A DFT study on electronic structure and elastic properties of AuN in rock salt structure

Jameson Maibam¹, Kh. Kabita¹, Indrajit Sharma B¹✉, Thapa RK², Brojen RK³

1. Department of Physics, Assam University, Silchar-788011, Assam, India
2. Department of Physics, Mizoram University, Tanhri, Aizawl-796 009
3. School of Computational and Integrative Sciences, JNU, New Delhi 110067, India

✉Corresponding Author: Department of Physics, Assam University, Silchar-788011, Assam, India, E-mail: indraofficial@rediffmail.com

Received 12 March; accepted 18 April; published online 01 May; printed 16 May 2013

ABSTRACT

The electronic structure and elastic properties of gold nitride (AuN) in rock salt structure have been calculated within the framework of density functional theory (DFT) using the full-potential linearized augmented plane wave (FP-LAPW) method. The exchange correlation potential was calculated with the generalized gradient approximation (GGA). The equilibrium volume, bulk moduli (B₀), pressure derivative of bulk moduli (B’₀), elastic constants are determined and compared with the available other results. The elastic constants (C₁₁, C₁₂, and C₄₄) are found positive and the conditions for stability: (C₁₁-C₁₂)>0, (C₁₁+2C₁₂)>0, C₁₁>0, C₄₄>0 are satisfied. Thus AuN in rock salt structure may be a stable compound. The energy band diagram shows the valence band and the conduction band overlaps each other at Fermi level and thus implies it exhibits metallic in nature.

Keywords: Density functional theory, energy band structure, density of states and elastic constants.

1. INTRODUCTION

The transition metal carbides and nitrides possess many interesting properties such as high melting points, extreme hardness, good corrosion resistance, high superconducting critical temperature (Toth, 1971, Francavilla, et al., 1981). Their hardness, brittleness and high melting points are related to their unusual electronic bonding: ionic, covalent and metallic. The complex bonding in these compounds makes it very difficult to give a simple interpretation of the electronic structures of these compounds. Based on recent synthesis of noble metals (Devia, et al., 2006, Yua, et al., 2005, Quintero, et al., 2008, Kanoun, et al., 2007) and their suggestions of possibility to form nitrides with noble metals such as Au, Ag and Cu, we have chosen to do theoretical calculations to study more in the electronic structure and elastic properties which was not done much earlier.

The elastic constants play an important role in the physics of materials as they characterize the behavior of the crystal in the field of external forces. It can also be foreseen that AuN could have improved hardness as in transition metals, preserving the high electrical conductivity of pure Au. The calculations have been done using the full-potential linearised augmented plane wave (FP-LAPW) method (Perdew, et al., 1996, Singh, 1994, Blaha et al., 1990) based on the density functional theory. The paper is organized as follows. In section 2, we briefly present the methods of calculation for electronic structure and elastic constants. In section 3, we give results and discussion. Conclusion of the overall work is given in section 4.

2. METHODS OF CALCULATION

Within the formalism of Density Functional Theory (DFT) (Cottenier, 2002, Hohenberg et al., 1964, Kohn et al., 1965), the total energy can be expressed as a functional of density (ρ) of electron system and can be written by the following functional.
The elastic constants $C_{ij}$ are listed extensively tested and is typically in an iterative process. Thus the energy band is calculated using FP-LAPW method (Blaha, et al., 2001). The exchange and correlation potential is incorporated by using GGA parameterized by Perdew et al. (Perdew et al., 1996). This method has been extensively tested and is among the most accurate methods for performing electronic structure calculations of crystals. For this calculation, the unit cell is divided into non-overlapping atomic spheres whose centre is at atomic position and interstitial region. Inside the muffin tin region, we used a linear combination of radial function multiplied by spherical harmonics and outside the muffin tin sphere, augmented plane wave expansion. We choose the muffin tin radius for Au and N as 2.1 atomic units and 1.95 atomic units respectively. The convergence of the basis set is controlled by a cutoff parameter $RMTK_{max} = 9.0$ where $K_{max}$ gives the plane wave cutoff. For every case the wave functions inside the MT spheres which are expanded into spherical harmonics are up to $l = 10$. The number of k points used for the integration procedure is 7000 which reduces to 220 irreducible k points inside the Brillouin zone including five high symmetry points W, L, Γ, X and K. The calculation was performed at the equilibrium lattice constant which is determined from a plot of total energy against the unit cell volume by fitting to the Murnaghan equation of state (Murnaghan, 1949, Brich, 1938). The overall simulation work is carried out using Wien2k code (Blaha et al., 2001).

3. RESULTS AND DISCUSSION

3.1. Structural and Elastic properties

The unit cell of AuN in rock salt structure is generated as a first step of the calculation. For the optimization of thus generated structure, total energy of the different sizes of the unit cell is calculated. Figure 1 shows the total energy curve as a function of volume of a molecule of the AuN. This curve is fitted with Murnaghan equation of state (Murnaghan, 1949) and the fitting parameters are obtained. Thus the structural parameters such as equilibrium lattice constant, bulk modulus and its pressure derivatives obtained from the Murnaghan fitting are listed in Table 1. The elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ are determined based on the volume conservative techniques. The values of the elastic constants are listed in Table 1. The elastic constants show the conditions for the stability, $(C_{11}+2C_{12})>0$, $(C_{11}+2C_{12}+2C_{44})>0$, $C_{12}>0$, $C_{44}>0$, are satisfied and hence the AuN in rock salt structure can exist as a stable compound.

3.2. Electronic structure

The total, partial density of states (DOS) and the energy band diagram of AuN are shown in Figure 2 (a,b,c) and Figure 3 respectively. In the total DOS of AuN as shown in Figure 2a, one can clearly observe that there is no separation between valence band and conduction band at Fermi level. In the sense that there is overlapping both the band as confirmed in energy band diagram as shown in Figure 3. It clearly indicates that AuN crystallizes in rock salt structure exhibits metallic nature. As
seen in the partial density of states in Figure 2b and Figure 2c, one can observe that the metal Au 5d states and the N 2p states are strongly hybridized in the total density of states in Figure 2a. Also referring to Figure 2b, it is seen that the band crossing the Fermi level in band diagram is mainly attributed to N 2p orbital. The lowest band in the band structure in Figure 3 is mainly N 2s orbital. They do not contribute to the bonding. Above this band, there lies the 2p non-metallic band complex. These band states overlap and mixed in ∆. The 5d metal state is further decomposed to dt_{5/2} and dt_{3/2} originating at Γ. E_{F}-E_{Np} gives the energy gap between the Ns band and the valence band complex. These band structure parameters are listed in Table 1.

4. CONCLUSION

The energy band diagram of AuN clearly shows the overlapping of the valence band (which is mainly contributed from the p band of N, partly d band of Au) and the upper conduction band at Fermi level. It implies that AuN (rock salt structure) exhibits metallic nature. Our structural data and energy band parameters are found to be comparable to those obtained from the other theoretical studies. The elastic constants (C_{11}, C_{12} and C_{44}) are found positive and satisfy the stability conditions: (C_{12}−C_{11})>0, (C_{11}+2C_{12})>0, C_{11}>0, C_{44}>0. Thus the AuN crystalizes in rock salt structure is a stable compound. Although the calculated parameters show interesting results, there is less experimental work on AuN. Thus experiments need to be performed to understand the true nature of AuN.

ACKNOWLEDGEMENT
Financial support under the Fast Track Project (SR/FTP/PS-33/2006 dt.06.05.2006) from Department of Science and Technology (DST), Government of India is gratefully acknowledged.

REFERENCE

10. Murnaghan FD. Proc. USA Natl. Acad. Sci., 1994, 30, 244