Structural, Electronic and Thermal Properties of NbN Superconductors

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Abstract—**Self consistent first principle calculations on hard superconducting material NbN have been performed to understand their fundamental characteristics of the structural, electronic and thermal properties. The bulk modulus (B_0), Debye temperature (θ_D), density of states (N (E_F)) and electronic specific heat coefficient (γ) have been computed in terms of the electronic structure results obtained by using the tight-binding linear muffin tin orbital (TB-LMTO) method based on the density functional theory (DFT) within the local density approximation (LDA). Structural, Electronic and Thermal properties calculated here are found to corroborate well with the experimental and theoretical results of literature.**

Keywords-B1 phase; superconductors; band structure; specific heat coefficient; Debye temperature.

I. INTRODUCTION

Extensive theoretical and experimental work have been carried out on the hard superconducting material such as transition metal nitrides due to their outstanding mechanical, thermal and superconducting properties of the material [1,2]. The mechanical property of the material have been studied by Vickers indentation method and the Vickers hardness in close to sapphire, while its bulk modulus is close to the cubic boron nitride [1,3]. The detailed mechanical properties of NbN based on DFT have been studied by Wang et al. [4]. The elastic and thermo dynamical properties have been studied by Ren Da-Hua et al., based on the DFT method combined with the quasi-harmonic Debye model [5]. The superconducting transition temperature (T_c) of NbN alloy is found to be above 17 K [6] which is equivalent to the A15 phase superconductors such as Nb_3Sn and V_3Si [7, 8]. Here we have carried out the band structure calculation by TB-LMTO method, to understand the basic electronic structure and thermal properties of NbN .

II. METHODOLOGY

The calculation of the present work are performed using tight binding linear muffin tin orbital method [9]. Exchange and correlation contributions to both the atomic and crystalline potentials have been included through the von Barth–Hedin parameterization scheme [10]. The NbN alloy crystallize into the B1 phase (NaCl-type) with cubic crystal structure (space group: Fm-3m; 225) with lattice constant a= 8.2979 a.u. [11]. The tetrahedron method [12] of Brillouin zone integration was used to calculate the density of states. *E* and **k** convergence are also checked carefully. A mesh of 14×14×14 was taken in the irreducible wedge of Brillouin zone. To find the equilibrium lattice constant, the total energies were computed by reducing the crystal volume from $1.20V_0$ to $0.80V_0$, where V_0 is the equilibrium volume. The computed electronic total energy with respect to relative volume were fitted using the Murnaghan equation of state [13] to obtain the ground state properties.

III. RESULT AND DISCUSSION

The total energy of NbN is estimated using the band structure studies and is plotted for different Wigner-Seitz volumes in Fig. 1. The minimum of the curve defines the equilibrium cell volume, which is found to be 575.337 a.u.^{3} corresponding to the lattice parameter 8.3171 a.u. These results are tabulated in Table 1 and agree well the available theoretical and experimental values. The Bulk modulus is calculated from the relation $B = -V\mathrm{d}P/\mathrm{d}V$ and these are also presented in Table 1. Here our bulk modulus results found reasonable agreement with the Amriou et al. [14] from the full potential calculation by the use of LDA.

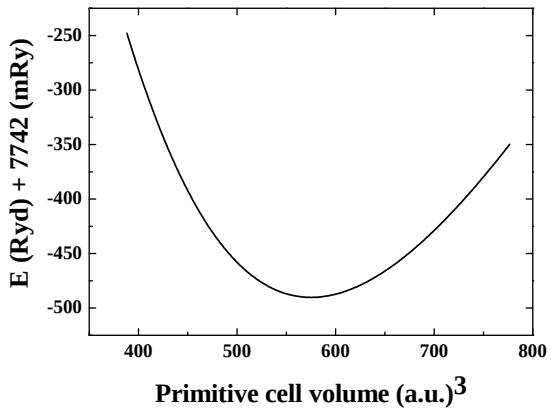

Figure 1. Calculated electronic total energy vs. primitive cell volume of NbN.

TABLE I. CALCULATED PARAMETERS OF NbN COMPOUND.

Calculated Parameters	Computed Values	References
Lattice constant, a_0 (a.u.)	8.317	8.297 [11]
Bulk modulus, B (Mbar)	3.342	3.499 [14]
Wigner-Seitz radius, S_0 (a.u.)	4.338	-
Density of states, $N(E_F)$ (states/Ryd. cell)	11.258	11.025[14]
Electronic specific heat coefficient, γ ($mJK^{-2}mol^{-1}$)	1.946	2.20 [6]
Debye temperature, θ_D ($^{\circ}K$)	383.29	335 [16]

Fig. 2a and 2b show the plots of the band structures along the high symmetry directions and total density of states (DOS) for NbN from the calculated equilibrium lattice constant. From the band structure we can see the low lying band arises between -2 Ryd to -1 Ryd due to the s-states of non-metal atom which is not responsible for metallic nature of the alloy. Below the Fermi level the bands mainly arises due to the p-states of both Nb and N atom. At higher energies there is a possibility of p-d hybridization occurs from the non-metal and the metal atom respectively which is responsible for the metallic nature of the alloy. The DOS histogram reveals the same nature of metallic character. A minimum is observed below the Fermi level which separate the bonding bands and antibonding bands. The sharp peak arises around the Fermi region due to the band overlapping observed in the band structure from the contribution of p-states of non-metal atom and the d-states of metal atom. Fig. 3 shows the partial DOS histogram of each band from Nb and N atom. The total DOS at Fermi level $N(E_F)$ have been deduced given in Table 1 which is close to the value by full-potential calculation [14]. From the density of states, the electronic specific heat coefficient (γ) is calculated by using the relation given in (1) and the data given in Table 1 found corroborate well with the previous results.

$$\gamma = \frac{\pi^2}{3} k_B^2 \, N(E_F). \qquad (1)$$

Moruzzi et al., [15] derived a simple relation to obtain Debye temperature from the electronic structure given by (2).

$$\theta_D = 41.63 \sqrt{\left(\frac{S_0 B}{M}\right)} \qquad (2)$$

where B is the bulk modulus evaluated at the equilibrium Wigner-Seitz sphere radius S_0 and M is the atomic mass. Although Moruzzi et al., [15] verified the validity of this expression for elemental metallic solids, we assume its validity for the alloy by considering M to be the concentration average of the masses of the component atoms. Our calculated Debye temperature shows reasonable agreement with the earlier experimental results of pseudobinary NbC_xN_{1-x} alloys by Roedhammer et al., [16] were given in Table 1.

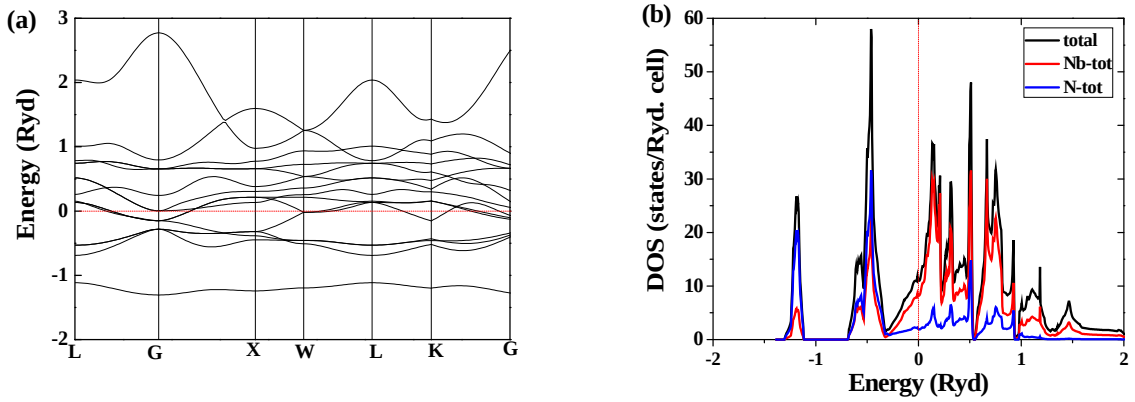

Figure 2. Band structure and total DOS of NbN are shown in (a) and (b). Dotted lines represent the Fermi level.

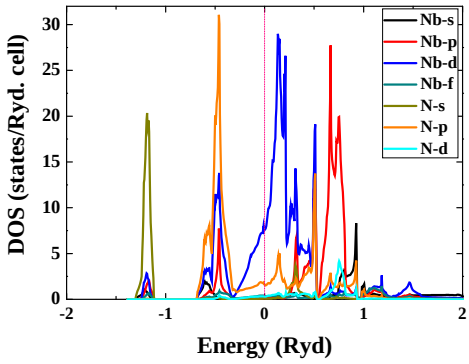

Figure 3. Partial Density of States of NbN. Dotted lines represent the Fermi level.

IV. CONCLUSIONS

The electronic band structure studies of NbN compound is carried out using the self-consistent tight binding linear muffin-tin orbital method. The electronic band structures show a strong hybridization between p-and d-bands of non metal and metal atom. The sharp peak observed in the DOS histogram due to overlapping of bands around

Fermi region. The electronic properties such as DOS at Fermi level, specific heat coefficient have been calculated and found good agreement with the available literature. The important thermal property such as Debye temperature is calculated from the Bulk modulus results. Therefore the Debye temperature is associated with the phonon frequency of the material and the specific heat coefficient associated with the electronic properties of the material.

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