Grain-boundary diffusion rates inferred from grain-size variations of quartz in metacherts from a contact aureole

TAKAMOTO OKUDAIRA,¹,* HIKARU BANDO,¹ AND KENTA YOSHIDA²

¹Department of Geosciences, Osaka City University, Osaka 558-8585, Japan
²Department of Geology and Mineralogy, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

ABSTRACT

We evaluate a temperature-dependent coefficient for grain-boundary diffusion in quartz aggregates using grain size data from a contact aureole, based on the coupling of a numerical model for the temperature-time history of the contact aureole with a model for the kinetics of diffusion-controlled grain growth. The metachert samples were collected from the contact aureole of the Hanase-Bessho quartz diorite at Hanase Pass, Kyoto, Japan. The quartz grain sizes vary systematically with distance from the quartz diorite. We calculated the temperature-time history using a one-dimensional thermal model, validated by peak metamorphic temperature estimates that are based on the degree of graphitization of carbonaceous material in metapelites, as characterized by Raman microspectroscopy. To minimize the sum of the squares of the errors between the measured and calculated grain sizes, based on the normal grain growth law together with the temperature-time history, we estimated the activation energy and pre-exponential factor in the Arrhenius function for oxygen diffusion rates in quartz aggregates to be estimated as 208 kJ/mol and 1.1 × 10⁻⁸ m²/s, respectively, assuming a grain-boundary width of 1 nm. The grain-boundary diffusion rates for temperatures in the greenschist and amphibolite facies are similar to those determined in natural or laboratory grain-coarsening experiments, but differ significantly from those determined in tracer diffusion experiments. During grain-size-sensitive deformation, “effective” grain-boundary diffusion rates may be intermediate between the rates of diffusion along and across the grain boundary, and would be higher than the grain-boundary diffusion rates estimated by grain-coarsening experiments, and lower than those by tracer diffusion experiments.

Keywords: Grain-boundary diffusion, quartz aggregates, grain sizes, contact aureole, normal grain growth

INTRODUCTION

Understanding and predicting the rheological behavior of many common crustal rocks requires knowledge of the mechanical properties of quartz crystals and aggregates, because quartz is one of the most abundant rock-forming minerals in the Earth’s continental crust. Diffusion contributes to most of the important deformation mechanisms, including grain-size-sensitive diffusion creep/grain-boundary sliding and insensitive dislocation creep (e.g., Okudaira and Shigematsu 2012). To evaluate the relative importance of these different mechanisms for quartz deformation, the diffusion kinetics of the major ionic species in quartz crystals and aggregates must first be known.

The grain-boundary (or bulk) diffusion coefficients of Si or O have been estimated from tracer diffusion experiments (Farver and Yund 1991a, 2000a), and from natural or laboratory grain-coarsening experiments (Joesten 1983, 1991; Tullis and Yund 1992). According to Farver and Yund (2000a), based on the data obtained by isotopic tracer (¹⁸O) and standard step-scan analysis using an ion microprobe, the temperature dependence of silicon bulk diffusion in novaculite for hydrothermal experiments at 600–800 °C and 150 MPa confining pressure, and dry experiments at 800–1100 °C and 1 atm (in a stream of dry N₂), respectively, is described by the Arrhenius parameters

\[ D_0 = 3.7 \times 10^{-10} \text{ m}^2/\text{s} \text{ and } E = 137 \pm 18 \text{ kJ/mol} \text{, and } D_0 = 6.2 \times 10^{-9} \text{ m}^2/\text{s} \text{ and } E = 178 \pm 38 \text{ kJ/mol}. \]

Assuming volume diffusion to be negligible (i.e., type C kinetics; Saal et al. 1990), the measured bulk diffusion rates (\( D_{\text{bulk}} \)) can be related to grain-boundary diffusion rates (\( D_{\phi} \)) through the expression

\[ D_{\phi} = \tau D_{\phi} \delta/d, \]

where \( \tau \), the tortuosity factor, represents the ratio of the true path length to the length of the measured profile (e.g., Watson 1991), \( \delta \) is the grain-boundary width, and \( d \) the average grain size. The value of \( \tau \) depends on the grain geometries, and estimates typically range from 1.5 to 2.0 (e.g., Farver and Yund 2000a).

On the other hand, variations in the grain sizes of quartz in five nodular chert samples from the Christmas Mountains contact aureole were matched by a normal grain growth model in which the temperature dependence of the Arrhenius function, along a temperature-time history, was calculated by one-dimensional thermal modeling (Joesten 1983). Assuming a grain-boundary width of 1 nm, the data permit the coefficient for the grain-boundary diffusion of oxygen in quartz aggregates to be estimated as

\[ D_{\phi} = 8.07 \times 10^{-10} \exp(-210/RT) \] for the temperature range of 600–1000 °C. Tullis and Yund (1982) determined grain growth rates for quartz aggregates between 800 and 1000 °C at 200–1500 MPa, and based on the data from a grain-growth experiment of Tullis and Yund (1982), Joesten (1991) recalculated the values of \( D_0 \) and \( E \) as \( 2.3 \times 10^{-7} \text{ m}^2/\text{s} \) and 262 kJ/mol, respectively.

The values of the grain-boundary diffusion coefficients...