University of Texas at San Antonio

Department of Physics & Astronomy

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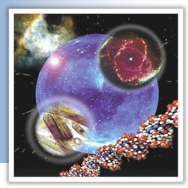
Time: 3:00 p.m.-4:00 p.m.

Recent Findings on Nanotructural Response and Bio-Nano Interaction

Due to the limitation of experimental techniques available and the need for cost-effective designs, Simulation-Based Engineering and Science (SBES) is playing an increasingly important role in engineering practice. In this presentation, an introduction will be given on multi-scale model-based simulation. Recent research findings on nanostructural responses and bio-nano interactions will then be presented to illustrate the potential of SBES. In particular, molecular dynamics simulation results are given to demonstrate the nanostructural response to extreme loading conditions. It is found that the impact response at nanoscale is size-dependent while the aspect ratio has a negligible effect. It is also observed that the evolution speed of disordered atoms diffused from the impact surface first approaches the shock wave speed, and then slows down to form dislocations. The thermal gradient in the target is mainly due to the temperature difference between hcp zones and fcc atoms. The continuum equation relating the stress to the particle velocity, which is based on the half-space derivation without considering the impact surface corner effect, is not valid for the finite nano structures. In addition, the recent simulation results related to the interaction between nano particles and living cells are shown to explore the effects of nano technology on the environment and life science. The future research directions in SBES will be discussed to conclude the presentation.



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