Melting of Cubic Boron Nitride Nanoparticles: A Molecular Dynamics Study

Hsiao-Fang Lee[1], Keivan Esfarjani[1], Assimina A. Pelegri[1], Bernard H. Kear[2], and Stephen D. Tse[1*]

[1]*Mechanical and Aerospace Engineering, Rutgers University, Piscataway, NJ 08854, US*
[2]*Material Science and Engineering, Rutgers University, Piscataway, NJ 08854, US*

Abstract

Molecular dynamics (MD) simulations on cubic Boron Nitride (c-BN) nanoclusters are presented in this study. Using a Stillinger-Weber potential, the stability of the nanoparticles is determined to be strongly surface dependent. The surface energies of the (100), (110) and (111) facets of c-BN are found to be Υ_{100}=-1.0438, Υ_{110}=-1.9524 and Υ_{111}=-2.1240, respectively. Hence, a faceted octahedron nanoparticle is most stable due to its (111) facet termination, while surface reconstruction is observed on the (100) facet termination of c-BN nanoparticles. Nanoparticles have a much higher surface-area/volume ratio than the corresponding bulk material, so surface phenomena become more important in nanoclusters, including melting of c-BN nanoclusters. The melting behavior of our nanoparticles is unlike bulk materials having critical melting points where a phase transition of the entire crystal occurs, instead our nanoparticles possess a core versus shell melting property.