Thermodynamic approach to grain boundary premelting in a binary eutectic system

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The structure of a weak asthenosphere and a rigid lithosphere constitutes the essential element of plate tectonics. The weakness of asthenosphere has been attributed to the partial melting of rocks. However, in the recent experimental study by using a rock analogue (borneol + diphenylamine binary eutectic system), anelastic relaxation and viscous creep were significantly enhanced from just below the eutectic temperature, where melt does not exist (Yamauchi and Takei, 2016). The mechanisms of anelasticity and viscosity are related to grain boundary sliding and grain boundary diffusion respectively, which implies that thesechanges in the mechanical properties resulted from the changes in grain boundary properties. That means that the “weak asthenosphere” can be explained by “weak grain boundaries” at near solidus temperatures without invoking melt. However, the mechanism causing the change in grain boundary properties is unclear.

In the areas of material science and physics, it is known that the grain boundary is disordered just below the melting temperature or solidus, which is called grain boundary premelting. The results of experiment are expected to be explained by grain boundary premelting. In this study, we investigate the possible occurrence of grain boundary premelting in the upper mantle and its effects on the mechanical properties of rock by using a theoretical model developed in these areas.

In this study, we use a thermodynamic model called phase-field model. We consider a two component bicrystal containing a single grain boundary at x=0. Tang et al. (2006) modeled this system by using three field parameters, composition c(x), crystal orientation θ(x), and crystallinity η(x).(η is sometimes called order parameter or phase-field parameter.) Using the theory of Cahn and Hilliard (1958), they phenomenologically derived the free energy of this nonuniform system as a function of c(x), θ(x), and η(x). By calculating the condition which minimize the free energy, we can predict the equilibrium composition and crystallinity of the grain boundary as functions of temperature. Occurrence of grain boundary premelting can be predicted as an increase in grain boundary disorder (decrease in η at x=0) near the eutectic temperature. We investigate the effects of various model parameters, such as melting temperature, melting enthalpy, and grain boundary misorientation, on the grain boundary crystallinity.

Keywords: premelting, phase-field model

