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MOLECULAR DYNAMICS STUDY OF STRUCTURAL PROPERTIES OF Ti57 NANOCLUSTER

Recently, there has been a renewed interest in the experimental and theoretical studies of atomic molecular clusters. Small nanoclusters exhibit physical and chemical properties that are often different from the bulk phase due to the large fraction of surface atoms. It is in this context that we initiated this study to investigate how the nanocluster behaves concerning an increase in temperature. Particularly, the titanium metal clusters have not been extensively studied. Molecular dynamics simulations were carried out for Ti57 nanoclusters in a vacuum using Gupta potentials for metal-metal interactions potentials. The classical molecular dynamics simulation software (DL_POLY) was used to investigate the temperature effects on pure Ti57 metal nanocluster. The dynamical properties vacuum environment were interrogated by subjecting the nanoclusters to various temperatures in the range of 300 – 2400 K. The radial distribution functions (RDFs), diffusion coefficient, density profiles and Mean square displacement (MSD) were examined to study the structural changes as a function of temperature. It was found that the vacuum structures melting point reasonably correspond with the experimental data. The phase transitions from solid to liquid have been identified by a simple jump in the total potential energy curve. Furthermore, the RDFs and density profile peaks decrease as the temperature is increased and the potential energy increases as a function of temperature. The density profiles depicted the solid-like features indicated by the distinct peaks at lower temperatures.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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