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Mechanical and Thermal Properties of Nickel by Molecular Dynamics

Hassan Chamati, **Kostadin G. Gaminchev**

Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee, Blvd. 1784 Sofia, Bulgaria

Abstract. We study the thermal and mechanical properties of Nickel at low temperatures and high pressures via Molecular Dynamics in conjunction with embedded-atom method [1-3], its modified counterpart modified [4] and the angular-dependent potentials [5]. We computed the linear-thermal expansion coefficients, mean-square displacements, velocity-auto correlation functions, phonon-dispersion curves, as well as elastic moduli of the element under positive loading at finite temperatures.

The results from the above mentioned three potentials are compared to experimental data, when available. The differences between the results obtained with these potentials are discussed.

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