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The thermodynamic phase transitions in Ti17 metal nanocluster: A molecular dynamics study

Titanium clusters are one of the central theme in cluster science to investigate the evolution of the electronic, structural and magnetic properties of the metal clusters as a function of cluster size. Nanoclusters provide a nice prototype to investigate and understand the thermodynamics of finite systems. Small nanoclusters exhibit physical and chemical properties that are often different from the bulk phase. In particular, the titanium metal clusters have been shown to strongly dependent on their internal clusters energy which dictates the geometrical arrangement and growth patterns. In this study, classical molecular dynamics simulation software (DL_POLY), on normal queue, using 8 notes and 24:00 walltime was used to investigate the temperature effects on pure Ti17 metal nanocluster. The dynamical properties were interrogated by subjecting the nanoclusters to various temperatures in the range of 300 – 2400 K. The radial distribution functions, density profiles and potential energies were examined to study the structural changes as a function of temperature. It was found that the vacuum structures undergo several transitions as a function of temperature. The phase transition from solid to liquid has been identified by a simple jump in the total potential energy curve. Furthermore, the RDF's peaks decrease as the temperature is increased and the potential energy smoothly increases with temperature. These observations are important in the production of titanium metal and development of titanium metal components for industrial and aerospace applications

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