A topological model for defects and interfaces in complex crystal structures

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ABSTRACT

A topological model (TM) is presented for the complex crystal structures characteristic of some minerals. We introduce a tractable method for applying the TM to characterize defects in these complex materials. Specifically, we illustrate how structural groups, each with a motif containing multiple atoms, provide lattices and structures that are useful in describing dislocations and disconnections in interfaces. Simplified methods for determining the shuffles that accompany disconnection motion are also described. We illustrate the model for twinning in albite owing to its potential application for constraining the rheological properties of the crust at conditions near the brittle-plastic transition, where plagioclase is a major constituent of common rock types. While deformation twins in plagioclase are often observed in crustal rocks, the interpretation of the stress states at which they form has not advanced. The concept of structural groups makes an analysis of the twinning process easier in complex minerals and explicitly predicts the interface structure of the deformation twins.

Keywords: Twinning, mineral, structural group, dislocations, disconnections, topological model

INTRODUCTION

Topological theory, based on crystal symmetry with added symmetry elements at interfaces (Pond and Vlachavas 1983), was developed to describe interfaces and defects in crystals (Pond 1989). It was expanded to include a formal description of defects called disconnections (Hirth and Pond 1996). The topological model (TM) entails the application of these ideas to describe dislocations and disconnections at interfaces, including those that provide the mechanism for growth of a phase normal to the interface (Pond et al. 2007). The same defects account for interface structure and misfit accommodation. While almost all applications have dealt with simple metals and simple compounds (e.g., Medlin and Yang 2012), the TM has many potential applications in Earth and planetary sciences, for a wide range of minerals. However, there are added factors that must be considered for more complicated minerals (i.e., with low symmetry and/or a large number of atoms in the unit cell) such as the plagioclase feldspars. Here, we review the topological model and then introduce new concepts useful in the application of the TM to more complicated mineral structures.

Disconnections are linear interface defects with both a step character and dislocation components characterized by the Burgers vector. Motion of the disconnection can be envisioned to occur by a simple engineering shear associated with motion of the dislocation part, and local rearrangements of atoms (shuffles) associated with motion of the step part. These components of the TM and a view of a disconnection are illustrated in Appendix A for the case of a twin in a simple cubic structure. In metals, step heights are small and shuffles are either absent or simple. Minerals often have complex structures containing many atoms, so step heights and corresponding Burgers vectors can be large and the associated shuffles are numerous. To facilitate application of the TM to these complex mineral structures, we propose the concept of a lattice of structural groups and show that this yields the Burgers vector in the TM description. While these ideas are general and can be extended to other processes such as phase transformations and grain boundary sliding (as outlined in the discussion), we introduce these concepts for twinning, using the example of low albite.

Defect properties can be determined by circuit mapping (e.g., the familiar Burgers circuits for dislocations) or by line integrals of symmetry elements. These two techniques were compared in Pond and Hirth (1994) and shown to give equivalent results for defects in twinning and phase transformations, where translation and rotation are the principal symmetry elements. For complex crystal structures, the new concept of a lattice of structural groups makes the circuit mapping technique significantly more tractable. Our focus is on disconnections, interface defects that provide the mechanism for shear-type phase transformation and twinning (reviewed in Hirth et al. 2013, 2016) and grain boundary processes (reviewed in Han et al. 2018). More general symmetry considerations and other types of defects are treated in Pond (1989).

REFERENCE SPACES

As reviewed in Howe et al. (2009), early work indicated that transformation defects have step character. Building on the early work, the TM precisely defined the Burgers vector and step height of a disconnection in reference spaces. In the next sections, we describe three perfect reference spaces in the TM, analogous to reference structures for the familiar Burgers circuits for dislocations (Anderson et al. 2017). The volume