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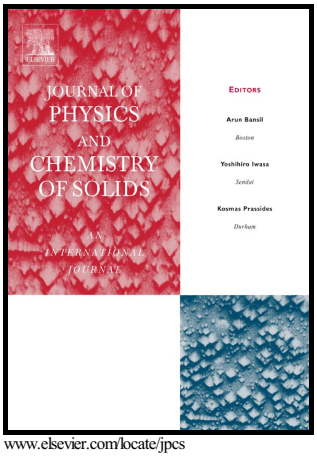

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A first-principles study of the properties of four predicted novel phases of AlN

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Abstract

Structural, elastic, thermodynamic, electronic and optical properties of four predicted novel AlN phases (*Pmn2$_1$*-AlN, *Pbam*-AlN, *Pbca*-AlN and *Cmcm*-AlN) are calculated using first-principles according to density function theory (DFT). These phases were found using the CALYPSO method but have not yet been synthesized experimentally. Here we predict some of their properties. The properties are analyzed by means of GGA-PBE and PBE0 respectively. The more precision results are obtained by PBE0. *Cmcm*-AlN owns better plasticity and it's Young's modulus has clearer anisotropy than *Pmn2$_1$*-AlN, *Pbam*-AlN and *Pbca*-AlN. The Debye temperature, under higher temperature, shows weak temperature dependence and approach to a constant value. The Dulong-Petit limit of all four novel AlN phases and *wz*-AlN is about 48J mol^{-1}K^{-1} and they have almost the same temperature law. The band structures show that the four AlN are the wide direct band gap semiconductors, which band gaps are 5.95 (*Pmn2$_1$*-AlN), 5.99 (*Pbam*-AlN), 5.88 (*Pbca*-AlN) and 5.59 eV (*Cmcm*-AlN). The bonding behaviors are the combination of covalent and ionic nature. The dielectric constants, refractive index, reflectivity, absorption, loss spectra, conductivity and Raman spectra are also calculated in detail. All four phases have a lower plasma frequency than of wz-AlN.

Keywords: Aluminium nitride; Novel phases; Physical properties; First-principles calculations

1. Introduction

The III-V groups of nitrides have been given close attention because those have the properties of wide band gap, super-hardness, high power conversion efficiency, and high thermal conductivity [1–6]. As a larger band gap semiconductor material, AlN has many favorable properties, and it is the more suitable material for constructing devices in the violet region, such as light emitting diodes (LED's), high power and high temperature field effect transistors [7–12].

For the AlN semiconductors of both the wurtzite and zinc-blende structures, the band structure and quasi-particle excitation energies were studied [13]. A direct nitridation process was proposed for the manufacture of sinterable AlN at the pilot scale [14]. The measurements of second-order Raman scattering for perfect AlN crystals and the Raman-scattering data for strongly disordered samples were given under the conditions of the room and low temperatures [15]. The hydrolysis behavior of AlN was analyzed when it is immersed in the aqueous solutions for various pH values [16]. High-pressure structural, dielectric properties and phonon dispersions of wurtzite, zinc-blende and rocksalt AlN were analyzed [17–19]. The high-pressure behaviors of amorphous AlN were investigated [20]. The deformation properties of single crystal AlN micropillars subjected to uniaxial compression were analyzed [21]. The thermal conductivity of the titanium nitride/titanium aluminum nitride multilayer coatings deposited by lateral rotating cathode was discussed [22]. In addition to research on the structures and properties of wz-AlN, zb-AlN, rs-AlN and other AlN, Liu et al. [23] predicted four novel high-pressure orthorhombic AlN crystal structures found by using CALYPSO method and proved all four structures are dynamically stable.

In this paper, the structural, elastic, thermodynamic, electronic and optical properties of the four predicted novel AlN phases (that is *Pmn2$_1$*-AlN, *Pbam*-AlN, *Pbca*-AlN and *Cmcm*-AlN) are calculated in detail using first-principles. Some properties of *wz*-AlN are also calculated for comparison. Of course, these results need to be further confirmed by experiment. A possible route to achieve the four novel AlN phases is adjusting the pressure