Equilibrium Time of System Temperature and Phase Transition Under High and Low Pressure and Temperature of ZnO Wurtzite Structure, a Molecular Dynamics Prediction.

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Abstract

The parallel molecular dynamics and dlpoly_4 are investigated to study the equilibrium time of system temperature of ZnO wurtzite phase under low and high temperatures and pressures using the range of 300-3000K and 0-200GPa respectively. The interatomic interaction is modelled by Buckingham-Coulomb potential, we analysed the equilibrium time of system temperature and system temperature evolution under different pressures and temperatures. Our work is in agreement with available data, which confirm the phase transition from the wurtzite phase to rocksalt .We tried to confirm that the equilibrium time of system temperature versus pressure can give the transition pressure. This technique needs more work for confirmation. Our results are important in industry, medicine, pharmacy, nanotechnoly, and geophysics.



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.*