Abstract

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The Effect of Pressure on System Temperatureof ZnO a Molecular Dynamics Prediction

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Abstract

The technique of Molecular Dynamics simulation is used to analyze the effect of pressure on the system temperature of Zin Oxide using dl_poly_4 software. In order to analyze our data we use an extended range of pressure and temperature 0-200GPa and 300-3000K respectively, we study in this work the effect of low and high pressure on the system temperature, and its evolution in time where at high temperature and low pressure thereis an oscillation of temperature around the equilibrium position.. The interatomic interaction is modeled by the Coulomb-Buckingham potential. Our data are in agreement with some available results due to no more work under the previous extreme conditions of pressure and temperature. This work has great importance in pharmacy, medicine, nanotechnology industry and in geophysics, but needs confirmation in future.

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Biography

Yahia CHERGUI is a lecturer in Electrical & Electronics Engineering Institute, Boumerdes Algeria. He has completed his PhD from Badji Mokhtar University in Annaba, Algeria. He did all his PhD work in Cardiff University in UK. His research field is Physics(condensed matter, simulation by molecular dynamics). He is a lecturer in Boumerdes University(Electrical & Electronics Engineering Institute) since 2012. He has many published articles and international conferences. He has been serving as a referee with condensed matter journal (IOP), Energy journal (Elsevier), and recently accepted to be a reviewer of American Journal of Modern Physics.

