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Temperature effect on Ti13 metal cluster: A molecular dynamics study

Titanium clusters is 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. 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 dictate the geometrical arrangement and growth patterns. In this study, classical molecular dynamics simulation software (DL_POLY), on normal queue, using 8 nodes and 24:00 walltime was used to investigate the temperature effects on pure Ti13 metal nanocluster. The dynamical properties were interrogated by subjecting the nanocluster to various temperatures in the range of 300K – 2300K. The radial distribution functions and MSD were examined to study the structural changes as a function of temperature. It was found that the structure melting point reasonably correspond with the experimental data. The phase transition from solid to liquid have been identified by a simple jump in the total potential energy curve. Furthermore, the RDF's peaks decreases as the temperature is increased and the potential energy increases as a function of temperature. This observations is important in the production of titanium metal and development of titanium metal components for industrial and aerospace applications. Centre for high performance computing Lengau cluster played a significant role in computing the dynamics on Ti13 system.

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