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Phase diagram and *P-V-T* equation of state of Al-bearing seifertite at lowermost mantle conditions

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Abstract

We investigated the properties of Al-bearing SiO_2 (with 4 or 6 wt% Al_2O_3) at pressures and temperatures corresponding to the lowermost mantle, using laser-heated diamond-anvil cell coupled with synchrotron-based in situ X-ray diffraction. The phase transition from $CaCl_2$-structured to α-PbO_2-structured (seifertite) polymorphs occurs between 113 and 119 GPa at 2500 K. The range of pressure where the two phases coexist is small. There is a slight decrease of the transition pressure with increasing Al-content. We propose a tentative phase diagram reporting the minerals composition as a function of pressure in the SiO_2-Al_2O_3 system.

We also refine the *P-V-T* equation of state of Al-bearing seifertite based on volume measurements up to more than 160 GPa and 4000 K [$V_0 = 92.73(10)$ Å^3, $K_0 = 304.2(3.0)$ GPa, $K_0' = 4.59$ (fixed), $\Theta_{D0} = 1130$ K (fixed), $\gamma_0 = 1.61(3)$]. At 300 K, the volume decrease at the $CaCl_2$ to α-PbO_2 transition is 0.5(1)%, a value slightly lower than the 0.6% reported previously for Al-free samples. At high temperature, the Grüneisen parameter of seifertite is found to be similar to that of stishovite. Nevertheless, the $\Delta V/V$ across the $CaCl_2$-form to seifertite transition is found to increase slightly with increasing temperature.

Across the phase transition, volume changes can be translated into density changes only when the Al substitution mechanisms in both $CaCl_2$-form and seifertite are defined. The analysis of all available data sets suggests different substitution mechanisms for the two SiO_2 polymorphs. Al-substitution could occur via O-vacancies in the $CaCl_2$-form and via extra interstitial Al in seifertite. This would result in a density increase of 2.2(3)% at 300 K for SiO_2 in basaltic lithologies. Alternatively, the same Al-substitution mechanism in both of the SiO_2-dominated phases would yield a density increase of 0.5(1)%.

Keywords: Seifertite, phase transition in SiO_2, *P-V-T* equation of state, lowermost Earth mantle