

SAIP 2011



Contribution ID : 319

The reduction of melting temperature with size in Gold

Wednesday 13 Jul 2011 at 17:00 (02h00')

Content :

The importance of gold for scientific use is of fundamental importance to research and technology developments. The bulk gold shows reluctance to participate in chemical reactions, the effect which has been corrected by the change in the size towards nanoclusters and, this makes the study of temperature effects on gold very important. We have performed molecular dynamics simulations on bulk and nanomaterials of gold at various temperatures to study the effect of size on the melting temperature. Melting temperature of bulk gold was determined to be 1320 K and this in good agreement with the experimental value of 1337 K. Different gold nanoclusters and nanotubes melt at temperatures lower than 1200 K which is a significant decrease in the melting temperature from the bulk. The face centered cubic (fcc) bulk gold structure remains intact at high temperatures while spherical nanoclusters and cylindrical nanotubes respectively transform into tetragonal structures and patches of spherical clusters.

Level (Hons, MSc, PhD, other)? :

PhD

Consider for a student award (Yes / No)? :

No

Short Paper :

Yes

Primary authors : Mr. MAHLADISA, Mokete (University of Limpopo (Turfloop campus))

Co-authors : Prof. NGOEPE, Phuti (University of Limpopo (Turfloop Campus)) ; Dr. ACKERMANN, Lutz (University of Limpopo (Turfloop Campus))

Presenter : Mr. MAHLADISA, Mokete (University of Limpopo (Turfloop campus))

Session classification : Poster1

Track classification : Track A - Condensed Matter Physics and Material Science

Type : Poster Presentation