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Abstract. The algebraic topological aspect of defects field is considered by using the useful topological invariant: Betti numbers. We suggest that the topological nature of the dislocation field is expressed in terms of "strength" of the dislocation corresponding to the change in the first Betti number. We also show that Frank vectors of the disclinations are related to the first Betti number.

1. Introduction

In order to make an idealized mathematical description of material deformation, we often assume that the material-space is closely approximated by continuum space. However, the natural material-space always contains topological defects, so the continuum description of the defects filed is necessary (EDELEN and LAGOUDAS, 1988; KLEINERT, 1989; YAMASAKI and NAGAHAMA, 2002), and apply to various fields such as cosmic strings, seismology, and geophysics (TESIIEYRE, 1995; KATANAEV and VOLOVICH, 1999; YAMASAKI, 2005).

One standard mathematical technique for describing defects fields is to use differential geometry in which the metric (a "measure" of space) plays an important role (BLOOM, 1979; MIRI and RIVIER, 2002; KATANAEV, 2005). The defects field such as dislocations and disclinations can be recognized as two geometric objects consist of metrics: Cartan torsion and Riemann curvature.

Another approach to defects field is to use non-metric geometry: topology (MERMIN, 1979; NAKAHARA, 2003). In the late 1970, it was recognized that the proper mathematical language to describe and classify topological defects in condensed matter is homotopy, rather than homology (e.g., MERMIN *et al.*, 1978). Both homotopy and homology have the useful concept of topological invariant such as the Betti numbers mainly used in algebraic topology (SINGER and THOPE, 1967).

According to Gauss-Bonnet theorem for an oriented and connected Riemannian 2manifold, the integral of the Gaussian curvature is related to the Betti numbers (SINGER and THOPE, 1967). This implies that the differential geometrical approach to the defects field is not irrelevant to the topological approach using the Betti numbers. However, an understanding of the Betti numbers of the defects field is still lacking. The purpose of this

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Fig. 1. (A) Lattices with an edge dislocation. (B) Corresponding perfect lattice and Burgers vector.

paper is to investigate the topological aspects of defects field by using Betti numbers.

This paper is structured as follows. In Sec. 2, we concisely review the Betti numbers. In Sec. 3, we reconsider the geometrical meanings of dislocations based on the first Betti numbers. In Sec. 4, we reconsider the topological aspects of disclinations. Section 5 is devoted to conclusions. In this paper, there may be still some conceptual shortcomings in assumptions or in mathematical treatments. But, the results seem to be meaningful. Therefore, this author decided to publish this work at this stage while leaving a room for improvement in future.

2. The Betti Numbers

In this section, we review the concept of the Betti number. We suppose that m points p_i are given in the *n*-dimensional Euclidian space. The *m*-simplex is defined as the group of points in terms of p_i as follows:

$$\sigma^m = \left\{ x = \sum_{i=0}^m \lambda_i p_i \middle| \lambda_i \ge 0, \sum_{i=0}^m \lambda_i = 1 \right\}.$$
 (1)

The *m*-simplex is constituted of the spaces inside the convex envelope of the *m* points p_i , together with its convex envelope. For instance, points (p_0) and segments (p_0, p_i) correspond to 0-simplex and 1-simplex, respectively. Let *K* be a finite set of 0- and 1-simplices. We call *K* a simplical complex when *K* satisfies the following two conditions:

(1) Any endpoint (a point connected to the simplex with a single bond) of a simplex from K is also in K.

(2) The intersection of any two simplices from K is either empty or is an endpoint for both of them.

In this paper, we regard the crystal lattice as a one-dimensional complex made of 0- and 1simplices, in which atoms and bonds correspond to 0-simplex and 1-simplex, respectively. A circuit on the crystal lattice is made of atoms and bonds so it is considered to be onedimensional complex made of 0- and 1-simplices.



Fig. 2. (A) Lattices with a screw dislocation. (B) Corresponding perfect lattice and Burgers vector. (C) Threedimensional expression of the screw dislocation. (D) Corresponding perfect lattice.

In a simplical complex, we can define Betti numbers that are topological invariants of a crystal lattice (the complex), i.e., they depend only on the topology of the space, so it is shared by any topological space homeomorphic to the space (see SINGER and THOPE, 1967 for rigorous definition). The zero Betti number b_0 is defined by the number of geometrical connection of K, that is, b_0 is the number of connected components. For instance, in Figs. 1, 2(A) and 2(B), we have $b_0 = 1$ in each crystal lattice. On the other hand, if the four crystal lattices constitute a set K while separated from each other, we have $b_0 = 4$. The first Betti number b_1 is defined by the number of independent circuits. According to Homology theory, the alternative sum of the *n*th Betti number b_n gives the Euler characteristic of a crystal lattice (the complex) χ :

$$\chi = \sum_{n=0}^{1} (-1)^n b_n = b_0 - b_1.$$
⁽²⁾

Euler characteristic is also called the Euler number or the Euler-Poincare characteristic. The Euler characteristic of a lattice is made of 0- and 1-simplices. On the other hand, Euler formula for a crystal lattice (the complex) gives





Fig. 3. (A) Lattices with a dislocation whose "strength" is one. (B) Corresponding perfect lattices. (C) Lattices with a dislocation whose "strength" is two. (D) Corresponding perfect lattices.

$$\chi = \sum_{n=0}^{1} (-1)^n \alpha_n = \alpha_0 - \alpha_1,$$
(3)

where α_n is the number of *n*-simplex. Since we regard crystal lattice as one-dimensional complex made of 0- and 1-simplices, so we ignored the higher order terms ($n \ge 2$) of Eq. (3). From Eqs. (2) and (3), the first Betti number is given by

$$b_1 = b_0 - \alpha_0 + \alpha_1. \tag{4}$$

For instance, the first Betti number of lattices in Figs. 1 and 2 are $b_1^{\text{ED}} = 1 - 14 + 20 = 7$, $b_1^{\text{ED}(\text{PL})} = 8$, $b_1^{\text{SD}} = 9$ and $b_1^{\text{SD}(\text{PL})} = 10$ (the meaning of the abbreviation will be mentioned in the next section.). This means that the first Betti number is useful for classifying the four lattices that cannot be distinguished by the zero Betti number ($b_0 = 1$). In the following sections, we will consider the physical meanings of the first Betti number in the crystal lattice as a one-dimensional complex.

3. Dislocations and the First Betti Number

First, to clarify the relationship between dislocations and the first Betti number b_1 , we take up the simple case in which the lattices include the edge and the screw dislocations have unit length (Figs. 1(A) and 2(A), see also Fig. 2(C)). To introduce Burgers vector, we



Fig. 4. (A) A positive disclination. (B) A negative disclination. (C) Corresponding perfect lattices.

image the perfect lattices that does not include the dislocations (Figs. 1(B) and 2(B), see also Fig. 2(D)). When we make a closed circuit around a dislocation in real lattices (Figs. 1(A) and 2(A)), there is a mismatch of one lattice vector in perfect lattices (the dotted arrows in Figs. 1(B) and 2(B)). This is called Burgers vector (e.g., HIRTH and LOTHE, 1982). The circuit is called Burgers circuit, which is a trace along the crystal lattice so it is also one-dimensional complex made of 0- and 1-simplices. In Figs. 2 (C) and (D), we make a closed circuit around a dislocation on the "surface" of the 3D graph, so we recognize the circuit as planar graph in essential. Let Δb_1^{SD} and Δb_1^{SD} be the change in the first Betti number, we have $\Delta b_1^{\text{ED}} = 8 - 7 = 1$ and $\Delta b_1^{\text{SD}} = 1$. This means that the existence of dislocations can be described by the change in the first Betti number in dependence of the type of edge and screw dislocations. This assertion is not proved rigorously, but so far as examined for several lattices including those shown in this paper, this seems valid.

Next, we take up more complicated lattices. In this paper, we define the "strength" of the dislocation as the number of bonds that lack atom due to the dislocation. For instance, the "strength" of the dislocations in Figs. 3(A) and (C) are one and two, respectively. Although dislocations have different "strength" in real lattices (Figs. 3(A) and (C)), the corresponding Burgers vectors are one in perfect lattice (Figs. 3(B) and (D)). We reconsider this case based on the first Betti number. To visualize the point in question, we blacken atoms of the closed circuit around the dislocation in real lattices, and draw atoms and lattices, needed to complete the perfect lattice, as dotted lines. Figure 3(B) shows an increase in one atom and two lattices when the "strength" of the dislocation is one. Figure 3(D) shows an increase in two atoms and four lattices when the "strength" of the dislocation is two. We can generalize theses results as follows. Let $\Delta b_1(n)$ be the change in the first Betti number in the case of the "strength" of the dislocation being *n*. The $\Delta b_1(n)$ -value can be estimated by Eq. (3). For instance, $\Delta b_1(n) = 0 - (+1) + (+2) = 1$ in Fig. 3(A) and $\Delta b_1(2) = 2$ in Fig. 3(B). Therefore, in the case of *n* (*n* atoms and 2*n* bonds are added), we obtain

$$\Delta b_1(n) = 0 - (+n) + (+2n) = n.$$
(5)

This is a topological expression of dislocations field: the "strength" of the dislocation

corresponds to the change in the first Betti number. The generality of Eq. (5) is not proved rigorously, but so far as checked for several examples including those shown in this paper, this assertion seems valid.

4. Disclinations and the First Betti Number

In this section, we consider a topological aspect of rotational dislocations, i.e., disclinations. In Sec. 3, we found that the existence of dislocations can be described by the change in b_1 . Let us estimate the corresponding quantity of disclinations. Figures 4 (A) and (B) show a disclination and its surrounding area. We blacken atoms of the cores of disclinations. From Eq. (3), we can estimate the core's b_1 as one. On the other hand, Fig. 4(C) shows that b_1 of the core of the perfect lattice is also one, therefore, the change in b_1 for disclinations is zero. That is, the core of disclinations cannot be described by the change in b_1 .

Now, a disclination is often called wide range defects. Then, we estimate b_1 of not only the core but also its surrounding area. Figures 4(A) to (C) show that b_1 of the core and its surround area are $b_1^{PD} = 7$, $b_1^{ND} = 11$ and $b_1^{PL} = 9$. Therefore, the change in b_1 of positive and negative disclinations are $\Delta b_1^{PD} = 2$ and $\Delta b_1^{ND} = -2$, respectively. That is, the absolute value of b_1 are independent of the type of disclinations, and the sign of b_1 depend on the type of disclinations. This result corresponds to Frank vector's value and direction.

5. Conclusions

We have shown that dislocations field can be described by the first Betti number b_1 in dependence of the types (edge or screw) based on the algebraic topology. Moreover, we have suggested the topological expression of dislocations field: the "strength" of the dislocation corresponds to the change in b_1 . Disclinations field is also described by b_1 : the absolute value of b_1 are independent of the type of disclinations, but the sign of b_1 depend on the type.

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