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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