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Effects of substitution on electronic and optic properties of Ga and P doped AlN nanosheets

İsmail Yücel[a,*], Seyfettin Çakmak[b], Ekrem Artuç[b]

[a] Süleyman Demirel University, Graduate School of Natural and Applied Science, 32260 Isparta, Turkey
[b] Süleyman Demirel University, Faculty of Arts and Sciences, 32260 Isparta, Turkey

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ABSTRACT

In this paper, the structural, electronic and optical properties of pure, Ga, P and Ga/P doped AlN nanosheets are investigated using the full potential linearized augmented plane wave (FP-LAPW) method within the density functional study (DFT). The exchange-correlation potential is formulated by the generalized gradient approximation (GGA). We have calculated bond length, bending length, band gap energies and density of states for all nanosheets. Besides, all optical parameters (real and imaginary parts of dielectric function, optical conductivity, energy loss function, absorption coefficient, reflectivity, refraction and extinction index) are calculated. We found from optical results that, optical properties are isotropic for both parallel and perpendicular electric field polarization. In addition optical conductivity calculations show that pure and doped AlN nanosheets have semiconductor characteristics.

1. Introduction

The nanomaterials like graphene [1–4], germanene [5–7], stanene [7,8–10], silicine [7,11,12], GaN [13–15], BN [16,17], ZnO [18,19] and SiC [20,21] have been attracted due to their desirable properties structural, electronic and optic properties. Group-III nitride semiconductor materials strong potential candidate for semiconductor lasers [22], light-emitting diode [23] and visible light photocatalayst [24]. The bulk AlN has a wurtzite structure with band gap energy 6.20 eV at room temperature [25]. Besides this, the AlN nanosheets have been smoothly synthesized on Si (001) substrates. Result of this study indicates that the nanosheets are uniformly stacked [26]. AlN nanomaterials such as nanowires [27], nanotubes [28], nanocones [29] and nanoribbons [30] have been studied recently. In this paper, we have investigated the effects of Ga and P doping on AlN nanosheets. In accordance with this scope, the structural, electronic and optical properties of pure and doped AlN nanosheets have been investigated by employing the generalized gradient approximation (GGA) based on density functional study (DFT).

2. Computational method

In this study, we have investigate the electronic and optic properties of P-doped, Ga-doped and P/Ga doped AlN nanosheets. The calculations have been performed using the WIEN2k [31–33] code within the framework density func-

* Corresponding author.
E-mail address: ismaillyucell@gmail.com (İ. Yücel).

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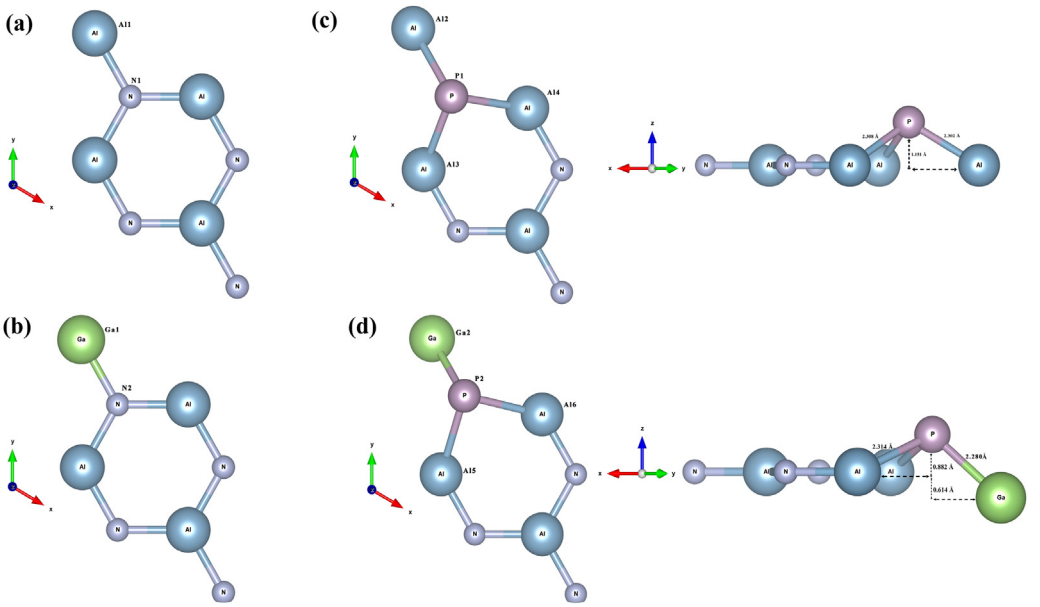

Fig. 1. The crystal structure of AlN nanosheets (a) pure, (b) Ga doped, (c) P doped and (d) Ga/P doped.

Table 1
The calculated bond lengths of pure and doped AlN nanosheets.

Atoms	Bond Lengths	
	Present Work	Other works
Al1-N1	1.802 Å	1.808 Å [36], 1.820 Å [37]
Ga1-N2	1.863 Å	1.851 Å [38], 1.869 Å [39], 1.880 Å [40]
Al2-P1	2.302 Å	2.340 Å, 2.290 Å [41]
Al3-P1	2.308 Å	2.340 Å, 2.290 Å [41]
Al4-P1	2.308 Å	2.340 Å, 2.290 Å [41]
Ga2-P2	2.280 Å	2.230 Å, 2.260 Å [42], 2.280 Å [43]
Al5-P2	2.314 Å	2.340 Å, 2.290 Å [41]
Al6-P2	2.314 Å	2.340 Å, 2.290 Å [41]

tional theory (DFT) [34]. The exchange-correlation potential is treated by the generalized gradient approximation (GGA) based on Perdew et al. [35]. In our calculations, the plane wave cutoff parameter is set to be $R_{mt} \times K_{max} = 7.0$, where R_{mt} is the smallest atomic sphere radius in the unit is cell and K_{max} is the magnitude of the largest K vector in equation. The radius muffin tin of atoms were set to be 1.60 a.u., 1.38 a.u., 1.61 a.u. and 1.77 a.u. for AL, N, Ga, and P atoms, respectively. For the electronic and optic calculations, the $2 \times 2 \times 1$ unit cells of nanosheets have been used with a vacuum space of 10 Å to avoid interlayer interactions between the neighboring cells. We take 100 k-points for the Brillouin zone integrations in the corresponding irreducible wedge. In addition optical properties of nanosheets have been calculated using 1000 k-points for the Brillouin zone integrations. The cut-off energy for separating core from valance states is set to be −8.0 Ry. The magnitude of the largest vector in charge density Fourier expansion is set to be G_{max}=12.

3. Result and discussions

3.1. Structural properties

The hexagonal cell of pure-, Ga-, P- and Ga/P-doped AlN nanosheets are presented in Fig. 1. The calculated bond lengths are available in Table 1. As can be clearly seen in Table 1 that, our calculations on bond lengths are in a good agreement with the literatures. There has been no structural change in pure and mono doped Ga nanosheets. On the other hand for the mono doped P nanosheet, the Al2-P1 bond length differs from Al3/4-P1 bond lengths. The differences of bond length causes structural deformations and the P1 atom moves the positive z direction. This displacement causes the bending of structure. The bending length is 1.151 Å. This bending can be seen clearly in Fig. 1(c). Finally, for the Ga and P doped nanosheet, Al5/6-P2 bond lengths is 0.034 Å bigger than Ga2-P2 distance. It means that P atom moves the positive z direction and Ga atom moves the negative z direction. As a result of these movements, the Ga/P doped structure has been bent in both positive and