

EVALUATION OF COOLING RATE CALCULATED BY DIFFUSIONAL MODIFICATION OF CHEMICAL ZONING: DIFFERENT INITIAL PROFILES FOR DIFFUSION CALCULATION. M. Miyamoto, A. Monkawa, E. Koizumi and T. Mikouchi, Space and Planetary Science, Graduate School of Science, University of Tokyo, Hongo, Tokyo 113-0033, Japan (miyamoto@eps.s.u-tokyo.ac.jp).

Introduction: Since chemical zoning in minerals provides information on their thermal history, it is often applied to calculating the cooling rate or burial depth by solving the diffusion equation on the assumption that chemical zoning is produced by diffusional modification or homogenization except for primary igneous zoning [e.g., 1]. There are several factors to have influence on the result. For example, although the atomic diffusion coefficient in minerals is one of the most important factors, there is often much difference among the reported values of the diffusion coefficient of an atom in a mineral.

It is sometimes difficult to determine the initial zoning profile for starting the diffusion calculation, because the zoning profile now observed is the result of diffusional modification or homogenization. It is, therefore, necessary to examine the difference in the cooling rate calculated by diffusional modification due to the difference in the initial profile. We, in this abstract, evaluate the cooling rate calculated by using the different initial (starting) zoning profiles for the Fe-Mg chemical zoning profile of pallasite olivine used in our previous study [2].

Calculations: We employed several initial profiles calculated by using the Rayleigh equation for the closed-system fractional crystallization and studied the difference in the cooling rate for the different initial profiles (Fig. 1). We used the distribution coefficient for Fe/Mg of 0.30. One of the variables for the equation is the fraction of liquid remaining (F). The initial profiles in Fig. 1 are shown for different F values. For our previous study [2], we used a uniform initial profile for the calculation.

Miyamoto et al. [3] evaluated the atomic diffusion coefficients of Fe-Mg in olivine (D_{Fe}) reported in several literatures on the basis of their diffusion experiments. They also extrapolated the Fe-Mg diffusion coefficient reported by Misener [4] by using an equation for variation with oxygen fugacity similar to that of Buening and Buseck [5], because D_{Fe} reported by Misener [4] is determined under the FMQ (fayalite-magnetite-quartz) buffer. This extrapolation enabled us to employ the Fe-Mg diffusion coefficient of Misener [4] under any oxygen-fugacity conditions.

The expression is:

$$D_{Fe} = 0.03163 \times 10^{-2} (f_{O_2})^{1/6} (0.41 + 0.0112C_{Fe}) \exp[-39.27 + 0.0905C_{Fe}/RT]$$

where f_{O_2} , C_{Fe} , R and T are oxygen fugacity in atm, the Fa component (=100 x Fe/(Mg+Fe)) in mol%, the gas constant in kcal mol⁻¹ K⁻¹ and temperature in K, respectively. Miyamoto et al. [3] concluded that the diffusion calculation by this expression for the Fe-Mg diffusion coefficient gives the best-fit to the observed zoning profile. Therefore, we employed this expression for the Fe-Mg diffusion coefficient of olivine in this study. In our previous study [2], we used D_{Fe} reported by Buening and Buseck [5].

A calculated Fe-Mg diffusion profile was fitted to the observed zoning in order to obtain the cooling rate [e.g., 1]. Diffusion calculations were started by assuming several initial profiles obtained by the procedures described above. For a given linear (continuous) cooling rate, a diffusion profile was calculated by numerically solving the diffusion equation. The best-fit cooling rate was determined to get the best fit between the calculated and observed zoning profiles by the non-linear least-squares method (Simplex method). The observed zoning profile (open circle in Fig. 1) is measured (by EPMA) for olivine in the Esquel pallasite that is the same as that used in our previous study [2]. The details of calculation procedures are similar to those described in [e.g., 1, 2].

Results and Discussion: Fig. 1 shows the initial (starting) zoning profile used in this study. The difference of the initial profile is shown as a function of the fraction of liquid remaining of the fractional crystallization model. In order to evaluate the difference in the cooling rate, we used the initial zoning profile for an extreme case (e.g., the fraction of liquid remaining (F) is 1%). Fig. 2 shows the results of the cooling rates calculated for the different initial profiles. The difference in the cooling rate is shown as a function of the fraction of liquid remaining. There is about one order of magnitude difference in the cooling rate. The smallest cooling rate is obtained for the initial profile for F of 1%, and the largest cooling rate is for the uniform initial profile. The maximum difference in the cooling rate due to the difference in the initial profile is about one order of magnitude. We note that the initial profiles used contain the extreme case. In practice, considering the shape of the initial zoning profiles shown in Fig. 1, the difference in the cooling rate due

to the difference in the initial profile is less than one order of magnitude.

Fig. 3 compares the results of the cooling rates obtained for the Fe-Mg diffusion coefficients reported by Buening and Buseck [5], Misener [4] with the oxygen-fugacity variation [3], and Chakraborty [6]. The largest Fe-Mg diffusion coefficient is that by Buening and Buseck [5], and the smallest is by Chakraborty [6]. The difference in these values is about two orders of magnitude [see 2]. Therefore, about two orders of magnitude difference in the cooling rate can be seen corresponding to the difference in the diffusion coefficient.

In fact, the difference in the diffusion coefficient has more influence on the cooling rate than that of the initial zoning profile. This result means that the accurate diffusion coefficient of an atom in a mineral is needed to determine the cooling rate on the basis of chemical zoning data.

References: [1] Miyamoto, M. et al. (1986) *JGR*, 91, 12804-12816. [2] Miyamoto, M. (1997) *JGR*, 102, 21613-21618. [3] Miyamoto M. et al. (2002) *Antarct. Meteorite Res.*, 15, 143-151. [4] Misener, D. J., (1974) in *Geochemical Transport and Kinetics*, ed. by A. W. Hofmann et al., Carnegie Inst. Washington, Publ. 634. [5] Buening, D. K. and Buseck, P. R. (1973) *JGR*, 78, 6852-6862. [6] Chakraborty, S. (1997) *JGR*, 102, 12317-12331. [7] Wood J. A. (1979) in *Asteroid*, ed. by T. Gehrels, pp. 849-891, Univ. of Ariz. Press, Tucson.

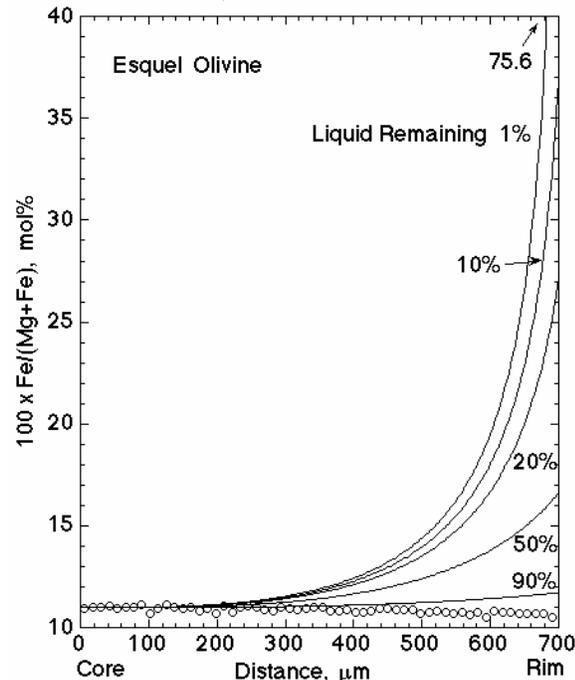


Fig. 1. Initial zoning profiles (solid curves) for starting the diffusion calculation. The profiles were

calculated by using the Rayleigh equation for the closed-system fractional crystallization. Numbers on curves show the fraction of liquid remaining. Open circles show the observed Fe-Mg zoning profile for the Esquel pallasite olivine [2]. A calculated Fe-Mg diffusion profile starting with the initial profile (solid curve) was fitted to the observed zoning profile (open circles) to obtain the best-fit cooling rate

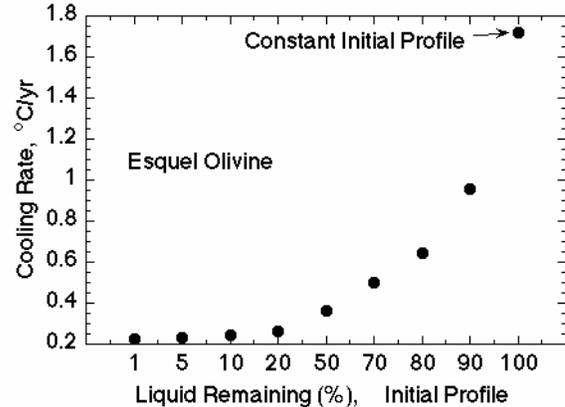


Fig. 2. The difference in the cooling rate due to the difference in the initial profile for diffusion calculation. The initial profile is shown as a function of the fraction of liquid remaining. Cooling is from 1150 to 650 °C.

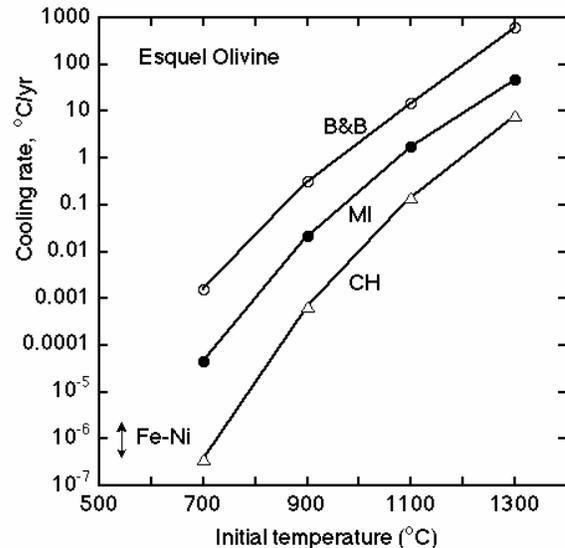


Fig. 3. Comparison of the cooling rate calculated by different Fe-Mg diffusion coefficients of Buening and Buseck (B&B) [5], Misener (MI) [4] with oxygen-fugacity variation [3] and Chakraborty (CH) [6]. The cooling rate is shown as a function of initial temperature of cooling [see 2 and 3]. Uniform initial profile was used. Fe-Ni (arrows) shows the range of the cooling rate obtained by Fe-Ni data [e.g., 7].