

First-principles investigations of structural and electronic properties of niobium nitrides under pressures

X. F. Li* and Z. L. Liu

College of Physics and Electronic Information, Luoyang Normal College, Luoyang 471022, China

Received 9 April 2011; Accepted (in revised version) 7 May 2011

Published Online 28 September 2011

Abstract. The ground structure, elastic and electronic properties of several phases of NbN are determined based on *ab initio* total-energy calculations within the framework of density functional theory. Among the five crystallographic structures that have been investigated, the hexagonal phases have been found to be more stable than the cubic ones. The calculated equilibrium structural parameters are in good agreement with the available experimental results. The elastic constants of five structures in NbN are calculated, which are in consistent with the obtained theoretical and experimental data. The corresponding Debye temperature and elastic anisotropies are also obtained. The Debye temperature of NbN in various structures consistent with available experimental and theoretical data, in which the Debye temperature of δ -NbN is highest. The anisotropies of ZB-NbN, NaCl-NbN, CsCl-NbN gradually increases. For hexagonal structure, the anisotropies of ϵ -NbN are stronger than that of δ -NbN. The electronic structures of NbN under pressure are investigated. It is found that NbN have metallization and the hybridizations of atoms in NbN under pressure become stronger.

PACS: 71.15Mb, 71.20.Be, 71.22.+i

Key words: phase transition, elastic constants, electronic structure, NbN

1 Introduction

The transition-metal nitrides are refractory compounds and put forward a technologically important series of materials. The compounds have a lot of interesting properties, such as high melting point [1], high hardness [2], superconductivity [3], magnetism [4] and so on. Because of these properties, they become the focus of view of fundamental studies. It is

*Corresponding author. Email address: lxfdjy@126.com (X. F. Li)

found that the superconducting temperature of solid solutions of NbN with rock salt structure reaches a maximum value of 17.8 K [5], which is comparable to that of Nb₃Sn and V₃Si [6].

Due to a great deal of attentions on NbN, several research groups have studied the physical properties of NbN theoretically and experimentally. Chen *et al.* [7] conducted the experiments on the high-pressure phonon spectra of transition-metal nitrides HfN, ZrN, and NbN by Raman-scattering measurements. Later using Raman scattering and x-ray diffraction Chen *et al.* [8] reported a quantitative study of pressure effects on the superconducting transition temperature T_c and the electronic stiffness of NbN, and they found that superconducting temperature T_c increases initially with pressure and then saturates up to 42 GPa. The equation of states, elastic properties and hardness of TMN (TM=Zr, Nb, Hf) [5] are investigated by angle-dispersive synchrotron powder x-ray diffractometry with a diamond anvil cell. It is found that NbN crystallized cubic structure and also have hexagonal structure experimentally [9]. The electronic structure of hex-NbN and NaCl-NbN are measured by X-ray photoemission spectroscopy and ellipsometric measurements [10]. Theoretically, the phase transition (NaCl→CsCl) and elastic properties of the selected transition metal nitrides are studied by two-body interionic potential theory [11]. The thermophysical properties of transition metal carbides and nitrides with NaCl structure were calculated using the Debye-Grüneisen model combined with *ab initio* calculations [12]. The elastic constants and electronic structure of transition metal nitrides and carbides are calculated using *ab initio* density functional perturbation theory [13]. The electronic structure and bonding mechanism of NbN and NbC are studied by means of the accurate first-principles total energy calculations using the full-potential linearized augmented plane wave method (FP-LAPW) [14]. The elastic constants of NbN (NaCl structure) are investigated under pressure up to 50 GPa within the framework of the density functional theory [5]. The mechanical properties of NbN in NaCl and NiAs structures have been reported by first-principles [15]. Wang *et al.* has calculated the structural phase transition in WC and NaCl structures and the hardness of NbN [16].

However, to our knowledge, the researches of fundamental physical properties of NbN focus on cubic structure, there are few reports on other hexagonal structures theoretically under pressure. In the present paper, we investigate the structure and fundamental physical properties of niobium nitrides for all possible cubic and hexagonal structures by the plane-wave pseudopotential density functional theory method through the Cambridge Serial Total Energy Package (CASTEP) program [17]. In this work, the mechanical properties and electronic structures of the five different structures of NbN are studied: NaCl structure (Fm-3m); CsCl structure (Pm-3m); ZB structure (F4-3m); hexagonal structure (δ) (P63/mmc) and tungsten-carbide-like structure (ϵ) (P-6m2).

2 Theoretical method

2.1 Total energy calculations

In the electronic structure calculations, the ultrasoft pseudopotentials introduced by Vanderbilt [18] have been employed for all the ion-electron interaction. The generalized gradi-