Molecular dynamics study of structural properties of Ti_{57} nanocluster

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SAIP 2021, 22-30 July

Introduction

Titanium and its alloys exhibit very attractive properties such as low density, high strength and good corrosion resistance that are exceptionally useful in various applications such as sporting to aerospace. Metallic nanoclusters have been of great importance in both theoretical and experimental researches due to their chemical, physical and electronical properties [1,2] which find them suitable for potential chemo – bio sensory materials. The melting process and thermodynamics properties of particles at nanometer length-scales are of interest because of their dramatically different behaviour from bulk materials [3,4]. Obtaining the structural information for small nano-sized particles from experimental work is, however, extremely difficult. Therefore, computational simulation techniques are often used as a complementary predictive tool or an aid in the analysis of experimental observations. Theoretical investigations of the melting behaviour of clusters and nanowires have been mostly studied by means of Monte Carlo (MC) and Molecular Dynamics (MD) computer simulations. The focus was mainly on investigating the melting temperature and thermal stability during the growth process, the structural evolutions and the relationship of structural characteristics with temperature. In the current study, we present the thermodynamic effect on the 57 atoms Ti cluster (Ti_{57}) at various temperatures.

Structures and Applications

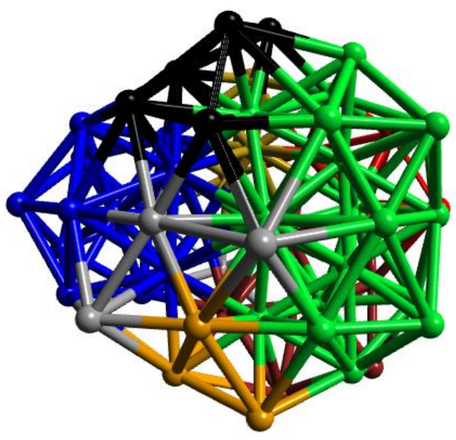

Figure 1: Ti_{57} nanocluster coordinated by icosahedral shape fragmentations.

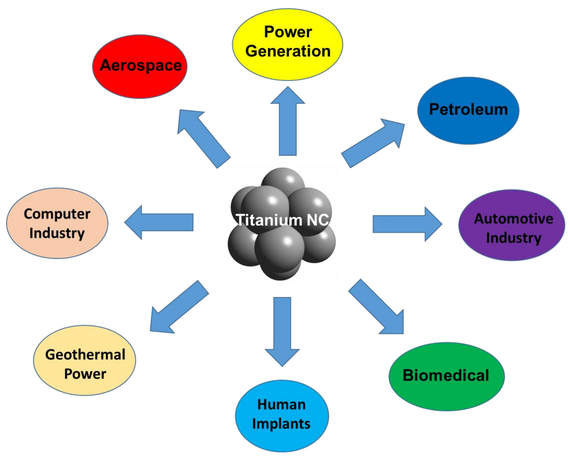

Figure 2: Schematic representation for various applications of titanium metal nanoclusters (Ti-M-NCs).

Results and Discussions

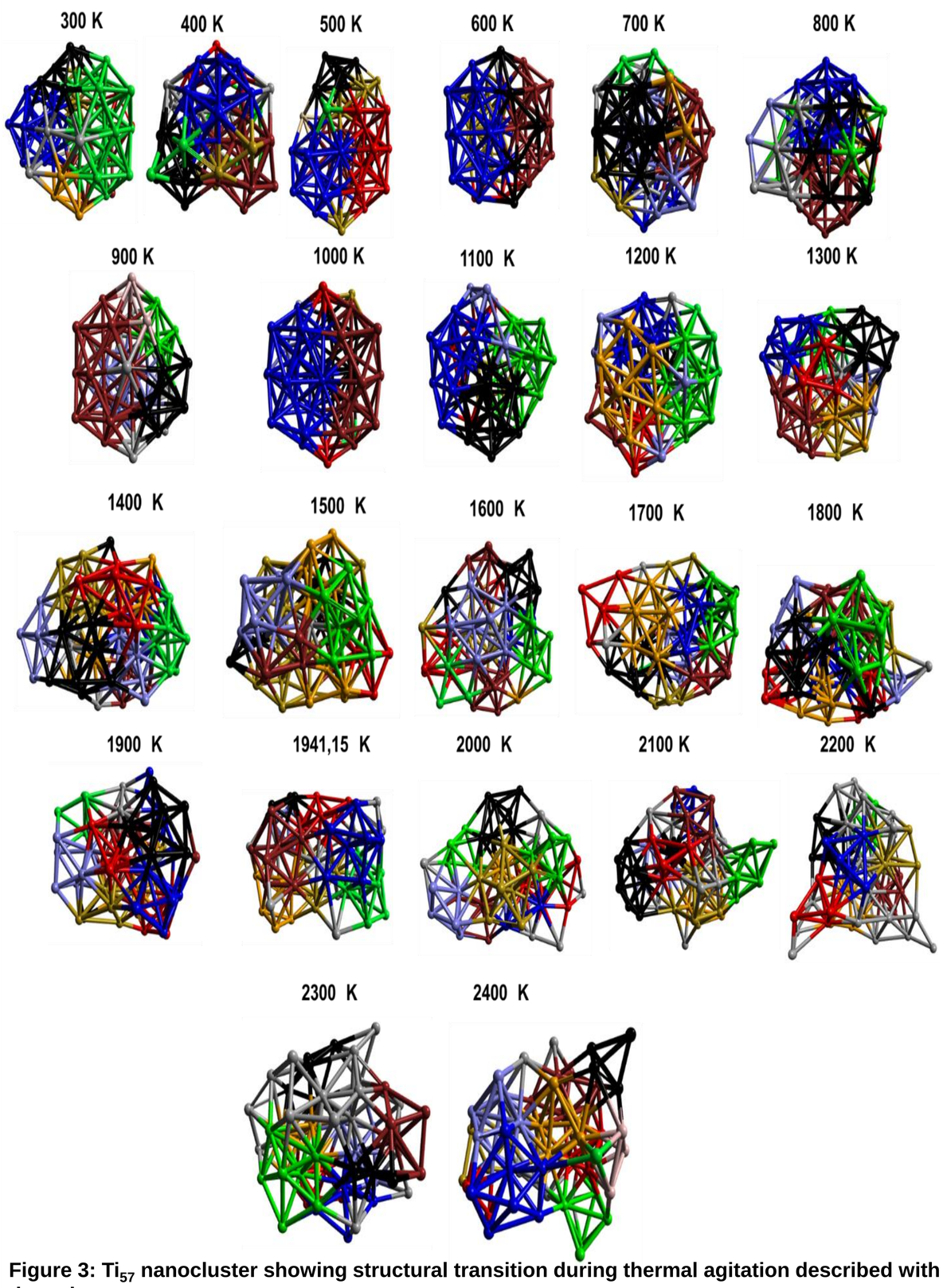

Figure 3: Ti_{57} nanocluster showing structural transition during thermal agitation described with the colors.

Figure 3 depicts the Ti_{57} nanocluster having structural transitions dominated by into two interpenetrating icosahedral isomers (mostly colored maroon, green, red and blue) and icosahedral isomers (black, blue and maroon) from **300 – 1200 K**. However, at elevated temperatures (**1800 – 2400 K**), the transitions of the nanocluster is dominated by pentagonal bipyramid which does not follow the transition patterns at moderate temperatures. The structural transition at the bulk Ti melting point (**1941.15 K**) is observed to be dominated by pentagonal bipyramid fragments. Furthermore, there is a dominants of triangular bi-pyramidal fragments at **2000 – 2400 K**.

Methodology

We used the Knowledge Led Master Code (KLMC) [5] with genetic algorithm (GA) to generate the lowest energy structures of Ti_N (N= 2-57). A GA search was done using an interatomic potential (IP) to identify the candidate structures for local minima up to clusters containing 57 atoms. MD simulations were employed to study the structural and dynamical properties of the Ti nanoclusters. The MD simulations were carried out in the canonical ensemble (NVT) with a time step of 0.001 ps. All of the simulations were made by the DL_POLY package [6]. Based on approximation of tight-binding theory, the Gupta potential [7] is introduced and the ion–ion interaction is described by an electronic band term and a repulsive term. These calculations were possible by using 8 nodes for nanoclusters from 2 to 57 atoms.

Results and Discussions

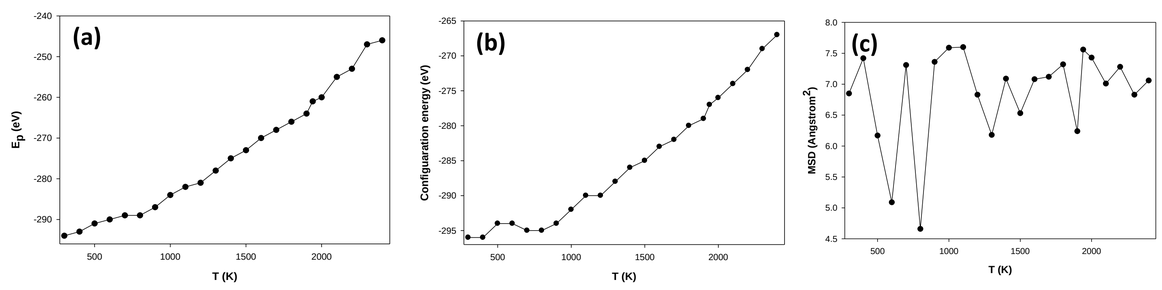

Figure 4: (a) Total energy, (b) configuration energy (c) Mean square displacement (MSD).

Figure 4 shows the total energy varying smoothly with temperature during thermal agitation. The configuration energy does not vary smoothly with temperature at **500 – 600 K**, however, stabilizes at 700 – 800 K. MSD shows a high degree of fluctuations from **300 – 1300 K** and the nanoclusters stabilizing at **1400 – 2400 K** temperature range. At **800 K** and **1900 K** the fluctuations are observed to be slightly steep more than their neighbouring thermal agitated configurations. These may be due to the nanocluster exhibiting molecular behaviour since the nanoclusters are below 500 atoms

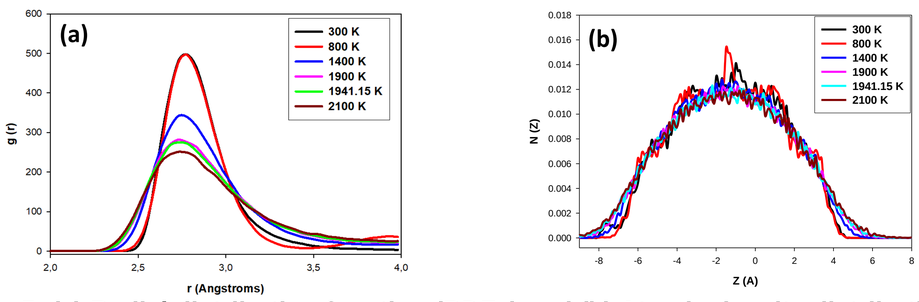

Figure 5: (a) Radial distribution function (RDFs) and (b) Atomic density distribution

Figure 5 shows the RDFs and density profiles which are suitable to measuring the structural variation at finite temperature. The RDFs and density profile peaks decrease with increasing temperature. Their peaks becomes broader and decrease with height due to randomly distributed atoms in liquid phase. Moreover, for atomic density distribution, the position of the peaks at **300 K** and **800 K** remains relatively similar, but the atomic distribution at **300 K** shifts from 4.7 Å to 5.8 Å as the temperature reaches **1400 K**. The peaks – peak separation is not that clear but there is a slight reduction in the magnitude of the peaks. The **2100 K** peak is observed to have a reduced magnitude and shifted from 4.7 Å at **300 K** to 7 Å **at 2100 K** along the z-axis, signaling the existence of solid-liquid transition above the melting point.

Conclusion

- The molecular dynamics study for Ti_{57} were determined.
- The thermodynamics analysis predicted transition of the nanocluster at lowest temperatures.
- The potentials energy varies smoothly with temperature. The configuration energy shows destabilization that is attributed to the loss of energies observed at **500 – 600 K** and stabilizing at **700 – 800 K**.
- The MSD depicted a high degree of fluctuations from **300 – 1300 K** and the nanoclusters stabilizing at **1400 – 2400 K** temperature range.
- The RDFs peaks become broader with increasing temperature. For the atomic density distribution, the position of the peaks at **300 K** and **800 K** remains relatively similar, but the atomic distribution at **300 K** shifts from 4.7 Å to 5.8 Å as the temperature reaches **1400 K**.

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Acknowledgments

Newton Fund, UCL, CHPC Centre for High Performance Computing, NRF National Research Foundation, University of Limpopo Faculty of Science and Agriculture, South African Institute of Physics

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