## 1.5.P02

# Analysis of thermal pressures and melting temperatures for pyrope minerals of the lower mantle

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To understand the composition of the lower mantle of the earth it is necessary to investigate the thermoelastic behavior of minerals under high pressures and at high temperatures. Basic data required for such a study are represented by pressure-volume-temperature relationships for minerals corresponding to a wider range of pressure and temperature. We shall study these relationships on the basis of equation of state based on phenomenological approaches. These equations of state have been used at high temperature by incarporating the contributions arising from the thermal pressure. The input data corresponding to reference pressure have been used in the calculations. The relationship between thermal pressure and melting temperature has been used to obtain the values of melting temperatures for lower mantle mineral -pyrope. The volume-temperature relationships along different isobars have also been studied using the values of thermal pressures. We have used isobaric equations of state for thermal pressure due to Shanker et al., Singh, and Shanker and Kushwaha. These equations have been recognized as improved equations for addressing the high pressure melting of geophysical minerals. The results have been discussed and compared with the values calculated from various equations of state.

### 1.5.P03

# Grain boundary diffusion of Mg and Ca in synthetic diopside aggregates

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We have determined experimentally the grain boundary diffusion coefficients of  $^{26}Mg$  and  $^{42}Ca$  in a synthetic, chromium bearing, iron free Diopside. The samples were almost 100% dense and had a grain size of approximately 1 $\mu$ m. For the diffusion experiments, specimens with isotopically doped surface layers were annealed, in air, at temperatures ranging from 800°C to 1000°C for times of up to 500 hrs. Diffusion profiles were measured using secondary ion mass spectrometry (SIMS). Values for the product of the diffusion coefficient (D'), and the effective grain boundary width ( $\delta$ ) were calculated using LeClaire's equation.

The calculated Arrhenius values for grain boundary diffusion are  $D_0$ ' $\delta$  = 2.88 x 10<sup>-14</sup> m<sup>3</sup>/s and Q = 147.3 kJ/mol for  ${}^{42}$ Ca, and 6.03 x 10<sup>-18</sup> m<sup>3</sup>/s and 112.6 kJ/mol for  ${}^{26}$ Mg. At 1000°C the D' $\delta$  values for <sup>42</sup>Ca and <sup>26</sup>Mg are 1.46 x 10<sup>-20</sup> m<sup>3</sup>/s and 3.01 x 10<sup>-20</sup> m<sup>3</sup>/s respectively. The calculated activation energy for Ca is half the value reported for volume diffusion in single crystal Diopside,  $284 \pm 10$  kJ/mol, at temperatures below  $1230 \pm 15^{\circ}$ C. The activation energy calculated for Mg is between 50 and 60% of that for volume diffusion in single crystal Diposide along the c axis (200.9 kJ/mol). The diffusion of Mg is faster than that of Ca over the temperature range studied, with a significantly lower activation energy, but shows less of an increase with temperature than Ca. At lower temperatures the two species yield near parallel trends, yet at temperatures above 900°C the Ca diffusion coefficient begins to converge with that for Mg. This change in the rate of diffusion could be the result of a change in the mechanism of diffusion of Ca which does not affect Mg.