14th World Congress on Computational Mechanics (WCCM XIV)
8th European Congress on Computational Methods in Applied Science and Engineering (ECCOMAS 2020)
July 19- 24, 2020, Paris, France

LATTICE BOLTZMAN METHOD FOR SOLIDS WITH POLYMORPHIC PHASE TRANSFORMATION IN EXTREME CONDITIONS

TRACK NUMBER 21….

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Key words: Multi-scale, thermodynamics, shock compression, condensed matter, phase transformation. Polymorphic behavior.

ABSTRACT

Many materials can experience polymorphic behavior under extreme conditions. Shock compression and high pressure result in extreme strain rates and high temperature and could result in polymorphic states, crystallization, densification, devitrification, and chemical reactions - many irreversible processes. To understand thermodynamics of this behavior under extreme conditions and develop Equation of State of these phases, experimental methods and diagnostics, are guided by computational methods to understand the conditions under which transformations occurred.

The Lattice Boltzmann Method LBM developed in the past three decades has proven to be a powerful computational method in hydrodynamics with many computational advantages when dealing with large number of microprocessors over other methods in solving Navier-Stokes equations in extremely complex computations.

The Mini-symposium is seeking papers on new computational codes, which are based on LBM approach and thermodynamic framework, thus incorporating Boltzmann thermodynamics equations, with conservation laws to formulate discretization of the continuum. Using this thermodynamic framework results in a true multi-scale computational approach, in addition it should dictate the scale of the molecular dynamics MD to the continuum, and the limits of discretization error.

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