

Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

Shock-Wave

Propagation

Study in Fe₂O₃+Al Energetic Nanocomposites Using Classical Molecular Dynamics Simulations VIKAS TOMAR, MIN ZHOU, Georgia Institute of Technology — Classical molecular dynamics (MD) simulation is an important technique for analyzing custom-designed nanostructured materials and nano-sized systems such as nanowires and nanobelts. This research focuses on the effect of shock wave propagation in Fe₂O₃+Al nanointerfaces. A generic potential form is used to describe the behavior of the Fe+Al+Fe₂O₃+Al₂O₃ system over a range of mechanical loading rate and temperature. The potential is able to describe bulk single crystal behavior of Fe, Al, Fe₂O₃, Al₂O₃ as well as interfacial transitions among them. Shock-wave propagation analyses over a range of plate impact velocities are used to reveal the effect of the correlation between nanoscale phase morphology and applied loading on the desired mechanical attributes. Effect of orientation of bicrystals interface on shock wave defect formations in various crystalline orientations of fcc-Al is also investigated.

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Date submitted: 31 Mar 2005

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