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AMORPHOUS MATERIALS: PROPERTIES, STRUCTURE, AND DURABILITY†

Atomic structure and transport properties of MgO-Al_2O_3 melts: A molecular dynamics simulation study

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ABSTRACT

Refractory oxide melts of the binary system MgO-Al_2O_3 have been studied by molecular dynamics simulation using an advanced ionic interaction model derived from first-principles. The simulations reproduce well experimental densities, structure factors, and transport properties. Anomalous behavior of the latter was observed as a function of melt composition. The minimum in the Al self-diffusion and the respective maximum in the shear viscosity around $MgAl_4O_7$ composition are explained by structural changes in the melt.

Keywords: Molecular dynamics simulation, Al_2O_3, MgO, melt, structure, viscosity, diffusion