J. At. Mol. Sci.
doi: 10.4208/jams.310810.200910a

Vol. **2**, No. 1, pp. 10-19
February 2011

Thermoelastic properties of nickel from molecular dynamic simulations

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Received 31 August 2010; Accepted (in revised version) 20 September 2010
Published online 17 January 2011

Abstract. The structures and elastic constants of face-centered-cubic (fcc) structured nickel at high temperature have been calculated for the first time using molecular dynamics (MD) with the direct method and the quantum Sutton-Chen (Q-SC) potential. The obtained thermoelastic constants are in excellent agreement with the experiment data. Calculated results for the radial distribution function show that the short-range atomic order of low-T is similar to the high-T solid with the applied temperatures. The thermoelastic constants, the bulk and shear modulus as a function of the applied temperature are presented. An analysis for the calculated parameters has been made to reveal mechanical stability of nickel up to 1300 K.

PACS: 46.25.Hf, 02.70.Ns

Key words: elastic properties, molecular dynamics, nickel

1 Introduction

Nickel, a d-band transition metal, is very important materials owing to broadly industrial applications such as catalysis, rechargeable batteries, and so on [1–3]. As an important transition metal in the field of condensed matter physics, it has recently attracted tremendous experimental and theoretical interest in its wide range of properties including the equation of state (EOS) [4], the elastic [5–7], transport properties [8–10], and melting properties [11–15], etc.

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Knowledge of thermoelastic constants is fundamental for describing the mechanical properties response of a material to applied sound velocity, anisotropy, thermoelastic stress, load deflection, fracture toughness, etc, so a complete set of single-crystal thermoelastic properties as a function of temperature is desirable. To date, several theoretical methods are applied to calculate the elastic constants, such as the tight-binding method (TB) [6], the $ab\ initio$ density-functional theory method (DFT) [7, 16], the full-potential linear muffin-tin orbital method (FP-LMTO) [17–19], and the molecular dynamic (MD) simulation methods [20–27]. For the fcc structured nickel, the theoretical investigations of elastic properties have been performed [6,7]. For example, Papanicolaou *et al.* [6] applied the tight-binding method (TB) and obtained the elastic constant, but C_{11} and C_{12} are relatively larger than experimental data [5].

In this work, we focus on the temperature dependence of elastic constants of the fcc structured Ni from MD simulation, in which the intramolecular forces are modeled by using the quantum Sutton-Chen (Q-SC) potential [28]. The validated of the Q-SC potential is confirmed by reproducing the density, cohesive energy, bulk modulus, surface energy, etc. In Section 2, the computational parameters for calculation will be presented in detail. In the following section, the theoretical result of the thermoelastic properties are listed and discussed. Finally, conclusions are summarized in Section 4.

2 Theoretical methods

In this work, we have adopted the quantum Sutton-Chen (Q-SC) potential as the reference potential. In the Q-SC potential [28], the total potential energy of the metal is given as follows

$$U_{tot}=\sum_i U_i=\sum_i \varepsilon\left(\sum_{j\neq i}\frac{1}{2}V(r_{ij})-c\sqrt{\rho_i}\right), \tag{1}$$

where $V(r_{ij})$ is a pair potential defined by the following form

$$V(r_{ij})=\left(\frac{a}{r_{ij}}\right)^n, \tag{2}$$

which accounts for a two body repulsive interaction between the atoms i and j, ρ_i is a local density representing the cohesion associated with atom i defined by

$$\rho_i=\sum_{j\neq i}\phi(r_{ij})=\sum_{j\neq i}\left(\frac{a}{r_{ij}}\right)^m. \tag{3}$$

In Eqs. (1)-(3), ε sets the overall energy scale, r_{ij} is the distance between the atom i and j, a is an arbitrary length parameter leading to dimensionless for $V(r_{ij})$ and ρ_i, c_i is a dimensionless parameter scaling the attractive term relative to the repulsive term, n and m are positive integer parameters such that $n>m$. The fitted parameters for Ni [28] are $n=10$, $m=5$, $\varepsilon=0.0073767$ eV, $c=84.745$ and $a=3.5157$ Å.