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Electronic Band Structure of Aluminium Nitride and Gallium Nitride Crystallizing in the Wurtzite and Zinc Blende Structures

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ABSTRACT We have studied the electronic band structure of aluminium nitride and gallium nitride crystallizing in the wurtzite and zinc blende structures. We have presented theoretical study of atom and orbital projected partial density of state for the group third nitrides. We have compared the energy distribution of electronic states in valence and conduction bands as calculated by means of linear muffintin orbital method. The direct comparison with the appropriate density of state was presented to indicate the extent to which we got direct information about allowed electron states by considering the positions of the maxima and minima of the intensity in spectra. The influence of the core level width and spectrometer broadening was also considered. The good agreement between structures observed in spectra and structures in the calculated density of state allowed for consistent analysis of results. We have compared the amounts of bonding and antibonding states near the band edges for different choices of cations and crystal structures. Since the device applications are based mainly on wurtzite type nitride, particular attention was given to this phase. We examined for wultzite structure the level of anisotropy in the formed chemical bonds. Two kinds of bonds π and σ are connected directly with bond lengths. We examined the amount of electronic states available for optical transition as a function of crystal structure, crystallographic direction and presence of cation semicore states. The hydridization between d and p states for different cations and nitrogen were studied. We found that d-p interaction affected the valence band edge and influenced magnitude of the fundamental gap. The obtained results were compared with previously obtained results of theoretical and experimental work and were found in good agreement.

KEYWORDS Electronic band, Zinc blende, wurtzite, density of state, cation, nitride, optical transition, hydridization.

INTRODUCTION

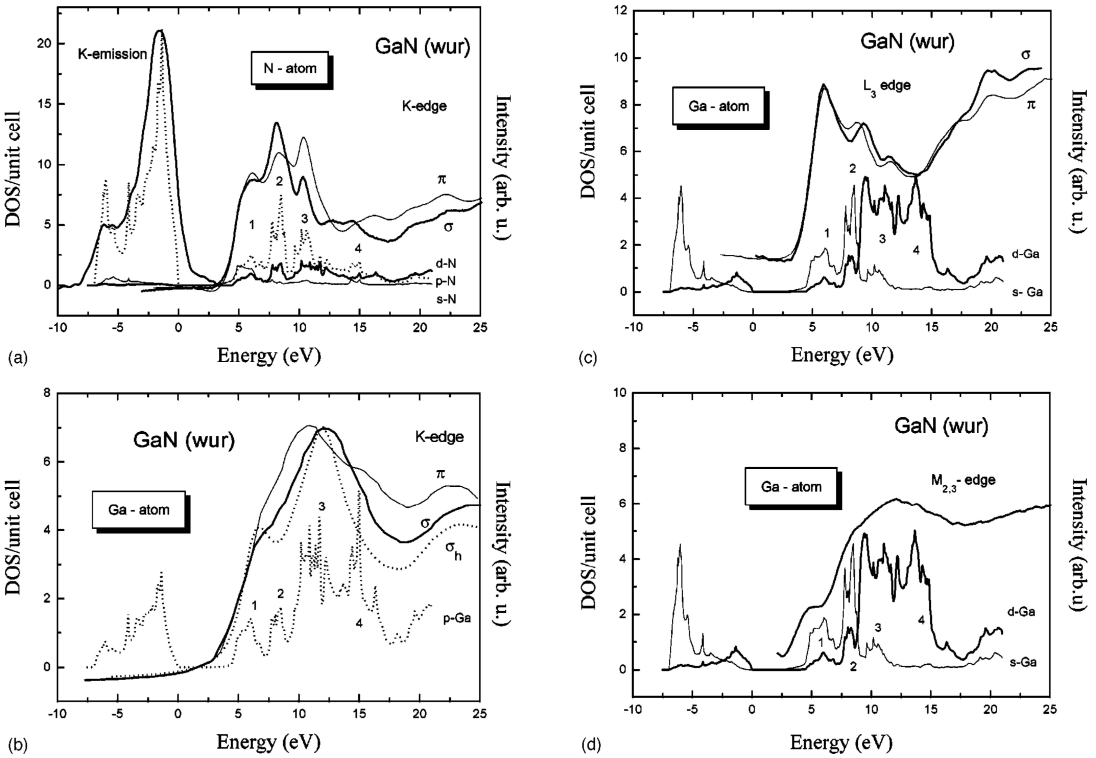
Christensen et al. [1], Lambrecht et al. [2] and Nian et al. [3] studied the III-V-group nitrides electronic band structures. A few experimental studies fo the band structure have been carried out by Martin et al. [4], Stagarescu et al. [5], Lawniczak et al. [6] and Duda et al. [7] concerning mainly for gallium nitride. They showed that the shape of x-ray spectra is a fingerprint of the particular chemical bound and makes it possible to identify the chemical nature of the bond formed by selected kind of atoms in different compounds. Photon absorption and emission involves an optical transition between electronic states of the atom in the sample. Sakai et al. [8] and Nakamura et al.[9] studied the group III nitrides and found that there are wide gap refractory semiconductors with application as basic materials in opto-electronic devices operating in the visible/ ultraviolet spectral range as well as in high temperature and high power microelectronic devices. Gubanov et al. [10] studied and found that several other metastable structures have been identified and also a fullerene like structure has been synthesized and characterized by Loiseau et al. [11]. The density of states, normalized to the unit cell were calculated by means of the tetrahedron technique [12]. Properties of cubic zinc blende silicon carbide nanowires with nitrogen impurities and vacancies along (111) direction were theoretically studied by means of atomistic simulations [13]. It was found that the thermoelectric figure of merit of silicon carbon nanowires can be significantly enhanced by doping nitrogen impurities together with making silicon vancancies. Vainorius et al. [14] investigated a large set of individual wurtzite/ zinc blende gallium arsenide heterojunction nanowires using transmission electron microscopy. They found a fairly deep emission that shows a strong blue shift with increasing excitation power density. The data gave a valence band offset of about 100 meV in excellent agreement with theoretical predications. Zhang et al. [15] reported a first principle study of the lattice dynamics of small graphene nanoribbon with zigzag edges. Nesting properties in the electronic band structure are very different for nanoribbons with unpolarized ferromagnetic and antiferromagnetic configurations. As a result the phonon spectrum and nesting related softening in phonon frequencies differ in these cases. The unpolarized and ferromagnetic structures showed nesting related phonon softening an considerable electron phonon line width, while for the antiferromagnetic structure, a band gap at the Fermi energy eliminates these effects. Saturating the nanoribbon edge with hydrogen has negligible effect on the phonon spectra for the magnetic structures while for unpolarized configuration all structures without hydrogen are unstable due to soft phonon modes.

METHOD

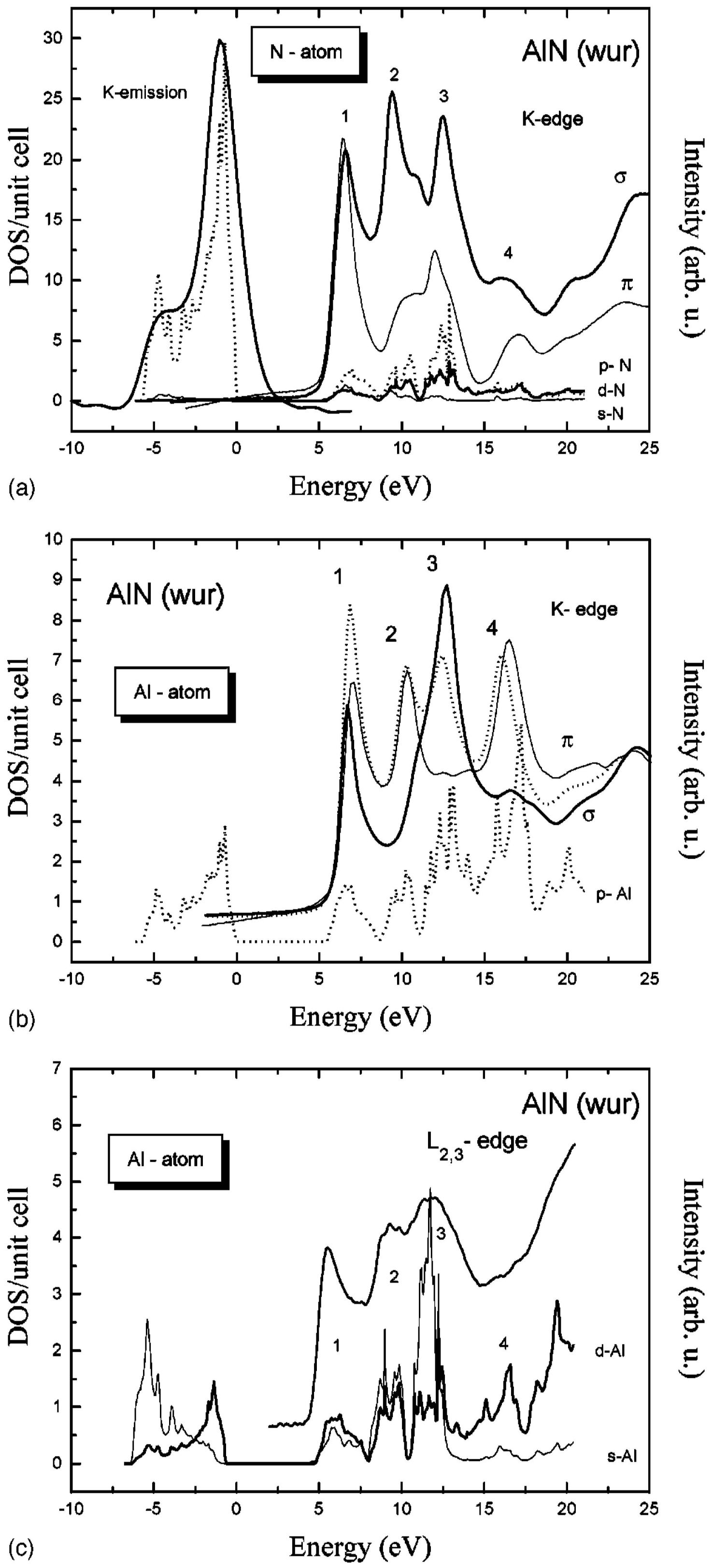
The band structure and density of states for the all group III nitrides in wurtizite and zinc blende structures have been calculated by means of the linear muffin tin orbital method in its scalar relativistic form in conjunction with the local density approximation to the density functional theory. We have applied the atomic sphere approximation but with the combined correction terms incorporated. The atomic sphere approximation version applies spherically symmetrized charge distributions and potentials in atomic spheres, i.e space filling and thus slightly overlapping spheres. Calculations for semiconductors included empty spheres located in the interstitial positions i.e. atomic spheres without nuclear charge. Each unit cell in the cubic zinc blende structure contains two real atoms cation and anion and two empty spheres. In the wurtzite structure we have eight atoms in the unit cell, four real and four empty. For calculations we have used the standard basis set, which includes partial wave of s, p, and d character on each atomic and interstitial site to give a total of 36 linear muffin-tin orbital per cubic unit cell. Energy eigen values and wave functions were obtained at 95(140) k points in the inrreducible part of the Brillouin zone. The densities of states normalized to the unit cell were calculated by means of tetrahedron technique. The calculations for wurtzite structure were performed under the assumption that the crystal structure was real.

RESULTS AND DISCUSSION

Graph (1) and (2) show the partial density of state for wurtzite and cubic gallium nitride and aluminium nitride. It was found that the energy zero corresponds to the valence band edge. On the left vertical axis the calculated total or partial s, p, d density of state per unit cell at the chosen atom has been indicated, which allowed to compare the absolute number of the available states. The number of atoms in the wurtzite unit cell is two times larger. On the right vertical axis the intensity of measured spectra in arbitrary unit is shown. The spectra obtained at different angles were normalized to the equal intensities before the onset of edge far above the conduction band edge where no polarization dependence is expected. Calculated partial density of state representing contribution of s, p and d states of nitrides are shown. The states are localized in easily seen subbands with energy position that agree with the maxima in observed emission and absorption spectra. The crystal field splits the valence states into two subbands and conduction states, in the considered energy range, into four separate subbands. P states dominate over all other states. The conduction band edge has also a significant contribution of nbitride s state. A similarity of the measured spectrum with the calculated partial density of state supported the dominant character of partial states in the valence and conduction bands. In graph 1 (c) and 1(d) absorption spectra of gallium are shown together with the calculated partial density of state of s and d symmetry. The similarity of cinduction band states of s and d symmetry. The similarity of conduction band states of s and d symmetry indicates strong hybridization of these states upto 12eV. The d partial density of state obtained from the calculations produced in the measured spectrum a broad maximum between 13 and 15 eV. From graph 1 (d) the spectral resolution is high and natural width of the 3p levels is small, only the first minimum and another one around 17.6 eV are well resolved. This is due to overlap of the spin-orbit-split bands. The features of wurtzite and cubic gallium nitride structures, the diominant character of p states, particularly at the nitrogen site, for both valence band and conduction band. The dominant contribution of s states of gallium at the bottom of the valence band for cubic structure and smaller contribution of these states for wurtzite structure are found. The aluminium nitride wurtzite partial density of state obtained are similar to those for gallium nitride but some differences also exist. One pronounced difference is that at the aluminium nitride conduction band edge the d states of cation dominate over s states contrary to the gallium nitride case. In valence band and conduction band the aluminium states of p as well as d symmetry are located at the same energy as the density maximum of nitride states of p symmetry, reflecting the strong hybridization of these states. In aluminium nitride the anisotropy of the p conduction states distribution is very pronounced at the anion as well as at the cation site which is shown in graph 2(a) and (b). Stronger anisotropy of the distribution of states in aluminium nitride seems to be connected with difference much larger than that in gallium nitride. Graph 2(b) also contains the mixed polarization spectrum which is compared directly with calculated p partial density of state. The obtained results were compared with previous obtained results and were found in good agreement.



Graph 1: The partial density of state as calculated for the wurtzite structure of gallium nitride.



Graph 2: The partial density of state as calculated for the wurtzite structure of aluminium nitride.

CONCLUSION

We have studied the electronic band structure of aluminium nitride and gallium nitrides crystallizing in the wurtzite and zinc blende structures. The electron transition is governed by dipole selection rule so obtained results of electronic states are also orbital resolved. The linear polarization of the synchrotron radiation allowed a separation of crystallographic direction dependent contributions from various constituents to the band states. The study of atom and orbital projected partial density of state of group three nitrides were used. The partial density of state distribution between the wurtzite and cubic structure of considered compounds were found in close similarity. For cubic structure more states are localized at the bottom of valance bond and in the conduction band and found that peaks are better separated and more visible than in the wurtzite structure. For aluminium we found pronounced anisotropy of bonds. For aluminium nitride and gallium nitride the agreement between structures observed in the calculated density of states and structures observed in experimental results are good in comparison. The obtained anisotropy of density of state distribution appeared in the anisotropy of various physical properties like reflective index, dielectric constant and elastic constant etc. More ionic bonding corresponded to higher valence electron density on the anion site but the density conduction staets on the cation site. The obtained results were in good agreement with previously obtained theoretical and experimental results.

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