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Study on the structural transition and thermal properties of Ni_3Nb-$D0_{22}$ phase: First-principles calculation

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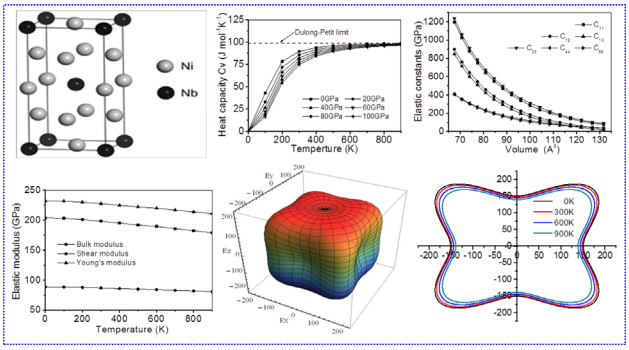
HIGHLIGHTS

- Structural transition and thermal properties of Ni_3Nb-$D0_{22}$ phase are studied by first-principles calculation.
- Structural transition from Ni_3Nb-$D0_{22}$ to Ni_3Nb-$D0_a$ occurs at the temperature range of 950–960 K.
- Heat capacity tends to Dulong-Petit limit when the temperature is higher than 900 K.
- Ni_3Nb-$D0_{22}$ phase is anisotropic and has a distinct dependence on crystal orientations.

GRAPHICAL ABSTRACT



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ABSTRACT

The structural transition and thermal properties (thermodynamic and thermoelastic properties) of Ni_3Nb-$D0_{22}$ phase are investigated by first-principles combined with quasi-harmonic approximation method. The computed results show that the structural transition from Ni_3Nb-$D0_{22}$ to Ni_3Nb-$D0_a$ primitively occurs at the temperature range of 950–960 K. The phase structure is thermally stable but easily compressed. The heat capacity tends to Dulong-Petit limit when the temperature is higher than 900 K. The computed thermoelastic properties of Ni_3Nb-$D0_{22}$ phase reveal the slight softening trends with the increased temperature, indicating that the Ni_3Nb-$D0_{22}$ phase is well heat-resistance. Additionally, Ni_3Nb-$D0_{22}$ phase is ductile at the temperature range of 0–900 K, and its hardness decreases with the increased temperature. Moreover, the Ni_3Nb-$D0_{22}$ phase is anisotropic and has a distinct dependence on crystal orientations. The strengths of chemical bond along [100] and [010] orientations on (001) plane are slightly weakened with the increase of temperature.

1. Introduction

Ni-based superalloys, which have marvelous performance including high strength, excellent erosion resistance and fatigue resistance at elevated temperatures, are widely used in aircraft industry [1–6]. During hot forming of superalloys, the phase stability and thermal properties are quite vital to in-service performance of final products. Usually, the thermal properties refer to heat capacity, thermal expansion, thermal

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Table 1
The specific parameters in geometry optimizing calculation and elastic constants calculation.

Parameters	Geometry optimizing calculation	Elastic constants calculation
Energy	1.0×10^{-5} eV/atom	2.0×10^{-6} eV/atom
Maximum force	0.03 eV/Å	0.006 eV/Å
Maximum ionic displacement	0.001 Å	2.0×10^{-4} Å
Maximum stress	0.05 GPa	\
Self-consistent field tolerance	5.0×10^{-7} eV/atom	\
Maximum strain amplitude	\	0.003 GPa

equilibrium volume and thermoelastic properties, which are used to identify high-temperature deformation capacity of materials. The morphologies and distribution of phases in the formed parts are affected by phase transition during hot working, which determine the plasticity, strength and hardness of products [7–10]. Generally, first-principles calculation can be used to study the phase transition and mechanical properties of some alloys [11–16]. Also, the structural or electronic properties of some other materials were investigated by first-principles method [17–20].

The mechanical properties of Ni-based superalloys are significantly affected by the final microstructures [21–23]. Especially, the Ni_3Nb phases greatly affect the hot deformation behaviors and mechanical properties of materials [24,25]. Ni_3Nb phase is an intermetallic compound which includes two main structures, one is ordered body-centered tetragonal crystal structure ($D0_{22}$) named γ″ phase, while the other is orthorhombic crystal structure ($D0_a$) named δ phase [26]. The γ″ phase usually precipitates at the temperature range of 868–1143 K, and is identified as the primary strengthening phase for the Ni-based superalloy containing Nb element [27]. Furthermore, γ″ and δ phases start to dissolve at the temperatures of 923 K and 1253 K, respectively. The complete dissolving temperatures of γ″ and δ phases are 1223 K and 1293 K, respectively [28]. Most γ″ phases would dissolve at 1173 K [29]. In addition, the mechanical properties, especially creep and tensile strengths, are vastly affected by the sizes of γ″ precipitates [30,31]. Lu et al. [32] found that γ″ phases have precipitation strengthening and coherency strain hardening below 923 K. The precipitation of γ″ phases can also improve micro-hardness of superalloys [33]. Wei et al. [34] presented a preferential oxidation mechanism of γ″ precipitates which significantly accelerate the crack growth in Ni-based superalloy. Devaux et al. [35] developed the coarsening kinetic model of γ″ precipitates according to Lifshitz-Slyozov-Wagner theory. Xu et al. [36] conducted low cycle fatigue tests on IN718 alloy, and found that the microscopic deformation process is dislocation shearing of γ″ precipitates. Recently, a method based on first-principles [37] was extensively used to study physical properties of Ni-based superalloys. Wang et al. [38] combined phenomenological modeling and first-principles calculations to evaluate the lattice misfit between γ and γ' in Ni-based alloys. Lin et al. [31] found that the Ni_3Nb-$D0_{22}$ phase exhibits ductile and high elastic anisotropy at elevated pressures by first-principles calculations. Wen et al. [39] found that the thermal stability

Table 2
Meanings of symbols used in calculations.

$E(V)$	Total free energy per unit cell	ν	Poisson ratio
$F_{vib}(\Theta(V);T)$	Helmholtz free energy	M	Molecular mass per formula unit
k	Boltzmann constant	γ	Grüneisen parameter
n	Number of atoms per formula unit	ħ	Reduced Planck constant
$D(\Theta/T)$	Debye integral	C_V	Heat capacity
Θ	Debye temperature (Assuming an isotropic solid)	α	Linear thermal expansion coefficient

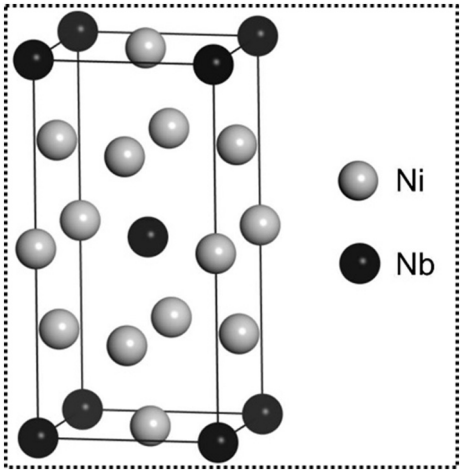

Fig. 1. The crystal structure of Ni_3Nb-$D0_{22}$ phase.

of Ni(001)/Ni_3Nb(001) interface is bad, but benefit for enhancing the mechanical properties of IN718 alloy. Dai and Liu [40] found that γ″ and δ phases have good ductility by first-principles calculations. Cao et al. [41] revealed that Ni_3Nb phase has a combination of ionic, metallic and covalent bonding properties by the first-principles calculations.

However, most previous researches mainly focused on the physical and mechanical properties of Ni_3Nb-$D0_{22}$ phase at 0 K and different pressures. Few reports systematically study the structural stability and thermal properties of Ni_3Nb-$D0_{22}$ phase at different pressures and temperatures. Meanwhile, it is quite hard to experimentally study the structural stability and thermal properties of Ni_3Nb-$D0_{22}$ phase at different pressures and temperatures. Nevertheless, the first principles calculation may be an available approach to research the related properties of Ni_3Nb-$D0_{22}$ phase at different temperatures and pressures. In the present paper, the influences of temperature and pressure on the phase stability, heat capacity, thermal expansion, elastic modulus, anisotropic elastic properties, Poisson ration and Vicker hardness are computed and discussed.

2. Computational methods

2.1. Computational parameters

The computations were executed with the CASTEP code in commercial software, Material Studio [37]. It is based on the implementation of the ultrasoft pseudopotential methods and the density functional theory [42]. The scheme of Perdew-Burke-Erzerhof was applied for the generalized gradient approximation [43]. The cut-off energy of plane wave and the k-point sampling of Brillouin zone were set as 420 eV and 10 × 10 × 8, respectively. Broyden-Fletcher-Goldfarb-Shanno methods was used to relax the structure [44]. The specific parameters

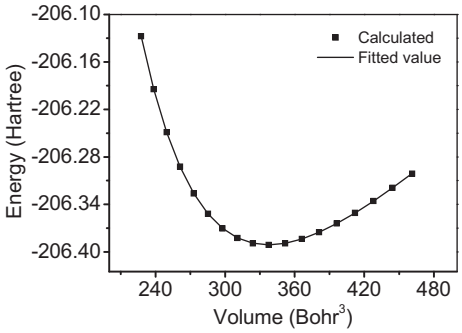

Fig. 2. Total energies versus the primitive cell volume of Ni_3Nb phase.