11th. World Congress on Computational Mechanics (WCCM2014)
5th. European Conference on Computational Mechanics (ECCM V)
6th. European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

Molecular Dynamics Simulation of the Rate-Dependent Nanostructural Transition under High Pressure

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Key words: Nanostructures, Soft-Hard Material Interaction, Molecular Dynamics.

ABSTRACT

Crystal plasticity under non-hydrodynamic loading is related to both external sample geometry and internal structure. We report our recent findings, with molecular dynamics simulation, on the rate-dependent nanostructural transition induced by hard (copper)-soft (krypton) crystal interaction under hydrodynamic loading. With copper crystals of different types of geometry being embedded into the hydrodynamically compressed krypton atoms, the size effect on the pressure-volume relation of copper, as observed from impact tests, diminishes while the stress state in copper deviates from hydrodynamic one to non-hydrodynamic one that results in the rate-dependent nanostructural transition in krypton. The mechanism governing this transition due to the hard-soft crystal interaction might be explained by the geometric effect on the indentation process in crystalline materials, and could provide a potential route to effectively make the nanocomposites with specific nanostructures in an extreme environment.