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FIRST PRINCIPLE CALCULATION ELECTRONIC AND OPTICAL PROPERTIES OF Si_3N_4

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Abstract. In presented article electronic band structure, density of state and the dielectric function of Si_3N_4 were studied were investigated by implementation DFT calculation. An imaginary part of the dielectric function in the range of optical frequencies was obtained by calculating the joint density-of-states (DOS) for optical transitions between the valence and conduction bands, using the Monchorst-Pack technique for integration over the BZ. The real part was obtained from the imaginary part by the Kramers–Kronig transformation.

Keywords: *Electronic properties, optical properties,* Si_3N_4*.*

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1. Introduction

Silicon nitride has very high concentrations of electron and hole traps ($10^{19}sm^{-3}$) (Gritsenko, 2003; Gritsenko, 1986), which are deep and have the energy W =1.5 eV (Roizin & Gritsenko, 2007). The higher dielectric constant of nitride (e = 7) compared to dioxide (e = 3.9) makes the former useful as an insulating layer in the holding capacitors of read access memories, for insulating multilevel metal interconnections, or as a blocking dielectric in floating gate flash memory elements. The spatial electron density distributions were calculated and analyzed for Si_3N_4 as a function of energy Ref. (Nekrashevich *et al.*,2010). First-principle calculations of the electronic band structure of the *a* and *b* phases of silicon nitride were performed in (Ren & Ching, 1981; Xu & Ching, 1995; Robertson, 1981;Shaposhnikov *et al*., 2007) using the density functional theory (DFT), currently the basic tool for such calculations.

2. Method

The electronic band structure, density of state and the dielectric function of Si_3N_4 were studied using ab initio calculations. Self-consistent electronic band structure calculations were performed with allowance for relativistic effects using a full potential linearized augmented plane wave method implemented in the Wien2k code (Blaha *et al.*, 2001). The exchange-correlation potential of the GGA suggested by Perdew et al. (Perdew *et al.*, 1996) was used. The convergence parameter RmtKmax, where Rmt is the muffin-tin sphere radius and Kmax is the size of the basis sets, was set to 7.0. Inside atomic spheres, the partial waves were expanded up to lmax = 10. Integrations in reciprocal space were performed using the tetrahedron16 method with 2000 k points in the first Brillouin zone (BZ) to determine the charge density in each self-consistency step.

The value of 2.0 was used for Rmt of N and Si. The cut-off energy for separation of the core and valence states was set to −8.5 Ry. Self-consistency was achieved with an energy convergence of 10−5 eV. The influence of relativistic effects on the electronic properties was taken into account in the scalar relativistic approximation. An imaginary part of the dielectric function in the range of optical frequencies was obtained by calculating the joint density-of-states (DOS) for optical transitions between the valence and conduction bands, using the Monchorst-Pack technique for integration over the BZ. The real part was obtained from the imaginary part by the Kramers–Kronig transformation.

3. Results and discussions

From calculated band structure the top of valence band and the bottom of conduction band were shown to be localized at different points on the surface of the Brillouin zone of the tetragonal lattice, namely along symmetry line Γ-A located top of valence band and at the symmetry point Γ located bottom of conduction band (Fig. 1). This in their turn indicates that Si_3N_4 is an indirect gap semiconductor with the indirect gap from Γ to Γ-A line of 4.21 eV, while the direct gap at the Γ-point is 4.36 eV. In (Fig. 1) zero of the energy scale shows the position of the Fermi level. The calculated valence bands below the Fermi energy agree well with

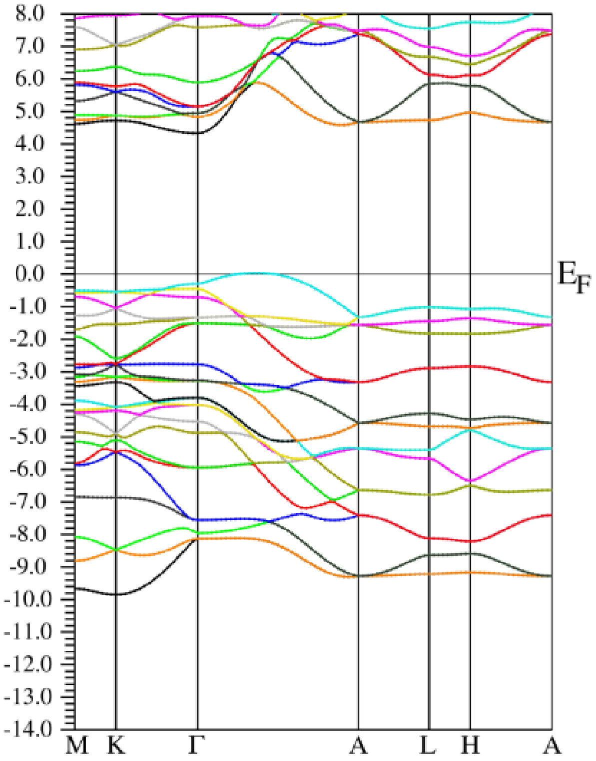

Fig. 1. Calculated band structure

other first principle studies. The band gap of Si_3N_4 was found to be close to 4.6 eV through first-principles calculations using the local density approximation (LDA) (Lu, *et* al., 2013).

Our calculated result is in good agreement with this result but smaller than the experimental result, probably due to a discrepancy in the GGA method. If we add a correction factor to this band gap, the results are found to be in excellent agreement with the experimental data.

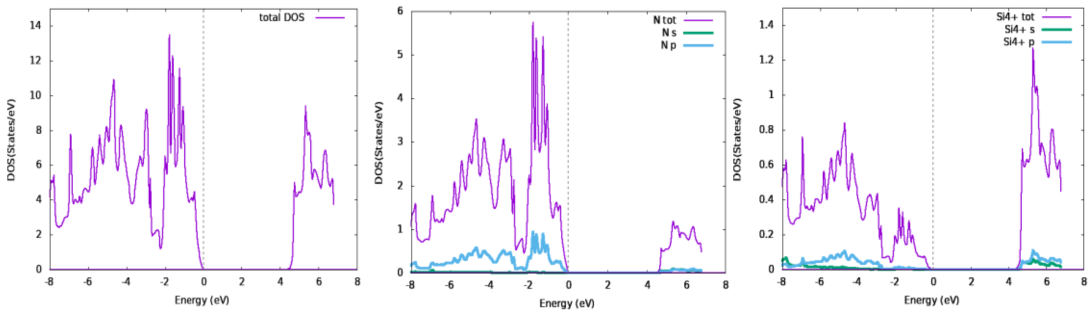

Fig. 2. Calculated DOS

The partial density of states (PDOS) of the N and Se atoms are shown in Fig. 2. The low-energy peak around -8 to -4 eV is a contribution mainly from the N1 p states, with a small component from the N2-p orbitals. The DOS peak at around -4 to -2eV mainly represents the contribution of the N2- p and Si- 4p states. Top of valence band mainly take their origin from p state of N1 atoms and partially from p state of N2 atoms. The Si-p state contribution to originate bottom of conduction band around energy range 4 to 6 eV. As well as this energy range partly take their origin from s state of Si atom.

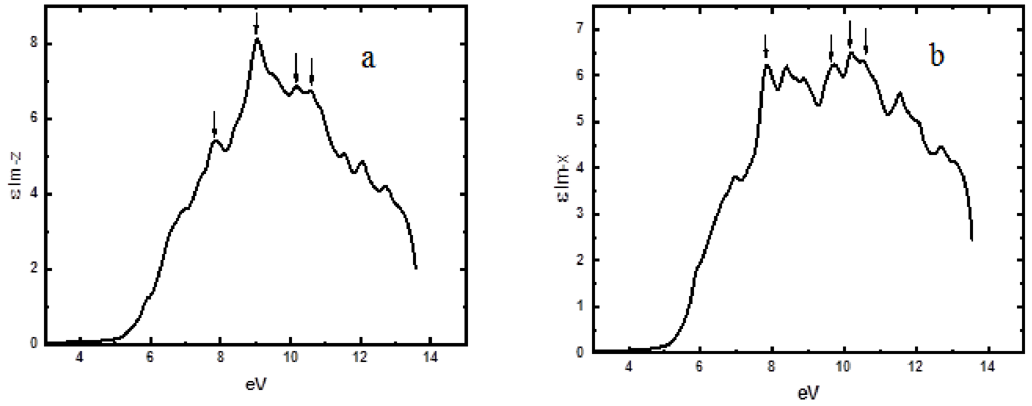

Fig. 3. Calculated dielectric function

The calculated imaginary parts ε⊥ and ε|| are shown in Fig. 3. Each exhibits four structures denoted as X1, X2, X3, and X4 [Fig. 3(a)] and Z1, Z2, Z3, and Z4 [Fig. 3(b)], respectively. According to the obtained band structure, the assignment of these peaks can be done in a manner shown in Fig. 3. The peak Z2 for ε⊥ positioned around 9 eV, have the highest amplitudes and are mainly due to interband optical transitions between N1-p +N2-p→Si p + Si s states. Structures X1 (Z1), X3 (Z3), and X4 (Z4) correspond to the transitions N2-p+Si-p → Si-p+Si-s respectively.

4. Conclusion

Carried out first principle calculation for investigation electronic band structure and optical properties of Si_3N_4 indicate that this compound is direct band gap compound. The indirect gap is from Γ to Γ-A line of 4.21 eV, while the direct gap at the Γ-point is 4.36 eV. The Si-p state contribution to originate bottom of conduction band around energy range 4 to 6 eV. Top of valence band mainly take their origin from p state of N1 atoms and partially from p state of N2 atoms.

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