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THE IMPACT OF PRESSURE ON THE LATTICE CONSTANT IN THE ROCK SALT SITUATION BINARY COMPOUND AGN

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Abstract:

First-principles simulations based on density functional theory (DFT) are used to study the structural, electronic, and optical properties of the Rock salt (RS) AgN bulk. When the pressure was zero, the lattice constant's magnitude was 8.23 Å, and the energy gap's quantity was 3.1 eV. However, when 20 kPa of pressure is applied, the lattice constant decreases to 6.5 Å, while the energy gap grows to 3.9 eV. Pressure generally lowers a solid's lattice constant. This occurs as a result of pressure forcing atoms closer together and decreasing the gap between them. A reduction in the lattice constant indicates that the crystal is being crushed since it represents the spacing between neighboring atoms in a crystal. Not every solid has the same impact of pressure on the lattice constant. Certain solids will compress more than others, which means that when pressure is applied, their volume will fall more dramatically. A solid's compressibility is determined by several variables, one of which is the kind of bonds that bind them together.

Keywords:

INTRODUCTION

When examining the characteristics of materials and how they behave under various circumstances, one crucial factor to examine is the impact of pressure on the lattice constant in such materials. The distance between a material's lattice points is known as the lattice constant, and variations in this constant have a significant impact on the material's characteristics. When a material is subjected to pressure, it is affected by forces that change its shape and size. The mesh constant decreases when the mesh points come closer together due to increased material stress. On the other hand, the lattice points move apart when the material's tension reduces, increasing the lattice constant. The mechanical characteristics of the material are influenced by the impact of material pressure on the lattice constant [1,2]. For instance, in solid materials, the hardness of the substance is determined by the lattice constant. The material becomes stiffer as the lattice constant lowers because the bonds between its molecules are stronger on the other hand, as the lattice constant rises, the material molecules' bonds weaken and its stiffness decreases. Furthermore, a material's thermal characteristics are influenced by its pressure [3-5]. Temperature variations cause the material's volume to fluctuate less when the lattice constant drops. On the other hand, temperature variations cause greater variations in the material's volume as the lattice constant rises. Additionally, a material's electrical and magnetic characteristics can be impacted by pressure. For instance, with semiconductor materials, rising pressure can result in higher conductivity, whereas falling pressure might result in lower conductivity. In general, the influence of pressure on the lattice constant in materials is determined by the kind of material as well as its atomic and molecular structures. Thus, investigating this effect aids to a better knowledge of material behavior under various situations, as well as the creation of novel applications [6].

Computational methods

Density functional theory and the CASTEP method were used in this study to compute the optical, magnetic, electric, phonon transport, and structural characteristics of a (RS) AgN bulk [7]. These characteristics include electric, magnetic, and optical. The PBE method and generalised gradient approximations (GGA) have been utilised to assess the exchange-correlation energy [8]. The system that has been created is a (RS) AgN bulk with 15 Å injected perpendicularly to it, in order to exclude any possible interactions between atoms. With 10 × 10 × 10 units per unit cell, the system that was built is a (RS) AgN bulk. When analysing plane waves, the 500 eV cutoff energy is employed. Every building has reached its condition of maximum relaxation. The size of the atomic force is less than 0.02 eV/Å, but the magnitude of the total energy affinity is 10^{-5} eV.

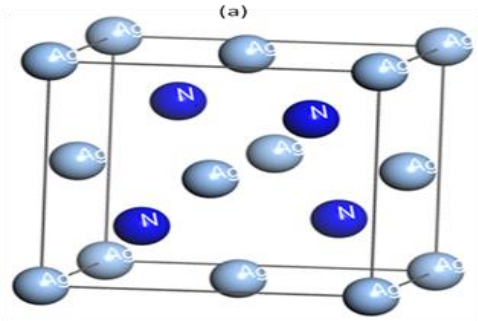


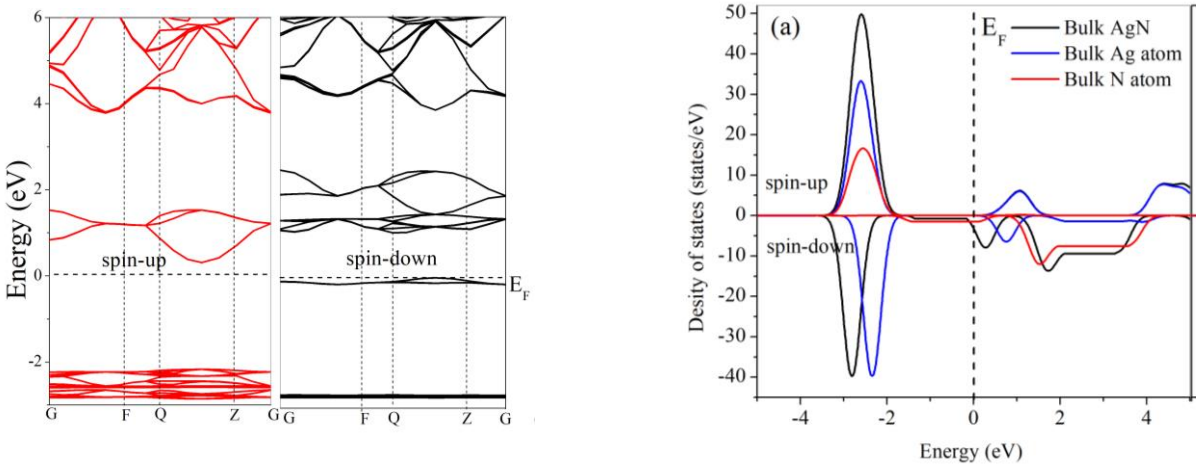
Figure 1: Crystal structure of (RS) AgN bulk

RESULTS AND DISCUSSION

3.1 Electronic structures of (RS) AgN bulk

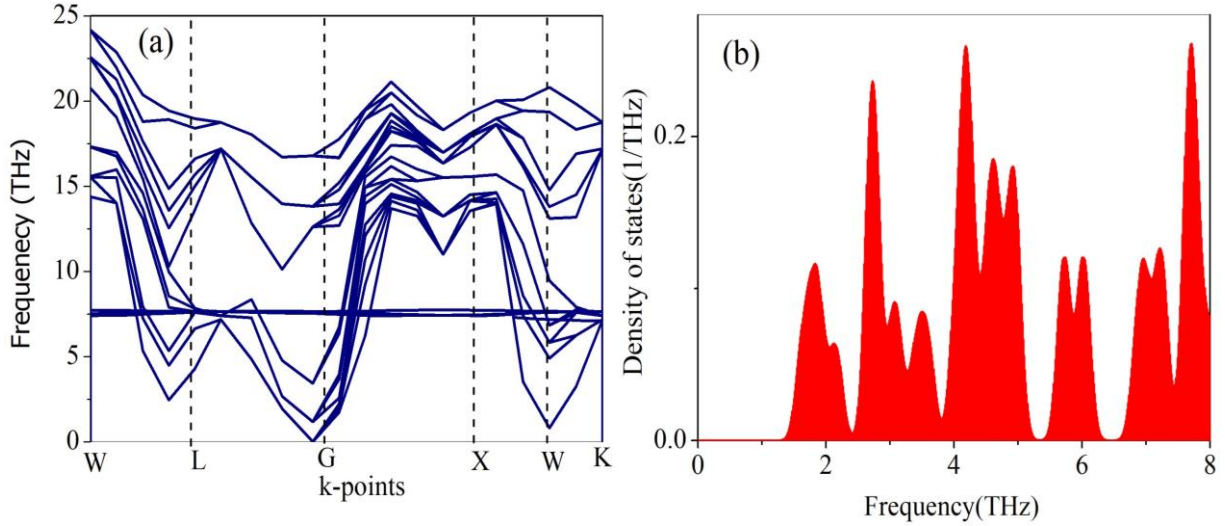
Because this compound has a modest lattice constant, as seen by the energy band and density of states in Figure 2, applying a pressure of 20 GPa will cause the energy gap to grow.

Figure 2: The densities of states in the bulk (RS) AgN (right) and the band structure (spin up and spin down) (left) by effected 20 GPa



3.2 phonon transport

Recent developments in the study of partially metallic materials have highlighted the need for a more comprehensive scientific understanding of heat transfer through materials. One useful method for figuring out the phonon scattering in the (RS) AgN is to use density functional theory (DFT) simulations of first-principles computations. Phonons must be



studied in materials physics. In actuality, phonons are necessary to produce a variety of physical properties, including electrical and thermal conductivity. Put another way, the smallest amount of energy that may be transferred from an auditory source to a physical medium is called a phonon. The phonon might be thought of in this context as the smallest amount of electromagnetic energy that can be transferred from an electromagnetic wave to a physical medium, or as an isotope of an electromagnetic wave [9].

Figure 3: Curves showing state density and phonon dispersion for bulk (RS) AgN

3.3 Optical Properties

Materials' optical properties are crucial for modern applications as well as fundamental research. Among other optical properties, we calculated the conductivity, dielectric function, loss function, refractive index, propagation constant (K), and absorption coefficient. It may be finished via the connection that is displayed below.

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1)$$

where the imaginary and real components of the dielectric function are represented by the $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, respectively. The electromagnetic field's propagative conduct has a connection to reality $\varepsilon_1(\omega)$ [10]. The Fermi golden rule is used for adding the occupied–unoccupied transitions to obtain the relationship for the imaginary part $\varepsilon_2(\omega)$ [11]. Figure 4 depicts the real and imaginary parts of the dielectric function. The (RS) AgN has a dielectric function (at zero energy) of is 15×10^5 and 65×10^5. Furthermore, the non-negative real dielectric function indicates that the (RS) AgN operates in the same manner as a semiconductor in this frequency range. UV radiation rapidly decreases with an increase in photon energy, but the insulation curve in visible areas expands and decreases with energy. It is generally known that materials that function effectively in visible and infrared light have gaps less than 1.8 eV. Consequently, the (RS) AgN will operate as a visible and infrared visual material [12].

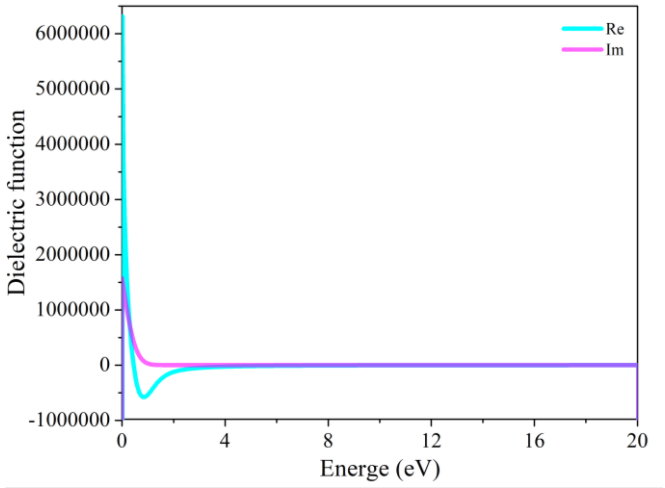
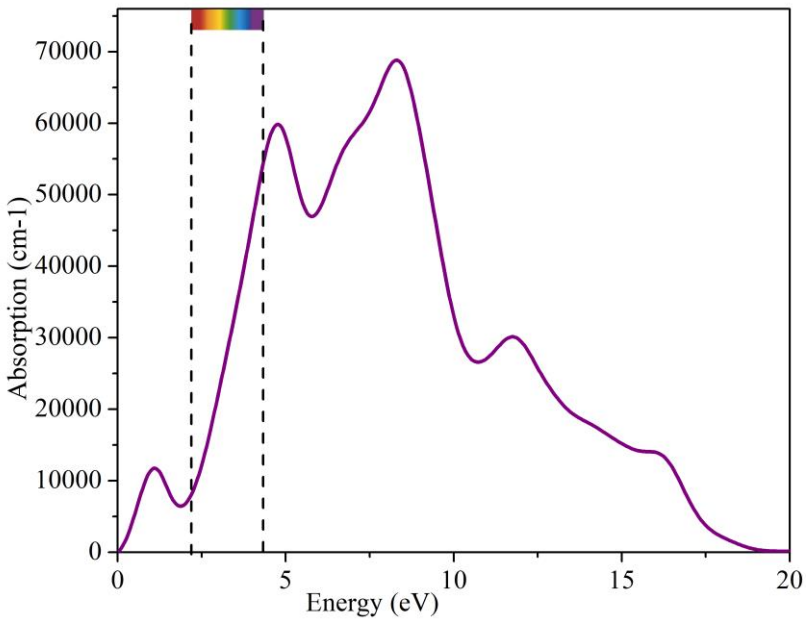


Figure 4: Real and imaginary parts of the (RS) AgN bulk dielectric function

The optical properties were studied in the energy range 0–20 eV. Figure 5 shows that absorption starts at energies lower than 1.27 eV in the infrared (IR) region. The existence of an IR absorption peak between (0.8 eV and 1.3 eV) was confirmed by our results. The absorption coefficient clearly indicates that the UV (8 eV) area is where its biggest



peaks are located. Visible light absorption, which begins in the range of (1.5 eV and 3 eV), is one of the most important research areas on light absorption that may be used in the creation of solar cells. Another observation is the high UV light absorption energy of a single layer of (RS) AgN, which might be used in photoelectronic devices such as UV detectors.

Figure 5: Optical absorption of (RS) AgN bulk

The refractive index and propagation constant of the (RS) AgN are shown vs photon energy in Figure (6). The (RS) AgN monolayer has a refractive index of 1.9 and a propagation coefficient (at zero energy) of 7.9. Conversely, at 2.5 eV, the propagation constant reaches its maximum value of 2.9. The refractive index finally begins to decrease with energy at high photon energies, while it tends to decrease with energy in the visible spectrum and with UV radiation. The infrared area is often where the bulk has the maximum refractive index. For the photon, the spectra of the refractive index (n) and propagation constant (K) decrease rapidly and stabilize at 20 eV.

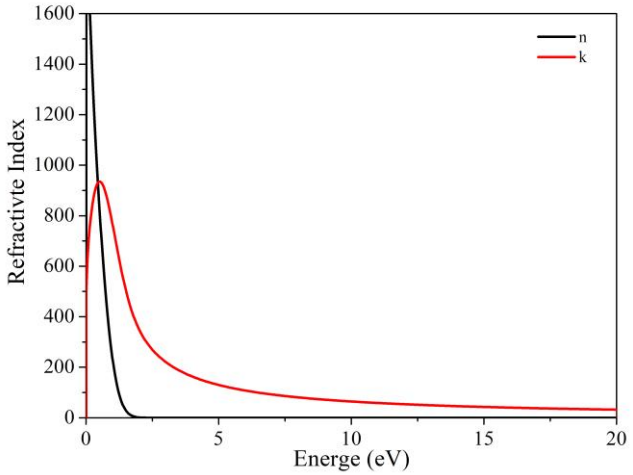


Figure 6: Refractive index of (RS) AgN bulk

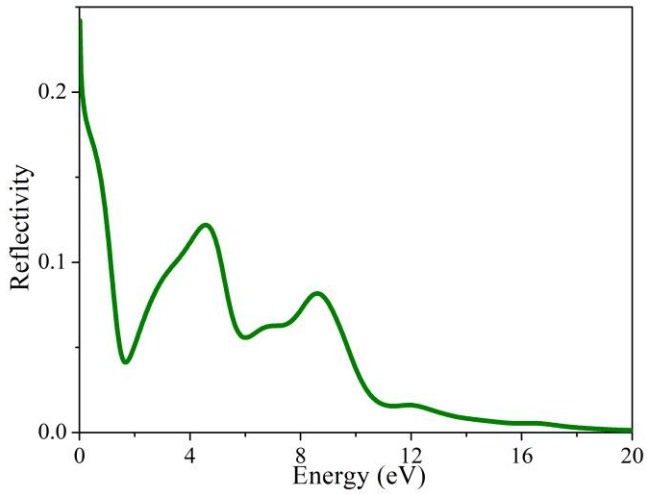


Figure 7: Reflectivity of (RS) AgN bulk

Figure 7 depicts the expected optical reflectance as a function of energy. At zero energy, optical reflectivity is 0.25.There is a single optically reflective peak for photon energy at 4.5 eV. The optical reflectivity curve decreases with energy in visible light and rapidly decreases with increasing photon energy in ultraviolet light. Based on Figure 8, we can observe that the loss function's maximum peak, with a value of 1.3, occurs at an energy of 10 eV.

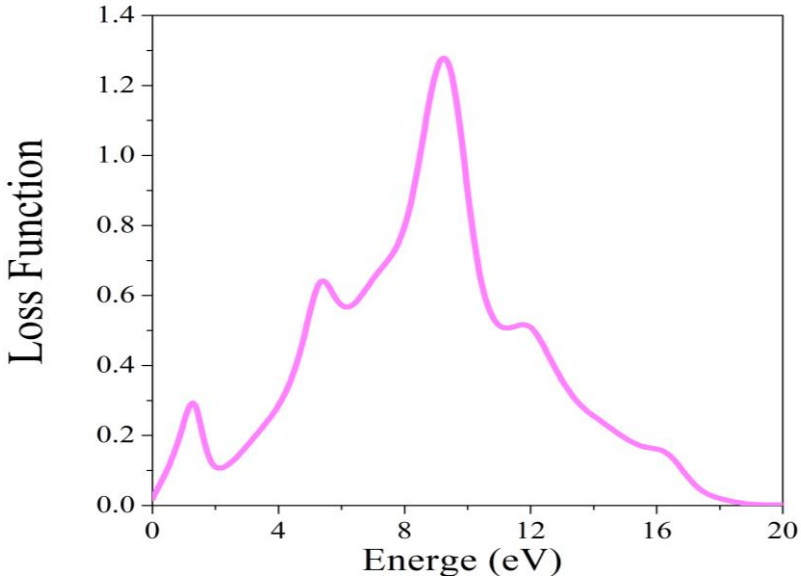


Figure 8: Loss function of (RS) AgN bulk

Optical conductivity as a function of photon energy is seen in Figure 9. The conductivity of the actual section of the (ZB) VTe bulk peaks at 1.3 eV in the infrared region of 95000. On the other hand, the highest values of the imaginary component of conductivity in the visible ray zone are 65000 at photon energies of 3 eV.

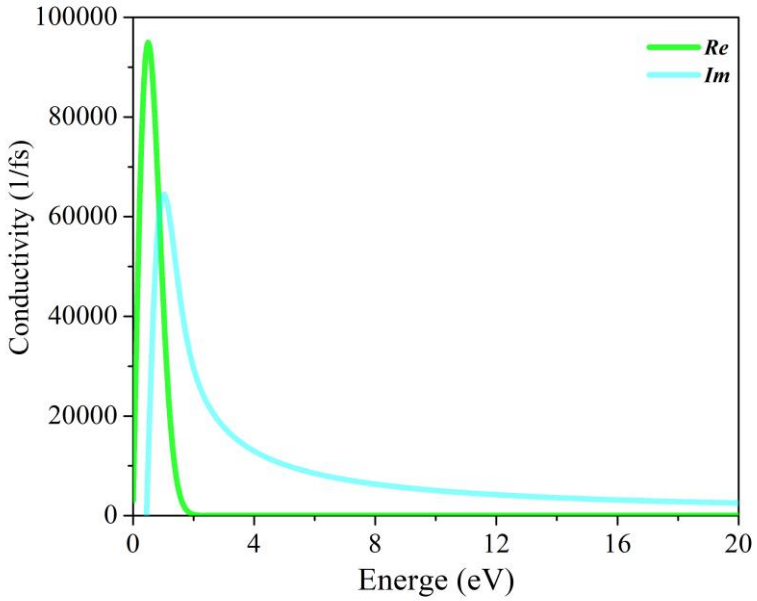


Figure 9: Optical conductivity of (RS) AgN bulk

CONCLUSION

This study employs a first-principles method to investigate the electrical structure, optical characteristics, and phonon transport of the (RS) AgN bulk. under an applied pressure of 20 GPa. The spin-down channel is a semiconductor while the spin-up channel is metallic, as evidenced by half-metallic features in the (RS) AgN bulk. In the bulk of (RS) AgN, the average magnetic moment per cell unit is 2μB. Throughout the entire Brillouin region, the absence of imaginary phonon vibration frequencies contributes to the dynamic stability of the (RS) AgN bulk. The (RS) AgN bulk is a good option for usage in microelectronic and electro-optical applications, according to the optical properties examined.

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