Molecular dynamics simulation of majorite solid solution

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A molecular dynamics method was applied to majorite solid solution $Mg_3Al_2Si_3O_{12}$-$Mg_4Si_4O_{12}$ by using two-body interatomic potential model CMAS94 (Matsui, 1994), in order to predict the compositional dependence of cell parameters, volume, bulk modulus, and molar enthalpy. The following two types of solid solutions were made: (1) Tetragonal solid solution with the ordering of Mg and Si on the two nonequivalent octahedral sites. (2) Cubic solid solution with the random distribution of Mg and Si in the octahedral site. In Al-enriched composition, the two solid solution models give almost the same values of molar volume, bulk modulus, and molar enthalpy. With the decrease in Al-content, the cubic solid solution becomes to show larger molar volume, smaller bulk modulus, and higher enthalpy.