Orowan's Formula, Differential Geometry and Four-dimensional Material Space

Kazuhito Yamasaki

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Department of Earth and Planetary Sciences, Faculty of Science, Kobe University, Kobe, 657–8501, Japan

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Introduction

In this paper, we explain the differential geometry description of continuum mechanics paid attention by theoretical geosciences in recent years (e.g., Yamashita and Teisseyre, 1994 ; Teisseyre, 1995 ; Takeo and Ito, 1997 ; Yamasaki and Nagahama, 1999 a ; Nagahama and Teisseyre, 2001). To explain the theory concisely, we do not expand the general frame of the theory. Instead, we take up the concrete phenomenon described by the well-known equation such as the rheology of rocks described by Orowan's formula :

$$\dot{\varepsilon} = \rho b v$$

(1)

where ε is strain, ρ is scalar density of dislocations, b is Burgers vector and v is velocity of dislocations. The purpose of this paper is to derive Orowan's formula from a viewpoint of the differential geometry.

Differential geometry description of defect field

One of the most famous correspondences between continuum mechanics and differential geometry is the definition of strain that is given by the difference of metric tensors : $\varepsilon_{ij} = (\delta_{ij} - g_{ij})/2$. It has been a center problem in differential geometry analysis of continuum mechanics to extend this correspondence even to the defect field. In this section, we explain concisely this result by considering the virtual circuit in crystal lattice.

Consider the closed curve: $A \rightarrow B \rightarrow C \rightarrow D \rightarrow A$, where A = A(u), B = A(u+du), $C = A(u+du+\delta u+\delta du)$, $D = A(u+\delta u)$ and $d\delta u = \delta du$ (Fig. 1(a)). We map point A to the Euclid tangent plane in point C along the curve : $A \rightarrow B \rightarrow C$ as follows

$$\underbrace{A + dA}_{A \rightarrow B} + \underbrace{\delta(A + dA)}_{B \rightarrow C}.$$

Next, we map point A to the Euclid tangent plane in point C along the curve $: A \rightarrow D \rightarrow C$ as follows

$$\underbrace{A + \delta A}_{A \to D} + \underbrace{d(A + \delta A)}_{D \to C}.$$

Therefore, when we map point A to the Euclid tangent plane in point A again along the closed curve : $A \rightarrow B \rightarrow C \rightarrow D \rightarrow A$, we obtain (Fig. 1 (b))

$$\underbrace{A + dA + \delta(A + dA)}_{A \to B \to C} \underbrace{-(A + \delta A + d(A + \delta A))}_{C \to D \to A}$$
$$= \delta dA - d\delta A = \varDelta A. \tag{2}$$

Now, when the base vector is set to be A_i , we obtain $dA = A_i du^i$. Because dA_i is also vector and $dA_i \rightarrow 0$ for $du^i \rightarrow 0$, it can be expand by using base vectors as follows : $dA_j = \Gamma^{i}{}_{jk} du^k A_i$, where $\Gamma^{i}{}_{jk}$ is affine connection. In this case, (2) becomes $\Delta A = \delta dA - d\delta A = \delta (A_i du^i) - d(A_i \delta u^i)$

 $= (\delta du^{i} + \Gamma^{i}{}_{jk} du^{j} \delta u^{k}) A_{i} - (d\delta u^{i} + \Gamma^{i}{}_{jk} \delta u^{j} du^{k}) A_{i}$ $= (\Gamma^{i}{}_{jk} - \Gamma^{i}{}_{kj}) du^{j} \delta u^{k} A_{i}.$

Because $\Gamma^{i}_{jk} = \Gamma^{i}_{kj}$ in Euclid space (or Riemann space), the discrepancy, ΔA , is zero. On the other hand, in the space with torsion, we have $\Gamma^{i}_{jk} - \Gamma^{i}_{kj} = 2\Gamma^{i}_{(jk)} = 2S^{i}_{jk} \neq 0$, where S^{i}_{jk} is called torsion tensor. Therefore, the discrepancy is expressed as

$$\Delta A = S^{i}_{\ ik} \varepsilon^{mjk} d\Sigma_{m} A_{i} \tag{3}$$

where $d \Sigma_m (=\varepsilon_{mjk} du^j \delta u^k/2)$ is infinitesimal area enclosed with closed curve. $\varepsilon^{\kappa\mu\nu}$ is Levi-Civita tensor. We have $\varepsilon^{\kappa\mu\nu}=0$ whenever two of the indicies coincide, and otherwise is given by $\varepsilon^{\kappa\mu\nu}$ $=\pm 1$ if sgn $(\kappa, \mu, \nu)=\pm 1$. For instance, $\varepsilon^{112}=0$, ε^{123} =1 and $\varepsilon^{132}=-1$. The discrepancy vector in the direction of *l* is given by

$$\Delta A = S^l_{jk} \varepsilon^{mjk} d\Sigma_m. \tag{4}$$

In crystal lattice, we can obtain similar discrepancy called Burgers vector. The curve that closes in a perfect lattice (Fig. 1 (c)) does not close in the lattice where the dislocation exists (Fig. 1 (d)). (When strictly saying, the discrepancy is defined by the naturalization in which non-Euclid material space with dislocations is mapped to Euclid material space without dislocations (Fig. 2).) This discrepancy increases in proportion to the dislocation density and the area enclosed with the curve. Therefore, Burgers vector, b^l , is given by the product of dislocation density tensor, α^{ml} , and infinitesimal area



Fig. 1 (a) Consider the closed curve ABCDA in the space with torsion. The area enclosed with this closed curve is infinitesimal enough, and we set AB=CD=d and BC=DA $=\delta$. (b) When this closed curve is mapped to the Euclid space, it does not close as shown in this figure. This is a result of the path dependency in the space with torsion, that is, the mapping result is different according to whether the path ABC passes or the path ADC passes even if the destination is the same point C. (c) In the perfect crystal where the dislocation does not exist, the closed curve can be drawn in an arbitrary region. (d) When the dislocation exists, there is a region where the closed curve cannot be drawn. This quantity of the discrepancy is called a Burgers vector.

enclosed with the curve, $d\sigma_m$:

$$b^l = \alpha^{ml} d\sigma_m.$$
 (5)

First and the second index of α^{ml} is the direction of dislocation line and Burgers vector, respectively. Therefore, if l=m, α^{ml} is a screw dislocation density, and if $l \neq m$, α^{ml} , is an edge dislocation density. From the comparison between (4) and (5), we can obtain the relations such as $\Delta A^{l} \Leftrightarrow b^{l}$, $S^{l}_{jk} \varepsilon^{mjk} \Leftrightarrow \alpha^{ml}$ and $d\Sigma_{m} \Leftrightarrow d\sigma_{m}$. In a word, the dislocation density is expressed geometrical by the torsion of the material space.

Geometrical description of dislocation density was derived by the mapping of the point. Next, we consider the mapping of the vector (Fig. 3(a)) in order to derive the geometrical description of disclination density. Here, a disclination is a generic name of rotating defects (a dislocations is a generic name of translational defects.). By the similar procedure to derive (3), we have

$$\begin{split} & \varDelta A_{j} = \delta dA_{j} - d\delta A_{j} = R^{i}{}_{jkh} du^{k} \delta u^{h} A_{i} \qquad (6) \\ & \text{where } R^{i}{}_{jkh} \left(= \partial_{h} \Gamma^{i}{}_{jk} - \partial_{k} \Gamma^{i}{}_{jh} + \Gamma^{l}{}_{jk} \Gamma^{i}{}_{lh} - \Gamma^{l}{}_{jh} \Gamma^{i}{}_{lk} \right) \\ & \text{is curvature tensor (Fig. 3 (b)). In crystal lattice,} \\ & \text{we can obtain similar discrepancy of vector} \\ & \text{called Frank vector. In the parallel shift in the} \\ & \text{perfect crystal, the direction of the vector turns} \\ & \text{to the same direction in the starting point and} \end{split}$$



Fig. 2 Consider the material space with a dislocation. First, take out the element that is small enough to be free from the dislocation. Second, the element is transformed elasticity to the eigenstrain-free state by cutting off from the surrounding and releasing it from the constraints of the surrounding. Finally, we reconstruct the material space by using these eigenstrain-free elements. This virtual process is called naturalization. Geometrically, this process is equivalent to the mapping of the non-Euclid space with torsion into the Euclid space. Burgers vector is defined as the discrepancy due to the naturalization.

the terminal (Fig. 3(c)). On the other hand, it is not for the same direction when the disclination exists (Fig. 3(d)). This discrepancy of the vector direction is called Frank vector. This discrepancy is proportional to the disclination density and the area of the closed surface as well as the Burger vector. In addition, it is also proportional to the size of the vector. Then, we have

 $f_j = \theta_j^{im} A_i d\Sigma_m$ (7) where f_j is Frank vector, θ_j^{im} is disclination density. From the comparison between (6) and (7), we have $\varepsilon^{mkh} R^i_{jkh} \leftrightarrow \theta_j^{im}$, that is, the disclination density is expressed geometrical by the curvature of the material space. In the ordinal analysis, the degenerated disclination density, $\varepsilon_{iml} \theta_j^{im}$ $= \theta_{il}$, is used.

Neither the dislocation density nor the disclination density are independent as known in the analysis of the liquid crystal. Next, we consider what kind of form the relation should be. The point of the above-mentioned analysis was to have expressed the physical quantities such as dislocations and disclinations by the geometrical quantity such as torsion and curvature of the material space. The curvature and the gradient of the torsion are in not independence but the following relations :

$$R^{a}_{[bcd]} = \partial_{[b} S^{a}_{cd]} \tag{8}$$

where we ignore the higher order terms of the affine connection. (8) is called the first Bianchi identity that is one of the basic relation in the differential geometry. The substitution of S^{a}_{cd} $\varepsilon^{bcd} = \alpha^{ba}$ and $\varepsilon^{bcd} R^{a}_{bcd} = \theta_{b}^{ab}$ into (8) leads to $\theta_{b}^{ab} = \partial_{b} \alpha^{ba}$. (9)

This means that the divergence of dislocations



Fig. 3 (a) Consider the parallel shift of the vector along the closed curve in the space with curvature. (b) When this closed curve is mapped to the Euclid space, the parallel shift of the vector is accompanied by the discrepancy in the terminal point. (c) In the parallel shift of the perfect crystal where the disclination does not exist, the direction of vector turns to the same. (d) When the disclination exists, the direction is not the same. This discrepancy of the vector direction is called a Frank vector.

is accompanied by disclinations. Disclinations does not exist in the ordinal material, so we have the well-known preservation law of the dislocation : $\partial_b \alpha^{ba} = 0$. Note that (9) is only the physical expression of the basic relation in differential geometry (8).

Orowan's formula and Cartan's structure equation in Four-dimensional material space

The first Bianchi identity (8) can be derived by the Cartan's structure equation. Abstract expression of this equation is

(torsion tensor) = (differential operator) (metric).

Because the torsion and the metric corresponds to dislocation density and strain, this becomes $\alpha^{ij} = \epsilon^{ikl} \partial_k \beta_l^{\ i}$. (10)

For detailed proof, refer to Yamasaki and Nagahama (1999 b) etc. (10) mean that the dislocation density is given by the rotation of the strain. If the distortion is integrable, it is given by the gradient of the displacement, then we have $\alpha^{ij} = \varepsilon^{ikl} \partial_k \partial_l u^i = 0$, that is, the dislocation density vanishes. In other words, the dislocation density is given by the non-integral term (non-holonomy term) of the strain. In the same way, the disclination density is given by the non-holonomy term of the bend-twist that is the gradient of rotational displacement. (In Taylor-Bishop-Hill model, all the non-holonomic terms vanish.)

Because (10) is the basic equation in describing dislocation field, it plays an important role in condensed matter physics (e.g., Edelen and Lagoudas, 1988; Kleinert, 1989), seismology (e.g., Yamashita and Teisseyre, 1994; Takeo and Ito, 1997) and geodesy (e.g., Yamasaki and Nagahama, 1999a). However, (10) does not include the effect of time, so we cannot derive the evolutional equation such as Orowan's formula (1). Then, in this section, we try to add time base to the coordinate system where the dislocation field is described. As known by special theory of relativity, if the velocity of light is multiplied by time base, it becomes the dimension of the space, so the spacetime can be described as the fourmanifold. Similarly, by multiplying the velocity of elastic wave by time base in the material space, the four-dimensional description of deformation field becomes possible. In the dislocation field, the dislocation current corresponds to the velocity, so we have

$$D^i = I^i \wedge dT + \alpha^i \tag{11}$$

where D_i is the four-dimensional dislocation 2 -form, $I^i(=I^i{}_A dx^A)$ is the dislocation current 1 -form, $\alpha^i(=\alpha^i{}_A dS^A)$ is the dislocation density 2 -form and \wedge is the wedge product. In this paper, we do not go deep into the explanation of the differential formalism. For detailed proof, refer to Edelen and Lagoudas (1988). In the same way, we can define the four-dimensional distortion (strain):

$$B^i = \nu^i \wedge dT + \beta^i \tag{12}$$

where B^i is four-dimensional distortion 1-form, ν^i is the velocity 0-form and $\beta^i (=\beta^i{}_A dx^A)$ is the distortion 1-form. It is followed from (10) that the differentiation of distortion is accompanied by the dislocation density. Then, we derive four-dimensional dislocation density as the differentiation of four-dimensional distortion :

 $D^i = dB^i$. (13) (The strict deriving of (13) is done by comparing the form numbers of the distortion and the dislocation. See Yamasaki and Nagahama (1999 b).) From (11) and (12), the concrete form of (13) is given by

 $I^{i} \wedge dT + \alpha^{i} = (d_{S}\nu^{i} - \partial_{t}\beta^{i}) \wedge dT + d_{S}\beta^{i}$ (14) where $d = dt \wedge \partial_{t} + d_{S}$ and d_{S} is the differentiation of space. By comparing coefficients, (13) is divided into the spatial component and the time component :

$lpha^i {=} d_S eta^i$	(15)
$I^i = d_S \nu^i \cdot \partial_t \beta^i.$	(16)

Because the differentiation of 1-form corresponds to the rotation in vector analysis, (15) is another expression of (10). Dislocation current is given by the product among scalar density, dislocation velocity and Burgers vector. Therefore, it is understood that the special one that the gradient of the velocity is disregarded in (16) corresponds to Owowan's formula (1). That is, Orowan's formula is nothing but the equation that looks at the physical expression of Cartan's structure equation from time base.

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