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Simulation study of Na-majorite

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Garnets, which are found as inclusions in diamonds, often have the excess of Na_2O and SiO_2 [Stachel, 2001]. Experimental studies suggest that Na is incorporated in pyrope-rich garnet via the coupled substitution Mg+Al=Na+Si [Bobrov et al., 2008]. This study is concerned with the determination of the structure and the thermodynamic properties of NaGrt ($Na_2MgSi_5O_{12}$), which is assumed to be the end-member of pyrope-rich garnets with the excess of Na_2O and SiO_2. Static lattice energy calculations were performed with the program GULP [Gale & Rohl, 2003] using the force-field model [Vinograd et al., 2007] for 200 structures of $Na_2MgSi_5O_{12}$ composition. These structures were prepared from Ia3-d pyrope $Mg_3Al_2Si_3O_{12}$ by replacing all octahedral Al atoms with Si and 2/3 of Mg atoms with Na. The distribution of Mg and Na was varied randomly. The static energies of these structures were cluster expanded using 8 pairwise effective cluster interactions (ECI). The ECIs were used to constrain Monte Carlo simulations within a 4×4×4 supercell (NNN exchangeable sites). The annealing experiments have shown that the lowest energy structure has the space group $I\bar{4}2D$. The temperature dependent properties were calculated in the range of 300-2000 K with a step of 50 K. A rapid increase in the enthalpy of disorder was observed at about 500 K. These results thus suggested that at temperatures below 500 K Na and Mg in NaGrt are ordered within the tetragonal structure, while at the higher temperatures NaGrt is disordered and has cubic symmetry. The equations of state of the tetragonal Na-majorite and Na-pyroxene (NaPx) of $NaMg_{0.5}Si_{2.5}O_6$ composition [Angel et al., 1988] were determined based on ab initio calculations using the CASTEP code []. The calculated volumes at 0, 5, 10, 15 and 20 GPa were fitted to the second order Murnaghan equation. The calculated bulk modulii of NaPx and NaGrt are 112.2 GPa and 165.5 GPa, respectively. Our calculations show that NaPx transforms to NaGrt at zero K at about 12 GPa. Our estimates based on lattice dynamics calculations suggest that the temperature is likely to shift the transformation boundary to a higher pressure.

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