = \operatorname{tr} \underline{A} = 3 \tag{18}
$$

In the next section we will see that the properties (16)-(18) of the point groups of the lattice are strictly connected with the topological classification of discrete linear lattice defects of nontranslational type.

3. DEFECTS OF THE CRYSTAL STRUCTURE

Let us consider a monoatomic crystal whose lattice is a Bravais lattice. In the local theory of the elastic response of such a material body, this response depends only on the actual configuration of atoms in the macroscopically small ("physically infinitesimal") neighborhood of each point of the crystal. In such a neighborhood the deformed lattice can be considered as being homogeneously deformed. This means that locally, the deformed Bravais lattice is also a lattice of such a type. Thus, the description of such a material continuum can be based on the consideration of a continuous distribution of the vector bases.

Let us denote by Λ the set of all Bravais lattices in E. It follows from the isomorphisms (12) that in the algebraic sense, this set has the structure of the quotient space $G^+(R^3)_*/S(Z^3)_*$, where $G^+(R^3)=R^3 \square GL^+(R^3)$, $S(Z^3)=Z^3 \square SL(Z^3)$, and G_* denotes the embedding of $G \subset G(R^3)$ in $GL(R^4)$, described in the Appendix [formulas (A1) and (A2)]. In other words, there exists a one-to-one correspondence (Rogula, 1976)

$$S \in \Lambda \leftrightarrow S_* \in G^+(R^3)_*/S(Z^3)_* \tag{19}$$

The topology in the set Λ can be introduced by the demand that the correspondence (19) should be a homeomorphism. With such a topology, Λ is a path-connected topological manifold (Rogula, 1976). This manifold reflects the deformation-transformation properties of the considered crystalline bodies in the following manner.

Let $\mathfrak{B}$ be a contractible, crystalline, three-dimensional body of the considered type and let

$$\begin{aligned} &\underline{\chi}: \quad \mathfrak{B} \times I \to \mathbf{E}, \quad I=\langle 0, \tau\rangle \\ &\underline{\chi}(P, 0)=\mathbf{OP}, \qquad O \in E \end{aligned} \tag{20}$$

describe the deformation of this body (see Section 4). If the crystal structure of the body in the nondeformed state is described by the field of bases $E_{T_0}=(\mathring{\underline{E}}_a)$ constant on $\mathfrak{B}$ and corresponding to the Bravais lattice S_0, then the field of bases $E_{T(P)}(t)=(\underline{E}_a(P, t)$ of the form

$$\begin{aligned} &\underline{E}_a(P, t)=\underline{F}(P, t)\underline{E}_a \\ &\underline{F}(P, t)=\nabla\underline{\chi}(P, t), \qquad \det\ \underline{F}(P, t)>0 \end{aligned} \tag{21}$$

describes locally certain Bravais lattices $S=S(P, t)$ with base vectors $\underline{E}_a(P, t)$, $a=1,2,3$. So, we can represent the deformation process of the considered body in the form of the deformation process of the crystal structure

$$\dot{\lambda}: \quad \mathfrak{B} \times I \to \Lambda \tag{22}$$

and that

$$\lambda(P, 0) = S_0 \tag{23}$$

The theory of discrete defects of the crystal structure can be formulated analogously to the theory of the irremovable distortions of that structure (Rogula, 1976). Namely, suppose that for the body considered, a certain local crystal structure $S_0 \in \Lambda$ is distinguished. The remaining structures $S \in \Lambda$ can be considered to be *distortions* of S_0, the distinguished structure S_0 being the *undistorted*. Let

$$S: \quad \mathfrak{B} \to \Lambda \tag{24}$$

describe the distorted crystal structure of the body in the form of the distortion field. The question is whether a continuous structure deformation process (22) exists such that

$$\begin{aligned} \lambda(P, 0) &= S_0 \\ \lambda(P, \tau) &= S(P) \end{aligned} \tag{25}$$

In the mathematical formulation, the question is whether the mapping S is null-homotopic. A mapping S that is not null-homotopic describes an *irremovable distortion* of the structure.

If the body $\mathfrak{B}$ is contractible, then each continuous distortion field describes a *removable distortion* of the structure (beacuse Λ is path-connected). This allows us to reduce the topologcal description of the distortion of the considered structure caused by the presence of the defect in the Bravis lattice to the consideration of Λ-space and a body that can itself be contractible but distorted in a discontinuous way. A contractible body from which a single, internal point is removed corresponds to a *point defect* distortion. An unbounded body from which a straight line was removed corresponds to a *line defect* distortion. It turns out (Rogula, 1976) that such a defined point defect does not determine the irremovable distortion of the structure. The linear defect determines the irremovable distortion of the structure. The counterpart to this conclusion, with the topologically different character of distortions caused by the occurrence of linear or point defects, is the following distinction, intuitively accepted in the literature concerning lattice defects (e.g., Kröner, 1960). Namely, the dislocations are defined as internal imperfections of the lattice. But the point defects, in the form of foreign atoms (so called extramatter), must be externally introduced into an ideal crystal or a crystal with dislocations, and that is why they should be called external imperfections of the lattice.

The topological classification of discrete linear defects of a crystal structure can be reduced to the consideration, in the set of matrices

$G^+(R^3)(GL(R^4))$, of the following relation ρ of affine equivalence (Rogula, 1976):

$$A_{1\rho}A_2 \Leftrightarrow \exists B \in G^+(R^3)_0 A_2 = BA_1B^{-1}$$

where A denotes the matrix in the form $(\underset{\sim}{a}, \underset{\sim}{A})$ $_0$Appendix, (A2)]. *Dislocations* (line defects of the translation type) correspond to the class $[\gamma]$ of this relation, where

$$\begin{aligned} \gamma &= (\underset{\sim}{a}, \underset{\sim}{I})^- \qquad \underset{\sim}{o} \neq \underset{\sim}{a} \in Z^3 \\ \operatorname{tr} \gamma &= 1 + \operatorname{tr} \underset{\sim}{I} = 4 \end{aligned} \tag{26}$$

Disclinations (line defects of the rotation type) correspond to the classes $[\gamma(\theta)]$, where [see (17) and Appendix, (A6)]

$$\begin{gathered} \gamma(\theta) = (\underset{\sim}{o}, Q(\theta))^- \qquad \theta \in (0, 2\pi) \\ \operatorname{tr} \gamma(\theta) = 1 + \operatorname{tr} Q(\theta) = 2(1 + \cos\theta) < 4 \\ Q(\theta) \in K(Z^3) \end{gathered} \tag{27}$$

There also exist *linear defects of simple shear type*, which correspond to the class of elements of the form [see (16), (18), and Appendix, (A5)]

$$\begin{gathered} \gamma(m, n, k) = (\underset{\sim}{o}, \underset{\sim}{A}(m, n, k)) \\ A(m, n, k) \in W(Z^3), \qquad m^2 + n^2 + k^2 \neq 0 \\ \operatorname{tr} \gamma(m, n, k) = 1 + \operatorname{tr} \underset{\sim}{A}(m, n, k) = 4 \end{gathered} \tag{28}$$

The element

$$e = (\underset{\sim}{o}, \underset{\sim}{I})^- \qquad \operatorname{tr} e = 4 \tag{29}$$

corresponds to an irremovable distortion, which can be realized in a ring by cutting it in the radial plane and turning one of the cut surfaces by 2π with respect to the other.

The discrete linear defects described by the formulas (26)-(28) are topologically nonequivalent, that is, we cannot reduce a linear defect of one of these types to a linear defect of another type through a continuous deformation of the structure. It follows from (27) that if $\operatorname{tr} \gamma(\theta_1) \neq \operatorname{tr} \gamma(\theta_2)$, then the linear defects of rotation type corresponding to the classes $[\gamma(\theta_1)]$ and $[\gamma(\theta_2)]$ are also topologically nonequivalent.

Usually, in the physically infinitesimal neighborhood of each crystalline body point, there are sufficiently many line (or point) defects to justify the assumption of a macroscopically continuous distribution in the body. In this case, the (macroscopic) continuity of distribution of base vectors of the distorted lattice is preserved, but it remains *nonintegrable*. This signifies the existence of the distribution of lattice groups

$$T = T(P), \qquad P \in \mathfrak{B} \quad (30)$$

determining the field (24) of distortions and such that, if

$$\begin{aligned} E_{T(P)} &= (\underline{E}_a(P)), \qquad P \in \mathfrak{B} \\ \underline{E}_a(P) &= \overset{\circ}{\underline{E}}_b S^b{}_a(P) \end{aligned} \tag{31}$$

where $\overset{\circ}{\underline{E}}_a$, $a = 1, 2, 3$, is a constant on the $\mathfrak{B}$ lattice base vector field corresponding to the undistorted structure S_0, then there does not exist a deformation of the body $\underline{\chi} : \mathfrak{B} \to \underline{E}$ such that

$$\begin{aligned} \forall P \in \mathfrak{B} \qquad \underline{E}_a(P) &= \underline{F}(P)\overset{\circ}{\underline{E}}_a \\ \underline{F}(P) &= \nabla\underline{\chi}(P) \end{aligned} \tag{32}$$

The nonintegrable distribution of the vector bases (31) endows the body $\mathfrak{B}$, as a subdomain of the Euclidean point space E, with an additional geometrical structure. We will take this into account, assuming that the body $\mathfrak{B}$, with the crystal structure distorted in the smooth way, is a three-dimensional and orientable differentiable manifold, which can be mappped diffeomorphically on a certain domain in the Euclidean, three-dimensional point space E. We will assume, in order to simplify the considerations, that this is a simply connected manifold of the C^∞ class. In each of tangent spaces $T_p(\mathfrak{B})$, $P \in \mathfrak{B}$, of that manifold $\mathfrak{B}$, there acts the lattice group $T(P)$ with the basic vectors $\underline{E}_a(P) \in T_p(\mathfrak{B})$, $a = 1, 2, 3$, determining the Bravais lattice $S(P)$ in this tangent space. But we cannot compute the metric parameters of the lattice $S(P)$, because the space $T_P(\mathfrak{B})$ does not possess the metric structure. In this paper we propose the following:

Postulate of Metric Uniformity. For each point $P \in \mathfrak{B}$, the space $T_P(\mathfrak{B})$ considered together with the proper system $\xi_{T(P)}$ of the lattice $S(P)$ has a geometric structure of the proper metric space associated with the proper system ξ_{T0} of an undistorted lattice S_0.

According to the above postulate, a metric space $R^3_{T(P)}(\xi^a)$ is assigned to each point $P \in \mathfrak{B}$, and has the following form [see formulas (3)-(7)]:

$$\begin{aligned} R^3_{T(P)}(\xi^a) &= (T_P(\mathfrak{B}), E_{T(P)}, \underline{g}_{T_0}, V_{T_0}) \\ V_{T_0} &= (\det \underline{g}_{T_0})^{1/2}, \qquad \underline{g}_{T_0} = \| g_{ab} \| \end{aligned} \tag{33}$$

This means defining on $\mathfrak{B}$ a Riemannian metric tensor $\underline{g}(P)$, $P \in \mathfrak{B}$, such that

$$\underline{E}_a(P)\underline{g}(P)\underline{E}_b(P) = g_{ab} = \text{const} \tag{34}$$

i.e., the metric structure of the distorted lattice is represented in the non-Euclidean space $\mathfrak{B}$ by the metric structure of the undistorted lattice S_0. This representation can be interpreted as corresponding to a distortion of the lattice (e.g., by dislocations) that has no influence on the local metric properties of the crystal structure of the body (Kröner, 1985).

The postulate of metric uniformity distinguishes the matrix group $SL(R^3)$ as the group acting in every one of the tangent spaces, and including local symmetries of the material structure described by the considered manifold [see formulas (15) and (16) and the commentary after formula (7)]. In this paper we will make use only of the orthogonal symmetries described by the group $O_g(R^3)$ formulas [(8) and (15)].

If the material structure is subject to an evolution process, then in the formulas (30)-(34) there appears a parameter in the form of time t, e.g.,

$$E_{T(P)}(t) = (\underline{E}_a(P, t)), \qquad P \in \mathfrak{B}, \quad t \in \langle 0, \tau \rangle \tag{35}$$

But since we consider only geometrical problems connected with the distribution of defects, this dependence on t is not essential, Therefore, we omit this parameter in the formulas.

4. DEFORMATION OF THE BODY

From the definition of the body (Section 3), it follows that there is a three-dimensional differentiable manifold $\mathfrak{B}$ such that there exist global diffeomorphisms

$$\kappa: \quad \mathfrak{B} \to E \tag{36}$$

The diffeomorphism (36) as well as the image $\mathfrak{B}_\kappa = \kappa(\mathfrak{B})$ are called the *configuration* of the body. Let κ be a certain distinguished configuration subsequently called a *reference configuartion.* Let us denote by X_κ the coordinate system on $\mathfrak{B}$, defined by

$$\begin{gathered} X_\kappa: \quad \mathfrak{B} \to R^3 \\ X_\kappa(P) = (X_\kappa^A(P)) \Leftrightarrow \mathbf{O\kappa(P)} = X_\kappa^A(P)\underline{\varepsilon}_A \end{gathered} \tag{37}$$

where $O \in E$ is a fixed point and $\underline{\varepsilon}_A$, $A = 1, 2, 3$, is a certain orthonormal base in $\mathbf{E}$:

$$\underline{\varepsilon}_A \cdot \underline{\varepsilon}_B = \delta_{AB} \tag{38}$$

If $\partial/\partial X_\kappa^A$ is the natural base of the coordinate system X_κ on $\mathfrak{B}$, i.e.,

$$\forall f \in C^\infty(\mathfrak{B}) \qquad \left.\frac{\partial}{\partial X_\kappa^A}\right|_P (f) = \frac{\partial(f \circ X_\kappa^{-1})}{\partial X_\kappa^A}(X_\kappa(P)) \tag{39}$$

then we will denote

$$\underset{\sim}{\varepsilon}_A[\kappa, P] = \frac{\partial}{\partial X_\kappa^A}\bigg|_P \tag{40}$$

The fixedness of the reference configuration κ allows us to identify the body $\mathfrak{B}$ with its image $\mathfrak{B}_\kappa$ under the mapping κ, and to identify the base $\underset{\sim}{\varepsilon}_A[\kappa, P]$ with the base $\underset{\sim}{\varepsilon}_A$. Then the moving frame on $\mathfrak{B}$ of the form

$$\underset{\sim}{E}_a(P) = \underset{a}{e}^A(X^B(P))\underset{\sim}{\varepsilon}_A[\kappa, P] \tag{41}$$

can be identified with the moving frame on $\mathfrak{B}_\kappa$ of the form

$$\begin{aligned} &\underset{\sim}{E}_a(X) = \underset{a}{e}^A(X^B)\underset{\sim}{\varepsilon}_A \\ &X \in \mathfrak{B}_\kappa, \mathbf{OX} = X^A\underset{\sim}{\varepsilon}_A \end{aligned} \tag{42}$$

and the tangent space $T_P(\mathfrak{B})$ with the fixed natural base of the form (40) can be identified with the vector space $\mathbf{E}$ with the fixed base (38).

The *deformations* of the body $\mathfrak{B}$ are called diffeomorphisms of the following form:

$$\lambda = \psi \circ \kappa^{-1}: \quad \mathfrak{B}_\kappa \to E$$

where ψ and κ are configurations. The *motion* of the body is called the ordered one-parameter family of configurations $\{\psi_t, t \in I\}$, where $I = \langle 0, \tau \rangle$ is a time interval. It is convenient to choose the configuration $\mathfrak{B}_0 = \psi_0(\mathfrak{B})$ as the reference configuration for the description of the deformation of the body in its motion. Let us denote

$$\begin{aligned} &\lambda_t = \psi_y \circ \psi_0^{-1}: \quad \mathfrak{B}_0 \to E \\ &\chi(X, t) = \lambda_t(X), \qquad X \in \mathfrak{B}_0 \end{aligned} \tag{43}$$

If $\Phi_O: E \to \mathbf{E}$ is a localization of the affinic strcture at the point $O \in E$ (see Appendix), then $\underset{\sim}{\chi}$ will denote the localization of the deformation χ at O defined by

$$\underset{\sim}{\chi}: \quad \mathfrak{F}_0 \times I \to \mathbf{E}, \qquad \mathfrak{F}_0 = \Phi_O(\mathfrak{B}_0) \tag{44}$$

$$\underset{\sim}{\chi}(\mathbf{OX}, t) = \mathbf{O}\boldsymbol{\chi}(\mathbf{X}, \mathbf{t})$$

If $D\underset{\sim}{\chi}_t(X)$, $\underset{\sim}{\chi}_t(X) = \underset{\sim}{\chi}(X, t)$, is the Frechet derivative, then the tensor $\underset{\sim}{F}(\underset{\sim}{X}, t) \in \mathbf{E} \otimes \mathbf{E}^* \cong \mathbf{E} \otimes \mathbf{E}$ such that

$$\forall \underset{\sim}{v} \in \mathbf{E}, \qquad D\underset{\sim}{\chi}_t(X)(\underset{\sim}{v}) = \underset{\sim}{F}(\underset{\sim}{X}, t)\underset{\sim}{v}, \qquad \underset{\sim}{X} \in \mathfrak{F}_0 \tag{45}$$

is called a *deformation gradient* and it is written as

$$\underset{\sim}{F}(\underset{\sim}{X}, t) = \nabla\underset{\sim}{\chi}(\underset{\sim}{X}, t) \tag{46}$$

We will also denote $\underset{\sim}{F}(X, t) = \underset{\sim}{F}(\mathbf{OX}, t)$.

In the coordinate description of the body motion, it is convenient, because of the independence of the motion from the choice of the reference configuration, to consider a second fixed orthonormal frame $x(0) = (0, \underset{\sim}{e}_k)$, different from the frame $X(0) = (0, \underset{\sim}{\varepsilon}_A)$ used in the description of the reference configuration:

$$\underset{\sim}{e}_k \cdot \underset{\sim}{e}_l = \delta_{kl} \tag{47}$$

The space E with the fixed frame $x(0)$ and the space $\mathbf{E}$ with the fixed base $(\underset{\sim}{e}_k)$ can be identified with the space R^3.

The deformation of the body during its motion can, with the already mentioned identification, be described by a vector function of the form

$$\begin{aligned} \underset{\sim}{x} &= \underset{\sim}{\chi}(\underset{\sim}{X}, t) = \chi^k(X^A, t)\underset{\sim}{e}_k \\ \underset{\sim}{x} &= x^k\underset{\sim}{e}_k; \qquad \underset{\sim}{X} = X^A\underset{\sim}{\varepsilon}_A \\ x_k &= \chi^k(X^A, t) \end{aligned} \tag{48}$$

Then the deformation gradient has the following form:

$$\begin{aligned} \underset{\sim}{F}(\underset{\sim}{X}, t) &= F^k{}_A(\underset{\sim}{X}, t)\underset{\sim}{e}_k \otimes \underset{\sim}{\varepsilon}^A \\ F^k{}_A(X, t) &= x^k{}_A(X^B, t) = \partial x^k(X^B, t)/\partial X^A \end{aligned} \tag{49}$$

Let us consider the deformation as the introduction on $\mathbf{E}$, by means of the formulas (48) and (49), of a one-parameter family of global curvilinear coordinate systems. Let us denote

$$\underset{\sim}{x} = x^k(X^A, t)\underset{\sim}{e}_k, \qquad \underset{\sim}{X} = X^A(x^k, t)\underset{\sim}{\varepsilon}_A \tag{50a}$$

$$x^k(X^A(x^l, t), t) = x^k \tag{50b}$$

$$x^k{}_A(X, t) = \frac{\partial x^k(X, t)}{\partial X^A}, \qquad X^A{}_k(x, t) = \frac{\partial X^A(x, t)}{\partial x^k} \tag{50c}$$

$$\underset{\sim}{x}_A = \underset{\sim}{x}_A(X, t) = \partial_A\underset{\sim}{x} = x^k{}_A(X, t)\underset{\sim}{e}_k, \qquad X = (X^A) \tag{50d}$$

$$\underset{\sim}{x}^A = \underset{\sim}{x}^A(x, t) = X^A{}_k(x, t)\underset{\sim}{e}^k, \qquad x = (x^k) \tag{50e}$$

where

$$\begin{aligned} &\underset{\sim}{e}_k \cdot \underset{\sim}{e}^l = \delta^l_k \\ &\underset{\sim}{x}^A(x(X, t), t) \cdot \underset{\sim}{x}_B(X, t) = X^A{}_k(x(X, t), t)x^k{}_B(X, t) = \delta^A_B \end{aligned} \tag{51}$$

The so-called *right Cauchy–Green tensor* is the metric tensor $\underset{\sim}{C}$ defined by

$$\underset{\sim}{C}(\underset{\sim}{X}, t) = \underset{\sim}{F}^t(\underset{\sim}{X}, t)\underset{\sim}{F}(\underset{\sim}{X}, t) \tag{52}$$

where AB denotes the simple contraction of tensors, and $\underset{\sim}{A}^t$ denotes the transposition of $\underset{\sim}{A}$. In the coordinates,

$$\underset{\sim}{C}(\underset{\sim}{X}, t) = C_{AB}(X, t)\underset{\sim}{\varepsilon}^A \otimes \underset{\sim}{\varepsilon}^B \tag{53a}$$

$$C_{AB}(X, t) = \underset{\sim}{x}_A(X, t) \cdot \underset{\sim}{x}_B(X, t) = x^k{}_A(X, t) x^l{}_B(X, t)\delta_{kl} \tag{53b}$$

Let

$$\begin{aligned} \partial_B \underset{\sim}{x}_A(X, t) &= \frac{\partial^2 x^k}{\partial X^B \partial X^A} \frac{\partial X^C}{\partial x^k} \underset{\sim}{x}_C(X, t) \\ &= \Gamma_{BA}{}^C(X, t)\underset{\sim}{x}_C(X, t) \\ \Gamma_{BAC}(X, t) &= C_{CD}(X, t)\Gamma_{BA}{}^D(X, t) \end{aligned} \tag{54}$$

Then (Goedecke, 1974)

$$\begin{aligned} \Gamma_{BAC}(X, t) &= \underset{\sim}{x}_C(X, t) \cdot \partial_B \underset{\sim}{x}_A(X, t) \\ &= \tfrac{1}{2}(\partial_B C_{AC} + \partial_A C_{BC} - \partial_C C_{BA}) \end{aligned} \tag{55}$$

i.e., $\Gamma_{AB}{}^C(X, t)$ is Levi-Civita connection for the right Cauchy-Green tensor. On the other hand, the field of vector bases $(\underset{\sim}{x}_A(X, t))$ determines the teleparallelism connection $\Lambda_{AB}{}^C(X, t)$ of the form

$$\Lambda_{BA}{}^C(X, t) = -X^C{}_k(x(X, t), t)\, \partial_B x^k{}_A(X, t) \tag{56}$$

Here we have

$$\begin{aligned} \Lambda_{BA}{}^C(X, t) &= -\underset{\sim}{x}^C(x(X, t), t) \cdot \partial_B \underset{\sim}{x}_A(X, t) \\ &= -\Gamma_{BA}{}^C(X, t) \end{aligned} \tag{57}$$

so that the condition of the symmetry of the Levi-Civita connection (54) covers with the condition of the vanishing of the torsion tensor of the teleparallelism connection (56):

$$2S_{AB}{}^C = \Lambda_{AB}{}^C - \Lambda_{BA}{}^C = \Gamma_{BA}{}^C - \Gamma_{AB}{}^C = 0 \tag{58}$$

where

$$\begin{gathered} \underset{\sim}{S} = -\underset{\sim}{x}_A \otimes d\underset{\sim}{x}^A = S_{AB}{}^C \underset{\sim}{x}^A \otimes \underset{\sim}{x}^B \otimes \underset{\sim}{x}_C \\ \underset{\sim}{x}_A \cdot \underset{\sim}{x}^B = \delta_A^B \end{gathered} \tag{59}$$

If $(\underset{\sim}{x}_A)$ is any field of vector bases, then the torsion tensor $\underset{\sim}{S}$ vanishes if and only if there exists a curvilinear coordinate system such that fields $\underset{\sim}{x}_A$, $A = 1, 2, 3$, are its natural base vectors [i.e., (50d) holds].

Because

$$\partial_C \, \partial_B \underline{x}_A = \frac{\partial^3 x^k}{\partial X^C \, \partial X^B \, \partial X^A} \underline{e}_k$$
$$= (\partial_C \, \Gamma_{BA}{}^D + \Gamma_{AB}{}^E \Gamma_{CE}{}^D) \underline{x}_D \tag{60}$$

then the tensor $R_{ABC}{}^D$ defined by

$$R_{ABC}{}^D = 2\underline{x}^D \cdot \partial_{[B} \, \partial_{C]} \underline{x}_A \tag{61}$$

covers with the curvature tensor of the Levi-Civita connection $\Gamma_{AB}{}^C$ (Goedecke, 1974)

$$R_{ABC}{}^D = 2\partial_{[B} \Gamma_{C]A}{}^D + 2\Gamma_{A[C}{}^E \Gamma_{B]E}{}^D \tag{62}$$

and vanishes:

$$R_{ABC}{}^D = R_{ABC}{}^D(\underline{C}(X, t)) = 0 \tag{63}$$

Conversely, if $\underline{C}(X, t)$ is a given metric tensor and the condtion (63) is satisfied, then there exists a deformation for which $\underline{C}(X, t)$ is a right Cauchy-Green tensor. Because of this, the condition (63) is called in continuum mechanics the *condition of compatibility* (Fosdick, 1966).

By R_{AB} and E_{AB} we denote the Ricci tensor and the Einstein tensor, respectively:

$$R_{AB} = R_{CAB}{}^C$$
$$E_{AB} = R_{AB} - \tfrac{1}{2} R C_{AB}, \qquad R = C^{AB} R_{AB} \tag{64}$$

and by e_{ABC} and e^{ABC} we denote the basic trivectors related to the metric tensor $\underline{C}$:

$$e_{ABC} = \varepsilon_{ABC} (\det \underline{C})^{1/2}, \qquad e^{ABC} = \varepsilon^{ABC} (\det \underline{C})^{-1/2} \tag{65}$$

where $\varepsilon_{ABC} = \varepsilon^{ABC}$ are alternating symbols. Let us denote

$$R_{ABCD} = C_{DE} R_{ABC}{}^{\mathrm{E}} \qquad E^{AB} = C^{AC} C^{BD} E_{CD} \tag{66}$$

We have the representations

$$E^{AB} = \tfrac{1}{4} e^{ACD} e^{BEF} R_{CDEF}, \qquad R_{ABCD} = e_{ABE} e_{CDF} E^{EF} \tag{67}$$

from which it follows that the condition (63) is equivalent to each of the following two conditions (Fosdick, 1966):

$$R_{AB} = 0 \tag{68}$$

or

$$E_{AB} = 0 \tag{69}$$

So, the deformation induces on the body the one-parameter family of the flat Riemannian metric tensors

$$\underline{C}(P,t)=C_{AB}(X^A(P),t)\,\underline{\varepsilon}^A[\kappa,P]\otimes\underline{\varepsilon}^B[\kappa,P] \tag{70}$$

where $\underline{\varepsilon}^A[\kappa, P]$ is the dual covector to the vector $\underline{\varepsilon}_A[\kappa, P]$ and $C_{AB}(X,t)$ is given by (53b). It is easy to observe that, irrespective of the choice of the reference configuration,

$$\underline{C}_t=\psi_t^*(\underline{\boldsymbol{\delta}}),\qquad \underline{C}_t(P)=\underline{C}(P,t) \tag{71}$$

where $\underline{\boldsymbol{\delta}}$ is the Euclidean metric tensor on $\mathbf{E}$, ψ_t is an actual configuration, and ψ_t^* denotes the "pullback" of tensors by ψ_t (Marsden and Hughes, 1978).

5. DEFORMATION OF THE MATERIAL STRUCTURE

Let us consider a crystalline material body with a continuous distribution of crystal lattice distortions, defined by the postulate of metric uniformity. In this case the "Euclidean picture" [cf. the formulas (37)-(42), (53), and (70)] of the body material structure is determined by the nonintegrable ("anholonomic") distribution of the basic lattice vectors $E_{T(X)}=(\underline{E}_a(X))$, $X\in\mathfrak{B}_0$ of the form

$$\underline{E}_a(X)-\underset{a}{e}^A(X)\underline{\varepsilon}_A,\qquad \underline{\varepsilon}_A\cdot\underline{\varepsilon}_B-\delta_{AB} \tag{72}$$

and by the metric tensor of the form [cf. (34)]

$$\begin{gathered}\underline{g}(X)=g_{AB}(X)\underline{\varepsilon}^A\otimes\underline{\varepsilon}^B=g_{ab}\underline{E}^a(X)\otimes\underline{E}^b(X)\\ g_{AB}=\overset{a}{e}_A(X)\,\overset{b}{e}_B(X)g_{ab}\end{gathered} \tag{73}$$

where $(\underline{E}^a(X), a=1,2,3)$ is the base dual to the base $E_{T(X)}$:

$$\underline{E}^a(X)=\overset{a}{e}_A(X)\underline{\varepsilon}^A,\qquad \underset{a}{e}^A(X)\overset{b}{e}_A(X)=\delta^b_a,\qquad \overset{a}{e}_A(X)\underset{a}{e}^B(X)=\delta^B_A \tag{74}$$

In general, the metric tensor $\underline{g}$ does not satisfy the condition of compatibility (63).

Let $X_0\in\mathfrak{B}_0$ be an arbitrary fixed point. Let us denote

$$\underline{E}_a=\underset{a}{e}^A(X_0)\underline{\varepsilon}_A,\qquad \underset{a}{S}^A=\underset{a}{e}^A(X_0) \tag{75}$$

From (72) and (75) it follows that [cf. (31)]

$$\underline{E}_a(X)=\mathring{\underline{E}}_bS^b{}_a(X),\qquad S^b{}_a(X)=\overset{b}{S}_A\underset{a}{e}^A(X) \tag{76}$$

i.e., the matrix

$$\underset{\sim}{S}_T(X) = \| S^a{}_b(X) \| \tag{77}$$

determines the field of distortions describing *nonintegrable distortion* of the crystal structure. It is the differentially geometric counterpart of the topological irremovability of structure distortions (Section 3).

Let $\underset{\sim}{F}(X, t)$ be a deformation gradient and [cf. (49) and (50)]

$$\begin{aligned} \underset{\sim}{x}_A(X, t) &= \underset{\sim}{F}(X, t)\underset{\sim}{\varepsilon}_A \\ \underset{\sim}{x}_a(X, t) &= \underset{\sim}{F}(X, t)\mathring{\underset{\sim}{E}}_a = S_a{}^A \underset{\sim}{x}_A(X, t) \end{aligned} \tag{78}$$

Then [cf. (53)]

$$\begin{aligned} \underset{\sim}{C}(X, t) &= \mathring{C}_{ab}(X, t)\mathring{\underset{\sim}{E}}^a \otimes \mathring{\underset{\sim}{E}}^b \\ \mathring{C}_{ab}(X, t) &= \underset{\sim}{x}_a(X, t) \cdot \underset{\sim}{x}_b(X, t) = \underset{a}{S}^A \underset{b}{S}^B C_{AB}(X, t) \end{aligned} \tag{79}$$

In plasticity theory so-called *elastic distortion* is considered, which in our case can be defined with the in general nonintegrable, tensor field $\underset{\sim}{A}(X, t) \in \mathbf{E} \otimes \mathbf{E}^* \cong \mathbf{E} \otimes \mathbf{E}$, such that

$$\underset{\sim}{x}_a(X, t) = \underset{\sim}{A}(X, t)\underset{\sim}{E}_a(X, t) \tag{80}$$

where $\underset{\sim}{x}_a(X, t)$, $a = 1, 2, 3$, is a field of deformed base vectors of the ideal reference lattice [equation (78)]. It follows from (72), (75), (78), and (80) that

$$\underset{\sim}{F}(X, t) = \underset{\sim}{A}(X, t)\underset{\sim}{P}(X), \qquad \det \underset{\sim}{F} = \det \underset{\sim}{A} \det \underset{\sim}{P} > 0 \tag{81}$$

where $\underset{\sim}{P}(X)$ (or $\underset{\sim}{P}(X, t)$ if the material structure of the body undergoes an evolution] is the nonintegrable, nonsingular tensor field of the form

$$\underset{\sim}{P}(X) = P^A{}_B(X)\underset{\sim}{\varepsilon}_A \otimes \underset{\sim}{\varepsilon}^B, \qquad P^A{}_B(X) = \underset{a}{e}^A(X)\overset{a}{S}_B \tag{82}$$

Because

$$\underset{\sim}{P}(X) = \underset{\sim}{1} \Leftrightarrow \underset{\sim}{E}_a(X) = \mathring{\underset{\sim}{E}}_a \tag{83}$$

then the field $\underset{\sim}{P}(X)$ can be identified with the so-called *plastic distortion* considered in plasticity theory. So, we have obtained, as is known from plasticity theory, the decomposition (81) of the deformation gradient for elastic and plastic distortions (Sidoroff, 1975).

From (52) and (81) the representation of the right Cauchy–Green tensor follows:

$$\underset{\sim}{C}(\underset{\sim}{F}(X, t)) = \underset{\sim}{P}(X)^t \underset{\sim}{C}(\underset{\sim}{A}(X, t))\underset{\sim}{P}(X) \tag{84}$$

or, equivalently,

$$\underset{\sim}{G}(X,t)=\underset{\sim}{P}(X)^{*}\underset{\sim}{C}(\underset{\sim}{F}(X,t))\underset{\sim}{P}(X)^{t} \tag{85}$$

where $\underset{\sim}{P}^{*}=(\underset{\sim}{P}^{-1})^{t}$, and

$$\underset{\sim}{G}(X,t)=\underset{\sim}{C}(\underset{\sim}{A})(X,t) \tag{86}$$

If

$$\underset{\sim}{A}(X,t)=a^{k}{}_{A}(X,t)\underset{\sim}{e}_{k}\otimes\underset{\sim}{\varepsilon}^{A} \tag{87}$$

then

$$\begin{aligned}\underset{\sim}{G}(X,t)&=G_{AB}(X,t)\underset{\sim}{\varepsilon}^{A}\otimes\underset{\sim}{\varepsilon}^{B}\\ G_{AB}(X,t)&=a^{k}{}_{A}(X,t)a^{l}{}_{B}(X,t)\delta_{kl}\\ &=\overset{a}{e}_{A}(X)\overset{b}{e}_{B}(X)\mathring{C}_{ab}(X,t)\end{aligned} \tag{88}$$

where $\mathring{C}_{ab}(X,t)$ is given by (79). The metric tensor $\underset{\sim}{G}(X,t)$ is invariant with respect to rotations in the configuration space, i.e.,

$$\underset{\sim}{C}(\underset{\sim}{Q}\underset{\sim}{A})=\underset{\sim}{C}(\underset{\sim}{A}),\qquad \underset{\sim}{Q}\underset{\sim}{Q}^{t}=\underset{\sim}{1} \tag{89}$$

and because of this, it is a more convenient measure of the material structure deformation than the elastic distortion. In plasticity theory the so-called *elastic strain tensor* is also considered defined by

$$\underset{\sim}{E}=\tfrac{1}{2}(\underset{\sim}{G}-\underset{\sim}{g}) \tag{90}$$

with the property [cf. (73), (79), and (88)]

$$\underset{\sim}{E}=\underset{\sim}{O}\Leftrightarrow\mathring{C}_{ab}(X,t)=g_{ab} \tag{91}$$

The tensor $\underset{\sim}{S}(X)$ of the form [cf. the formula (59)]

$$\underset{\sim}{S}=-\underset{\sim}{E}_{a}\otimes d\underset{\sim}{E}^{a}=S_{ab}{}^{c}\underset{\sim}{E}^{a}\otimes\underset{\sim}{E}^{b}\otimes\underset{\sim}{E}_{c} \tag{92}$$

can be associated with the distribution $E_{T(X)}$ of the lattice base vectors. This tensor we will call the *torsion tensor of the material structure.* Since

$$d\underset{\sim}{E}^{a}=S_{bc}{}^{a}\underset{\sim}{E}^{b}\wedge\underset{\sim}{E}^{c},\qquad S_{ab}{}^{c}=-S_{ba}{}^{c} \tag{93}$$

therefore, taking into account that $d(\underset{\sim}{E}_{a}\cdot\underset{\sim}{E}^{b})=0$, we obtain [see formula (57)]

$$\omega^{c}_{a}=-\underset{\sim}{E}^{c}\cdot d\underset{\sim}{E}_{a}=-S_{ba}{}^{c}\underset{\sim}{E}^{b} \tag{94}$$

which means that the geometric object $\Gamma=(\Gamma^{c}_{ab})$ defined by

$$\Gamma^{a}_{bc}=-S_{bc}{}^{a} \tag{95}$$

determines, together with the relations (74) and (94), a certain affine connection on the body. This is an affine connection of the form [see (37)-(42)]

$$\begin{aligned} \omega^a(P) &= \Gamma^a_A(X_\kappa(P))\underset{\sim}{\varepsilon}^A[\kappa, P], \qquad \Gamma^a_A = \overset{a}{e}_A \\ \omega^a_b(P) &= \Gamma^a_{bc}(X_\kappa(P))\omega^c(P), \qquad \Gamma^a_{bc} = -S^a_{bc} \end{aligned} \tag{96}$$

The formulas (96) define the infinitesimal "affine displacement," i.e., linear transformation, with components ω^a (translation) and ω^a_b ("affine rotation") generating one space tangent to $\mathfrak{B}$ (considered as an affine tangent space) from another (Bilby, 1968). So, this formula can be accepted as the basis for defining the infinitesimal counterparts of discrete, linear defects of the crystal lattice, discussed in the Section 3. Namely, we will assume that the nonintegrability of the forms ω^a describes the occurrence of line defects of translation-type dislocations in the body, whereas the nonvanishing of the forms ω^a_b describes the occurrence of line defects of the rotation or shear type. But now the lack of dislocations (that is, the integrability of the forms ω^a) also denotes the lack of other line defects [vanishing of forms ω^a_b together with the vanishing of the tensor $\underset{\sim}{S}$; see the commentary after (59)]. We suppose, therefore, that in the infinitesimal version, line defects of nontranslational type are a type of distribution of dislocations rather than a separate kind of line defect. Because the tensor $\underset{\sim}{S}$ is the torsion tensor for the teleparallelism connection determined by the distribution of the bases $E_{T(X)}$ [see formulas (56)-(59) together with accompanying commentary], therefore the above supposition is consistent with the generally accepted connection in the literature between the torsion tensor and the continuous distribution of dislocations in the body (e.g., Kröner, 1960; Bilby, 1968). However, the affine connection of the form (96) [just as the linear connection (95)] has not been considered in the literature. In Part II of this work we show that the appearance of the connection Γ^c_{ab} of the form (95) has a deeper meaning, both physically and geometrically.

6. CONCLUSIONS AND REMARKS

The introduced postulate of metric uniformity means that the material structure of the body is described by a certain teleparallelism and, parallel with respect to it, a Riemannian metric tensor [formulas (72)-(74)]. The affine connection, described in terms of the teleparallelism, but which is not its connection [formula (96)], is the support for the physical interpretation of this geometry as the one describing the distortion of the crystal by the continuous distribution of dislocations [commentary after formula (96)].

The teleparallelism also allows to define the basic measures of deformation used in plasticity theory: plastic distortion determined by the irremovable distortion of the crystal structure, and elastic distortion determined by the elastic (removable) deformation of that structure. The Riemannian metric tensor determines, together with the elastic distortion, another variable used in the theory of plasticity: the elastic strain of the distorted crystal structure. The appearance of the measures of deformation used in plasticity theory allows us to combine the torsion tensor of the material structure [formula (92)] and the considered Riemannian metric tensor with the internal forces acting in the body with the distorted material structure. This can be done in such a way that the second law of thermodynamics is satisfied (Sidoroff, 1975).

Finally, we observe that in continuum mechanics the description of the properties of a solid body by using both teleparallelism and the Riemannian metric tensor appears in the examination of the dependence of stresses on the deformation gradient (Wang and Truesdell, 1973). This dependence described indirectly the properties of the material of the body. In the case of a crystalline solid, such an approach has the imperfection that it introduces a dispensable element in the description of the geometry of the distorted material structure of the body—the notion of stress.

APPENDIX

In this paper we use the following designations;

$\boldsymbol{E}$ is three-dimensional real Euclidean vector space with scalar product designated by $\underline{a} \cdot \underline{b}$.

$GL(\mathbf{E})$ is the group of all nonsingular tensors $\underline{A} \in \mathbf{E} \otimes \mathbf{E}$.

$G(\mathbf{E})$ is the group of all nonsingular affine maps in $\mathbf{E}$, considered as the semidirect product of groups $(\mathbf{E}, +)$ and $GL(\mathbf{E})$, i.e.,

$$G(\mathbf{E}) = \mathbf{E} \,\square\, GL(\mathbf{E})$$

with the group structure in the form

$$(\underline{a}, \underline{A})(\underline{b}, \underline{B}) = (\underline{a} + \underline{A}\underline{b}, \underline{A}\underline{B})$$

$$(\underline{a}, \underline{A})^{-1} = (-\underline{A}^{-1}\underline{a}, \underline{A}^{-1}), \qquad e = (\underline{0}, \underline{1})$$

where $\underline{1}$ is the tensor realizing the identity map and the elements $(\underline{a}, \underline{A})$ act in $\mathbf{E}$ according to the rule

$$(\underline{a}, \underline{A})\underline{x} = \underline{A}\underline{x} + \underline{a}$$

$E(\mathbf{E})$ is the Euclidean group considered as the subgroup of $G(\mathbf{E})$ in the form

$$E(\mathbf{E}) = \mathbf{E} \,\square\, O(\mathbf{E})$$

where $O(\mathbf{E})$ is the orthogonal group on $\mathbf{E}$.

$SL(\mathbf{E}) = \{\underset{\sim}{A} \in GL(\mathbf{E})\colon \det \underset{\sim}{A} = 1\}$ is the group of all nonsingular tensors realizing the linear maps in $\mathbf{E}$ preserving the orientation and the volume (so-called special linear group).

E is the point space on $\mathbf{E}$, i.e., the set E in which the transitive and effective action $T(\mathbf{E})$ of the Abelian group $(\mathbf{E}, +)$ is defined in the form

$$T(\mathbf{E}) = \{\tau_{\underset{\sim}{a}}\colon E \to E,\ \underset{\sim}{a} \in \mathbf{E}\}$$

$$\tau_{\underset{\sim}{a}} \circ \tau_{\underset{\sim}{b}} = \tau_{\underset{\sim}{b}} \circ \tau_{\underset{\sim}{a}} = \tau_{\underset{\sim}{a}+\underset{\sim}{b}}$$

This action allows us to define the affine structure l in E by the rule

$$l\colon \quad E \times E \to \mathbf{E}, \qquad \mathbf{PQ} = l(P, Q)$$

$$\forall P \in E, \qquad l(P, \tau_{\underset{\sim}{a}}(P)) = \underset{\sim}{a}$$

The localization of this affine structure at the point $O \in E$ is the map Φ_O defined as

$$\Phi_O\colon \quad E \to \mathbf{E}, \qquad \Phi_O(P) = \mathbf{OP}$$

The localization Φ_O induces the action Φ in E of the group $G(\mathbf{E})$:

$$\Phi = \{\Phi_{(\underset{\sim}{a}, \underset{\sim}{A})} = \Phi_O^{-1} \circ (\underset{\sim}{a}, \underset{\sim}{A}) \circ \Phi_O : E \to E;\ (\underset{\sim}{a}, \underset{\sim}{A}) \in G(\mathbf{E})\}$$

If $\mathbf{E} = R^3$, then we identify $GL(R^3)$, $O(R^3)$, and $SL(R^3)$ with the groups of real 3×3 matrices respectively nonsingular, orthogonal, and unimodular with positive determinant. In the sense of this identification, the group $G(R^3)$ is isomorphic with the group of matrices $G(R^3)_* \subset GL(R^4)$ of the form

$$(\underset{\sim}{a}, \underset{\sim}{A})_* = \left\| \begin{matrix} \underset{\sim}{A} & \underset{\sim}{a} \\ 0 & 1 \end{matrix} \right\|, \qquad \underset{\sim}{A} \in GL(R^3),\ \underset{\sim}{a} \in \underset{\sim}{R}^3 \tag{A1}$$

so that, in the sense of matrix multiplication

$$\begin{aligned} (\underset{\sim}{a}, \underset{\sim}{A})_*(\underset{\sim}{b}, \underset{\sim}{B})_* &= (\underset{\sim}{a} + \underset{\sim}{A}\underset{\sim}{b}, \underset{\sim}{A}\underset{\sim}{B})_* \\ (\underset{\sim}{a}, \underset{\sim}{A})_*^{-1} &= (-\underset{\sim}{A}^{-1}\underset{\sim}{a}, \underset{\sim}{A}^{-1})_*, \qquad e = (\underset{\sim}{o}, \underset{\sim}{I})_* \\ (\underset{\sim}{b}, \underset{\sim}{B})_*(\underset{\sim}{a}, \underset{\sim}{A})_*(\underset{\sim}{b}, \underset{\sim}{B})_*^{-1} &= (\underset{\sim}{B}\underset{\sim}{a} + (\underset{\sim}{I} - \underset{\sim}{B}\underset{\sim}{A}\underset{\sim}{B}^{-1})\underset{\sim}{b}, \underset{\sim}{B}\underset{\sim}{A}\underset{\sim}{B}^{-1})_* \end{aligned} \tag{A2}$$

where $\underset{\sim}{I}$ is the identity matrix.

The *Iwasawa decomposition* of the group $SL(R^3)$ is its decomposition in the form (Barut and Rączka, 1977)

$$SL(R^3) = K(R^3) D(R^3) W(R^3) \tag{A3}$$

where $K(R^3) = SO(R^3)$, the group of proper orthogonal matrices [maximal compact subgroup of $SL(R^3)$], $D(R^3)$ is the diagonal matrix group [Abelian subgroup of $SL(R^3)$]:

$$D(R^3) = \{\underline{A} = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)\colon\ \lambda_1\lambda_2\lambda_3 = 1,\ \lambda_a \in R\} \tag{A4}$$

The group $D(R^3)$ describes the extensions in three perpendicular directions (preserving the volume). $W(R^3)$ is the nilpotent group called the Weyl group, consisting of matrices of the form

$$W(R^3) = \left\{ A = \underline{A}(\alpha, \beta, \gamma) = \left\| \begin{matrix} 1 & \alpha & \alpha \\ 0 & 1 & \gamma \\ 0 & 0 & 1 \end{matrix} \right\|,\ \alpha, \beta, \gamma \in R \right\} \tag{A5}$$

Weyl group matrices describe so-called simple shear, that is, the deformation changing a cube into a parallelepiped.

The designation of a rotation in R^3 by $Q(\theta)$ menas that the matrix of this rotation can be represented, in a suitably chosen Cartesian coordinate system, in the form

$$Q(\theta) = \left\| \begin{matrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{matrix} \right\|, \qquad 0 \le \theta \le 2\pi \tag{A6}$$

Lorentz transformation in R_1^3 [i.e., with the signature metric $(-++)$] can, modulo rotations around the "time" axis, be represented by a matrix of the form

$$\underline{L} = \| L^a{}_b \| = \left\| \begin{matrix} \gamma & \beta\gamma & 0 \\ \beta\gamma & \gamma & 0 \\ 0 & 0 & 1 \end{matrix} \right\|, \qquad \gamma = (1-\beta^2)^{-1/2}, \qquad |\beta| < 1 \tag{A.7}$$

In this representation, the matrix $\underline{L}$ describes a transformation on the hyperbolic plane (x^1, x^2) of the form

$$\begin{aligned} x'^1 &= \gamma(\beta x^2 + x^1) \\ x'^2 &= \gamma(x^2 + \beta x^1) \\ x'^3 &= x^3 \end{aligned} \tag{A8}$$

The formulas (A8) considered as the transformation on the Cartesian plane $x^3 = \text{const}$ describe the deformation called pure shear, i.e., the deformation changing a square into a rhomb, with the value of this shear $\beta = \operatorname{tg}\alpha$,

$|\alpha| < \pi/4$ (α is the shear angle). Conversely, the equations defining the pure shear on this plane (Żórawski, 1965)

$$\begin{gathered} L^1{}_1 = L^2{}_2 = \gamma \\ L^2{}_1 \colon L^1{}_1 = L^1{}_2 \colon L^2{}_2 = \beta \\ L^1{}_1 L^2{}_2 - L^1{}_2 L^2{}_1 = 1 \end{gathered} \tag{A9}$$

have a solution if and only if $\beta^2 < 1$. From (A9) it follows, then, that γ has the form in (A7) and the inequality $\gamma \geq 1$ resulting from it means the existence of the extension along the axes x^1 and x^2; $\beta = \operatorname{tg} \alpha$ means the rotation of the material fibres (initially parallel to the axis x^1 or x^2) by the angle α.

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