Contribution ID: **369** Type: **Oral Presentation**

Structure and dynamics of noble gas temperature control on Ti metal clusters

Thursday, 28 June 2018 10:20 (20 minutes)

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. The atomic structures and dynamics of nanoclusters have been of crucial importance in both experimental and theoretical studies owing to their useful physical and chemical properties in various industrial applications. 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, molecular dynamics simulation was used to investigate the temperature effects on pure Ti metal nanoclusters in both vacuum and under pressure of Argon gas. The effect of gas phase environment on the structural growth and dynamical properties was interrogated by subjecting the nanoclusters to various temperatures in the range of 300K – 2000K. The radial distribution functions and diffusivity were examined to study the structural changes as a function of temperature. It was found that the gas phase and the vacuum structures melting point correspond well with the experimental data. Furthermore, the diffusivity of both the gas phase and vacuum increases as the temperature is increased. This observations is important in the production of titanium metal and development of titanium metal components for industrial and aerospace applications

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Prof P. E. Ngoepe
Phuti.Ngoepe@ul.ac.za
University of Limpopo

Prof H. R. Chauke
Hr.Chauke@ul.ac.za
University of Limpopo

Primary author: Mr PHAAHLA, Tshegofatso Michael (University of Limpopo)

Presenter: Mr PHAAHLA, Tshegofatso Michael (University of Limpopo)

Session Classification: Physics of Condensed Matter and Materials

Track Classification: Track A - Physics of Condensed Matter and Materials