Supporting Information for "Modeling of the phase transformation of germanate olivine by using the phase-field method"

Sando Sawa[1], Jun Muto[1], Hiroyuki Nagahama[1]

[1]Department of Earth Science, Tohoku University, Sendai, Miyagi, Japan

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Introduction Text S1 describes a test against an analytical solution. Figure S2 shows an enlarged view of Run P3T1.2 (P = 3 GPa and T = 1200 K) at 35 s. Videos S1-S4 show animations of the grain growth of γ phase, von Mises stress evolution, shear plastic strain evolution, and shear eigen strain evolution in the deformation simulations at $P = 1$ GPa and T = 1200 K (Run P1T1.2), respectively. Videos S5-S8 show animations of the grain growth of γ phase, Mises stress evolution, shear plastic strain evolution, and shear eigen strain evolution in the deformation simulations at P = 3 GPa and T = 1200 K (Run P1T1.2), respectively. Videos S9-S10 show animations of the grain growth of γ phase and

Corresponding author: S. Sawa, Department of Earth Science, Tohoku University, Sendai, Miyagi, Japan. (sando.sawa.t1@dc.tohoku.ac.jp)

shear plastic strain evolution in the static simulations at $P = 5$ GPa and $T = 1200$ K (Run SP5T1.2), respectively. Videos S11-S12 show animations of the grain growth of γ phase and shear plastic strain evolution in the deformation simulations at $P = 5$ GPa and $T = 1200$ K (Run P5T1.2), respectively.

Text S1.

To test the numerical implementation of the elastic model in this study, we investigated the case of a single spherical particle Ω such as Steinbach and Apel (2006) and Ammar et al. (2011). The analytical solution for isotropic elasticity in x_1 direction from the center of the particle is given by Eshelby (1957):

$$\sigma_{ii} = \begin{cases} -\sigma_0 & \text{inside } \Omega; x_1 < r_p \\ -\sigma_0 \left(\dfrac{r_p}{x_1}\right)^3 & \text{for } i = 1; x_1 > r_p \\ \frac{1}{2}\sigma_0 \left(\dfrac{r_p}{x_1}\right)^3 & \text{for } i = 2 = 3; x_1 > r_p. \end{cases} \tag{1}$$

Here, r_p is the particle radius. σ_0 is calculated by

$$\sigma_0 = -\sigma_{ii} = -C_{iikl}(\varepsilon_{kl} - \varepsilon^*_{kl}) = C_{iikl}(S_{klmn}\varepsilon_{mn} - \varepsilon^*_{kl}), \tag{2}$$

where C_{ijkl} is the elasticity moduli, ε_{ij} is the total strain, ε^*_{ij} is the eigen strain, and S_{ijkl} is the eshelby tensor. At the plane strain condition (elliptic cylindrical inclusion), considering isotropic elasticity of Ω, S_{ijkl} is specifically given by Eshelby (1957) and Mura (1987):

$$\begin{aligned} &S_{1111} = S_{2222} = \frac{5 - 4\nu}{8(1-\nu)}, \\ &S_{1122} = S_{2211} = \frac{4\nu - 1}{8(1-\nu)}, \\ &S_{2233} = S_{1133} = \frac{\nu}{2(1-\nu)}, \\ &S_{3333} = S_{3311} = S_{3322} = 0. \end{aligned} \tag{3}$$

Here, ν is the Poisson ratio. According to (2) and (3), we obtain

$$\sigma_0 = -\sigma_{11} = -\sigma_{22} = \frac{\mu}{1-\nu}\varepsilon^*, \tag{4}$$

where μ is the shear modulus. We used the shear modulus $\mu = 72$ GPa and the Poisson ratio $\nu = 0.259$ of α phase (Liebermann, 1975). The eigen strain ε^* and the particle radius r_p is set to be 0.365 and 0.586 μm, respectively. The numerical simulation was conducted in a square domain of 60×60 μm^2 with discretizations Δx of 512×512

square meshes. The grain boundary thickness δ is set to be $5\Delta x = 0.585$ μm because $\delta = 4\Delta x \sim 7\Delta x$ is generally used for stability of the calculation (Takaki, 2014). Figure S1 shows the numerically simulated tangential (σ_{11}) and normal (σ_{22}) stress components and the analytical solution of Eq. (1) in a radial direction (x_1) from the center of the particle. The positive value of stress and strain means the compression of the material in this study. Calculated tangential and normal stresses correspond to the analytical solution inside Ω. However, both calculated stresses slightly shift to the outside from the analytical solution because we set a bit large grain boundary thickness of 0.585 μm caused by a square domain of 60×60 μm^2 with discretizations Δx of 512×512 square meshes. Therefore, we have to pay attention to overestimate stresses slightly near the grain boundary.

Figure S2.

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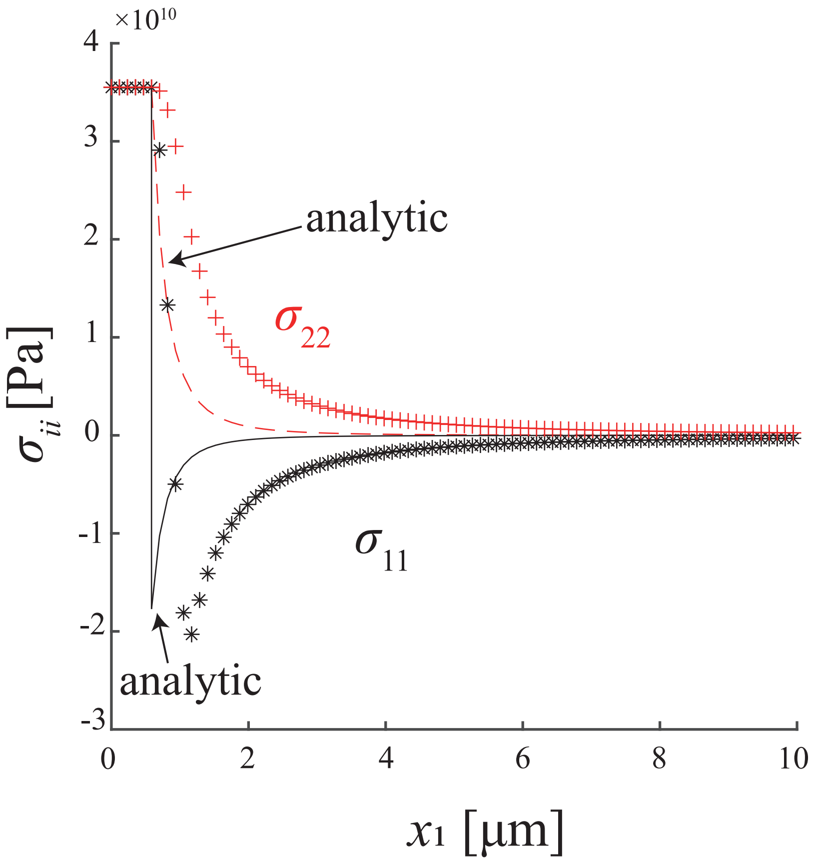

Figure S1. Calculated tangential (σ_{11}) and normal (σ_{22}) stresses components in a radial direction from the center of the particle in comparison with the analytical solution of Eq. (1)

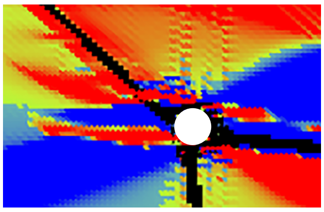

Figure S2. Enlarged view of Run P3T1.2 (P = 3 GPa and T = 1200 K) at 35 s. Red- and blue-colored pixels show postive and negative shear plastic strains, respectively. White-colored pixels shows γ grains. Pair of positive and negative shear plastic strain develops horizontally with γ grains at the core. Black line is a grain boundary of α grains.