Topological Gauge Theory Of General Weitzenböck Manifolds Of Dislocations In Crystals

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Abstract

General Weitzenböck material manifolds of dislocations in crystals are proposed, the reference, idealized and deformation states of the bodies in general case are unifiedly described by the general manifolds, the topological gauge field theory of dislocations is given in general case, true distributions and evolution of dislocations in crystals are given by the formulas describing dislocations in terms of the general manifolds, furthermore, their properties are discussed.

1. Introduction

Practical crystals always contain a lot of dislocations and are filled with them, the defects strongly affect the properties of the crystals. Some pioneers even in the fifties had researched the relations between the defect crystals and differential geometry. K. Kondo used torsion of material manifolds to study dislocations\textsuperscript{1}, and Nye\textsuperscript{2}, Bilby\textsuperscript{3}, Kröner\textsuperscript{4} etc studied the relations between the defects and torsion.

On the other hand, these defects are found having the features of elementary particles, and Kröner studied continuum theory of defects\textsuperscript{5}. Due to the great success of Yang-Mills gauge field theory describing the interactions of elementary particles\textsuperscript{6}, according to the research of gauge theory of gravitation, it can be discovered that geometry of Riemannian manifold essentially belongs to a kind of non-Abelian gauge theory\textsuperscript{7}. Gauge theory and topological properties of dislocations were researched, and many important conclusions in the fields were obtained by Toulous and Kleman\textsuperscript{8}, Kleinert\textsuperscript{9},
Trebin\textsuperscript{10} and so on. Duan and his associates showed a unified approach to the study of defect mechanics and their topological and geometric properties by applying vielbein field theory and gauge field theory to dislocation and disclination continuum\textsuperscript{11,12}.

Sect.2 of the paper constructs the general Weitzenböck manifolds of dislocations in crystals, gives a unified description of these reference, idealized and deformation states; Sect.3 unifiedly studies topological gauge theory of dislocations, gives the formulas describing dislocations, their properties are discussed; Sect.4 gives the discussions of overcoming the default; the last Sect. is summary.

2.General Weitzenböck Material Manifolds of Dislocations

The Weitzenböck manifold\textsuperscript{7} is the one whose $\nabla_i g_{jk} = 0$, $T^i_{jk} \neq 0$, $R^i_{jkl} = 0$, where $g_{ij}$, $T^i_{jk}$ and $R^i_{jkl}$ are, respectively, metric, torsion and curvature tensors of the manifold, when $T^i_{jk} = 0$, the manifold is reduced into Euclidean manifold. Since properties of dislocations correspond to properties of torsion tensor of a manifold\textsuperscript{1-4}, when considering dislocations, the corresponding manifold is thus taken as the Weitzenbock manifold. And the torsion tensor and metric tensor $g_{ij}$ of a manifold are all defined locally on the manifold\textsuperscript{13}, then we may naturally expect that the torsion tensor possesses different values, even zero, on different parts of the manifold, we call the manifold as the general Weitzenbock manifold, the corresponding different parts are just the corresponding submanifolds in the material manifold. In fact, the situations above just correspond to disappearance and appearance of dislocations for zero and non-zero of torsion tensor of the corresponding submanifold respectively. Therefore, we can use the above discussions to represent the complex situations of motion, disappearance and appearance of the dislocations.

Now we construct the general Weitzenböck material manifolds, relative to time parameter $t$, of dislocations in crystals.

It is well known that Weitzenbock manifold is an ensemble of lots of small coordinate pieces homeomorphic to some local Euclidean spaces, lying, however, to a certain degree amorphously, and the characters of the ensemble of lots of the small pieces can be described by means of affine connections of the small pieces. And the geometric properties of dislocations homeomorphically correspond to the geometric properties of torsions of the corresponding material manifold.

Owing to the periodic regular distributions of the lattice particles of per-
fect crystal, the position coordinate $x^a$ of lattice particles can be globally determined in Euclidean space in terms of their periodic rules, then we regard their corresponding material manifold as Euclidean manifold. Obviously, when dislocations appear, which means that we can not globally do the same in terms of their periodic rules, however, we can build up a lot of local coordinate systems in which the position coordinate $x^a$ of any particles in the crystal can be locally defined.

In general, for a crystal with dislocations in 3-dimensional Euclidean space, we assume that the body is made of N lattice particles, for any lattice particle $P_{ia}$, we can always construct local coordinate system $L_{ia}$ in local Euclidean space and presume that there are k lattice particles $P_{i1}, P_{i2}, \ldots, P_{ik}$ which are close adjacent to $P_{io}$, and the corresponding nonholonomic normalized frame fields are $e^a(a = 1, 2, 3)$, then the distance vector of any two close adjacent particles is

$$dr = e^a dx^a$$

(1)

the metric tensor is

$$\eta^{ab} = e^a \cdot e^b = \delta^{ab}$$

(2)

and the square of the distance, i.e., the square of the line element is

$$ds^2 = dr \cdot dr = \eta^{ab} dx^a dx^b = dx^a dx^a$$

(3)

where $dx^a$ is the corresponding nonholonomic coordinate difference.

Furthermore, for any particle $P_{il}(l \neq 0)$ discussed above, we can again construct a local coordinate system, and regard any such $P_{il}$ as a new $P'_{io}$, do further the same as the above discussions about the $P_{il}, \ldots$, up to all particles in the body.

For a open subset $V_\alpha \subset R^3$ of any local coordinate system discussed above, assume that there is an inverse homeomorphic map $\varphi^{-1}_\alpha : V_\alpha \rightarrow M_\alpha$ (where $M_\alpha$ is a family of open sets ) and $\bigcup V_\alpha = V_m$ ($V_m$ is the volume of the crystal in Euclidean space ) such that $\bigcup \alpha M_\alpha = M$ is topological space, which means that M is provided with family of pairs $\{(M_\alpha, \varphi_\alpha)\}$. Further assume that given $M_\alpha$ and $M_\beta(\alpha \neq \beta)$ ($M_\alpha \cap M_\beta \neq \phi$ ) the map $\varphi_\beta \circ \varphi^{-1}_\alpha$ from the subset $\varphi_\alpha(M_\alpha \cap M_\beta)$ of $R^3$ to the subset $\varphi_\beta(M_\alpha \cap M_\beta)$ of $R^3$ is infinitely differentiable. Consequently, the aggregation of the all coordinate pieces forms a general three dimensional differentiable material manifold\(^{13}\). Because the
general manifold inherits the topological and geometric properties of the dislocations in the body, and these properties correspond to properties of torsion of the manifold and can just be expressed by the torsion tensor of the manifold, therefore, there always exists the inverse map \( \varphi^{-1}_\alpha \) such that \( M \) is the manifold that the properties of the dislocations of the crystal may be represented by means of the torsion tensors of the manifold. Because the torsion of the general manifold may have different values on different parts of the manifold, the different parts may correspond to Euclidean and Weitzenböck material submanifolds of the general material manifold. Evidently, the local Euclidean and Weitzenböck material submanifolds can be locally included in the general Weitzenböck material manifold, which just corresponds to the real distribution situations of dislocations of the body.

The relationship\(^{15,16}\) between the normalized nonholonomic and holonomic frames is

\[
e^a = e^a_i e^i, \, a, \, i = 1, 2, 3
\]

where \( e^i = dx^i \) is holonomic coframe of the manifold and \( e^a_i \) is the vielbein, then we have metric tensor of the manifold \( M \)

\[
g_{ij} = e^a_i e^a_j
\]

Using the vielbein theory\(^7,14−16\) we can have

\[
dx^a = e^a_i dx^i
\]

Substituting (6) into (3) and using (5), we have

\[
ds^2 = dx^a dx^a = e^a_i dx^i e^a_j dx^j = g_{ij} dx^i dx^j
\]

which means that the square of the line element of a local Euclidean system in the crystal is equal to that of the line element of the general material manifold. Using the above discussions, furthermore, we can study their stress and so on. Therefore, the above discussions is essential for our further study.

If we take time \( t_0 \) to label the reference state of time \( t_0 \), when the body is experienced a deformation during time \( \Delta t = t - t_0 \) the corresponding deformed state is labelled by time \( t = t_0 + \Delta t \), in other words, at different time \( t \), the lattice particles possess different distributions by which the creating and moving of the dislocations with time \( t \) are represented, the general material manifold with time parameter \( t \) is thus obtained.
In elastic and plastic mechanics, the reference, idealized and deformation states are chosen. We now give a unified description of the states by means of the general manifold. The reference state is usually chosen as perfect or idealized states of an ordered material. By the discussions above of translating the discretum of a perfect crystal into the continuum, we obtain a Euclidean material manifold corresponding to the global vanishing torsion of the manifold. Usually the idealized state of the body is defined as an aggregation of lots of small pieces of the idealized material. In fact, the small pieces of the idealized material can always be viewed as having some ordered distributions of lattice particles, and our discussions about the piece distributions of the particles are general, i.e., our discussions are general, then the idealized state of the body is included in the states of the general Weitzeneböck material manifold M. For elastic and plastic deformation states, they can be represented in microscope as the changes of the displacement and interaction of any adjacent lattice particles. Analogous to the above discussions, evidently the elastic and plastic deformation states are included in the general state of the general manifold M, especially plastic deformation has cooperative motions of the many defects and lattice particles. Now we generally consider reference state (or called standard state) and deformation state of M, the line elements of their manifolds are generally defined, respectively, as

\[ ds^2_t = ds^2_{t_0} = g_{ij}(x(t_0), t_0)dx^i(t_0)dx^j(t_0) \]  
\[ ds^2_\eta = ds^2_\eta = g_{ij}(x(t), t)dx^i(t)dx^j(t) \]  
\[ ds^2_\eta = \eta^{ab}e^a_i(x(t), t)e^b_j(x(t), t)dx^i(t)dx^j(t) \]  

Similar to Ref.[11], the strain tensor is defined as

\[ E_{ij} = E_{ij}(x(t), x(t_0), t, t_0) = \frac{1}{2}[g_{ij}(x(t), t) - g_{ij}(x(t_0), t_0)] \]  

The general reference and deformation states and the strain tensor at any time t are useful for practical calculation, and it is convenient for acquiring different properties of a crystal, in fact, one usually compares reference states
with deformation states under different conditions and studies the evolution laws of the deformation states with time $t$.

It is important and useful to describe these different states in general case, we overcomes the difficulty of self-consistence that generally describes these different states in terms of differential geometry, give true distributions and evolution of dislocations with variances of time in the crystals by means of the differential manifolds, and may give useful tool of describing the defects.

3. Topological Gauge Field Theory Of Dislocations

We now discuss the topological gauge field theory of the defects. In physics, any physical law doesn’t depend on the choices of coordinates. For example, the square of the line element and Lagrangian of the system, there exist two kinds of indices $i$ and $a$ ($i, a = 1, 2, 3$) which is holonomic and nonholonomic indices respectively. For holonomic indices $i$, the coordinate transformations at a certain time $t$, i.e., at a certain state, are

$$x'^i(t) = x'^i\{x^j(t)\}$$

and

$$x^i(t) = x^i\{x'j(t)\}$$

The transformation of the nonholonomic indices is the local $SO(3)$ gauge transformation

$$dx'^a(t) = S^{ab}(t)dx^b(t)$$

where

$$\eta'^{ab} = \eta^{cd}S^{ac}S^{bd}$$

Using Eqs.(14), (15) and the discussions above, it is easy to prove that Eqs.(8-10) are all invariant under the two kinds of coordinate transformations.

In order to achieve the invariance of physical laws under the two kinds of coordinate transformations, the usual partial derivative should be substituted into two kinds of covariant derivatives as follows

$$\nabla_i e^a_j = \partial_i e^a_j - \Gamma^k_{ij} e^a_k$$

and

$$D_i e^a_j = \partial_i e^a_j - \omega^a_{ib} e^b_j$$
where $\Gamma^k_{ij}$ and $\omega^a_{i}$ are affine connection and $SO(3)$ gauge potential (spin connection). Eqs.(16) and (17) satisfy the general and gauge covariant principles respectively, but the total Lagrangian of the system is invariant under the both transformations$^{16}$.

Using the vielbein theory$^{11,12,16}$ we have the torsion tensor of the general manifold as follows:

$$T^k_{ij} = \Gamma^k_{ij} - \Gamma^k_{ji} = \epsilon^{ka} (D_i \epsilon^a_j - D_j \epsilon^a_i) = \epsilon^{ka} T^a_{ij}$$

(18)

where $T^a_{ij}$ is the torsion tensor with nonholonomic superscript $a$

$$T^a_{ij} = D_i \epsilon^a_j - D_j \epsilon^a_i$$

(19)

Analogous to Ref.$^{[12,17]}$, we may define the general tensor densities of dislocations of the body at any time $t$ in the following

$$\alpha^{ia}(x(t), t) = \frac{\varepsilon^{ilm}}{2 \sqrt{g(x(t), t)}} T^a_{lm}(x(t), t)$$

(20)

where $g = \text{det}(g_{ij})$, $\varepsilon^{123} = -\varepsilon^{132} = 1$, the coefficient $\frac{1}{2}$ is due to the tensor sums of subscripts $l$ and $m$. Then Burgers vector of dislocation can be defined as follows

$$b^a = \int_{\Sigma} \alpha^{ia}(x(t), t) \sqrt{g(x(t), t)} d\sigma_i$$

(21)

where $\Sigma$ is the surface including dislocations. The formulas (20) and (21) and $x(t)$ are all the functions of the time $t$ that labels the motions of the defects and deformations of a crystal, which includes the creations, motions and disappearances of the dislocations with evolution of time $t$ in the general manifold, therefore, these variances can be represented by Burgers vector, or the tensor density of dislocations, these variances correspond to the variances that Eq.(20) and Eq.(21) are equal to different values at different time and position. Then it is given that true distributions and evolution of dislocations in the crystals by the formulas describing dislocations at any time $t$ in the general manifold, and our theory is non-linear. Using gauge potential decompositions Duan and Zhang$^{12}$ gave the moving, geometric and topological descriptions of dislocations in terms of similar to Eqs. (20) and (21). Since the general Weitzenbock manifold is very general, then the corresponding
further discussions of (20) and (21) are similar to those in Ref.[12], therefore, one can arrive in their all results of topology, geometry and kinematics of the defects, thus we shall not repeat here.

The discussions about elastic and plastic dynamics and the generalization to a four dimensional general pseudo-Weitzenbock material manifold that concerns dissipative parts belonging to the fourth component of the vielbein fields will be written in a separated paper.

4. Summary
This paper proposes general Weitzenböck material manifolds, relative to time parameter $t$, of dislocations in crystals, in the manifolds the local Euclidean and Weitzenböck manifolds can be viewed as the submanifolds of the general Weitzenböck material manifold, furthermore, by analyzing the microscope structures and change, with time $t$, of the general manifolds, we obtain the unified description of reference, idealized and deformation states in terms of the general manifolds, and the general manifold with evolution of time parameter $t$ just represents the motions and the distributions of dislocations, and the topological gauge theory are acquired by leaving the physical laws invariant under the coordinate transformations. We overcome the difficulty of self-consistence that generally describes these different states in terms of differential geometry, give true distributions and evolution of dislocations in the crystals by the formulas describing dislocations to any time in general manifold, and their properties are discussed.

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