Geometry of Materials Manifolds with Defects

著者	Inoue Kazutoshi
学位授与機関	Tohoku University
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博士論文

Geometry of Materials Manifolds with Defects

(欠陥をもつ材料多様体の幾何学)

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Geometry of Materials Manifolds with Defects

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Kazutoshi Inoue

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Abstract

It is well-known that crystallographic structures are commonly observed in solid. The structures in reality are not globally perfect, but there are defects of from 0 to 3 dimension instead. Defects are regarded as a singular set which violates symmetries of the crystal. In this thesis, we mainly study 1-dimensional defects, called *dislocations* and 2-dimensional defects, called *grain boundaries*. Dislocations and grain boundaries are closely related. There are two types of dislocations: of an edge type and of a screw type. Mixed types of those, however, are common in general. The results of this thesis contain as follows:
1. mathematical formulations for selected topics on the study of dislocations in materials science,
2. determination of the stress fields over a manifold with a mixed dislocation and the stability of a mixed dislocation, and
3. a joint work on the study of grain boundaries with materials scientists.

Crystallographic structures are distorted as a consequence of the existence of dislocations. A material body is considered as a continuum body from a macroscopic viewpoint and defects has been studied in terms of the curvature tensor of the Levi-Civita connection of some appropriate metric in the framework of Riemannian geometry since more than a century ago. In another approach, defects can be expressed by the torsion tensor of a connection compatible with the metric. In this thesis, we stand at the latter position following the formulation of K. Kondo[44]-[46], S. Amari [2]-[4], E. Kröner[48], and A. Yavari and A. Goriely[79]-[80]. The 3-dimensional non-Riemannian geometry (Riemann-Cartan geometry) with nonzero torsion matches the concept of the Burgers vector which has been used to describe the orientation and the magnitude of a dislocation in materials researches. It is said that one of the motivations E. Cartan introduced torsion in geometry was to express the existence of defects in a material body. Yavari and Goriely reformulated the dislocation models via modern differential geometry. Then they studied the stress fields on a 3-dimensional locally flat manifold with nonzero torsion tensor. We consider a mixed dislocation and derive ordinary differential equations the metric tensor satisfies. And then we calculate stress fields and the stability conditions of a mixed dislocation from a macroscopic viewpoint.

In recent years, technological developments enable materials scientists to directly observe atomic structures. One can apply information of defects to estimate the geometrical structure of a materials body and predict properties or design new materials. Thus we need microscopic viewpoints; it is done by *discrete geometry* rather than geometry in *continuum.*

We regard a crystalline structure as a lattice in $\mathbb{R}^3$ where atoms are vertices (and, if necessary, bonds between adjacent atoms are edges) in the usual way. The term lattice always refers to a graph corresponding to a crystalline structure. In this thesis, we discuss the conditions for "good matching" of two lattices which form an interface. Especially, we study the commensurability of two lattices whose vertices are shared at the interface. If the intersection of two lattices

is not empty, then points in the intersection usually form a sublattice of those two and we term it a coincidence-site lattice (CSL). In this thesis, we review the 2-dimensional CSL theory and the O-lattice theory. The CSL theory was generalized to the O-lattice theory by W. Bollmann[11]-[18] in the 1960's and applied to materials researches. Though CSLs appear only when two lattices are in particular configurations, one can define an O-lattice for arbitrary configurations of lattices if they are related by a linear transformation. In this sense, the O-lattice theory is a way of generalization of the CSL theory. However, the method was not fully understood in the materials community and not so many researchers apply the theory nowadays. The author was motivated by an experimental result by M. Saito et al.[67] on a near CSL configuration of cubic lattices. We revealed that the distribution of rational numbers implied the periodicity of certain grain boundary structures in near CSL configurations due to the O-lattice theory. We present contributions of our theory to the grain boundary physics as a collaborative work with Y. Ikuhara et al.[34] as the main result of this thesis.

The first part of this thesis studies defects from macroscopic viewpoints while the latter from microscopic viewpoints. In Chapter 2, we review the classification of defects due to the homotopy theory which was well-studied in the 1970's. In Chapter 3, we give an overview of geometrical methods in the elastic deformation theory and introduce a dislocation model studied by Kondo, Amari, Kröner and others. We review the reformulated dislocation model due to Yavari and Goriely and generalize their results in the case of mixed dislocations. In Chapter 5, we determine the stability conditions for a mixed dislocation under appropriate assumptions. We mention a two-body interaction energy between dislocations at the end of the chapter.

We introduce microscopic viewpoints in Chapter 6. Main results are presented as an application of the O-lattice theory to materials science.

Contents

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