MOLECULAR DYNAMICS/STATICS SIMULATION OF NI-AL NANOPARTICLES SINTERING

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ABSTRACT

Keywords: Sintering, Powder Material, Ni-Al, Molecular Dynamics, Molecular Statics.

Molecular dynamics (MD) [1] and molecular statics (MS) [2] simulations using embedded-atom method (EAM) potential [3] were performed to investigate the sintering process [4] of Ni-Al nanoparticles system. The effects of simulated crystal orientation on different physical quantities, i.e. sintering geometry, self-diffusion coefficient D, per-atom stress, centro-symmetry parameter, the radial distribution function and the coordination number for sintered particles, were studied. The objective of the studies is to estimate the parameters of the sintering model at micro-scale.

In molecular dynamics simulations the values of critical time steps are usually of the order of 10^{-15} s [1] while the sintering time is counted in minutes [4]. Technique of increasing the critical time step by mass scaling is widely used in explicit finite element simulations as well as in the discrete element analyses [4]. The use of similar concepts in molecular dynamics simulations of the sintering process and even a replacing the molecular dynamic calculations by molecular static ones [2] were also investigated.

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