THERMODYNAMIC PROPERTIES OF ALUMINUM OXIDE FROM DENSITY FUNTIONAL THEORY-BASED CALCULATIONS

A. A. Rykounov

FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin», Snezhinsk, Russia

The thermodynamic properties of aluminum oxide (III) in its solid, molten and warm-dense-matter states were predicted through calculations by density functional theory methods. The range of thermodynamic quantities is much wider than in the previous atomistic simultions due to the use of the extended first principles molecular dynamics (ExtFPMD) method. It covers densities from 4 to 17 g/cm^3, temperatures from 0 to 1.5 MK, and pressures from 0 to 720 Mbar which allows direct comparison between calculations from first principles and calculations with one-center models. Calculated results are shown to be in good agreement with data from experiments on the static and shock loading of the materail (in the form of corundum, sapphire and ruby) as well as with other non-empirical calculations.