Molecular dynamics simulation of mixing properties in forsterite-monticellite system

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The mixing properties in forsterite (Fo) - monticellite (Mnt) system were studied using molecular dynamics (MD) simulations. Calculations based on two models were carried out, one is the model randomly putting the Ca ions into M2 site in the MD cell (random model) and another is the model putting the Mnt-cluster constructed by various Mnt-cell size into the MD cell (Mnt-cluster model). MD simulations of random model shows that Vex, bex and cex are positve values and do not conform to the experimental result obtained by Adams and Bishop (1985). On the other hand, MD simulations of various Mnt-cluster models are not entirely in agreement on the experimental data, but in some Mnt-cluster model, some of Vex, bex, and cex have negative values and are consistent with the experimental data. These results show that Mnt-cluster model is more appropriate than random model.