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Theoretical Investigations on Structural, Electronic and Optical Properties of Wurtzite $In_xGa_{1-x}N$ (x=0, 0.25, 0.5, 0.75 and 1)

Ang Yang Yu

Liaoning University of Petroleum and Chemical Technology, Fushun, China

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Abstract

Wurtzite InGaN solid solutions have been designed with indium's incorporation into GaN crystal. In this work, electronic structure and optical properties have been theoretically investigated in order to improve the optoelectronic performance of GaN semiconducting material. Lattice parameters of title materials have been provided, which shows very good agreement with experimental values, thereby making them a good choice for further studies, including delving into optical properties. It is found that the optical wavelength range has been enlarged when doping GaN with indium and the increased proportion of indium makes absorption curves shift towards lower energies, which covers the whole visible light region. Because of excellent performance of these materials, a lot of new applications can be expected in the near future.

***Corresponding author**: Ang Yang Yu, Liaoning University of Petroleum and Chemical Technology, Fushun, China.

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Introduction

As one kind of group III-nitride semiconductors, GaN material has many favorable properties, including its wide band gap (3.4eV at room temperature), high electron mobility and high thermal conductivity, which has thus drawn a lot of attention [1]. GaN-based semiconductor has already been used to fabricate short-wavelength light-emission diode, laser detector, ultraviolet detector and high-temperature microelectronic devices, including high temperature big power field effect transistor, bipolar transistor, as well as high electron mobility transistor, which have already played important roles both in scientific research and in practical applications of daily life [2,3]. Therefore,

we can believe that GaN semiconductor has great potential and bright future in the market. There has been considerable interest in wurtzite GaN, which prefers to crystallize in hexagonal structure.

InGaN solid solution, which is formed through the introduction of indium into pure GaN semiconductor, has greatly improved the properties of host material. This system is very interesting, and deserves investigations both in experimental work and in theoretical calculations. GaN and its solid solution can have perfect applications in optoelectronics devices in the frequency range from microwaves to ultraviolet region. In this paper, a comparative study of structural, electronic, and optical properties of wurtzite InGaN solid solution ($In_xGa_{1-x}N$) is presented [4,10]. The structural parameters were obtained based on first-principles calculations. Then, the optical properties, including the dielectric function and absorption are computed and analyzed.

Computational Methods

In the present work, InGaN solid solutions, namely, $In_xGa_{1-x}N$ with x=0, 0.25, 0.5, 0.75 and 1, are obtained through the incorporation of different proportional indium into wurtzite GaN model. The geometric parameters of $In_xGa_{1-x}N$, starting from a 16-atom 2×2×1 wurtzite GaN supercell, are optimized by performing the ab initiopseudopotential plane-wave method and making use of density mixing scheme and conjugate gradient (CG) method [11,12].

Exchange and correlation effects are treated by a functional PBE, as a version of the generalized-gradient approximation (GGA) [13]. The total energy and charge density are integrated in the Brilorine zone by means of Monkhorst-Pack scheme. In order to ensure the accuracy of results with an efficient calculation, a suitable plane wave cutting kinetic energy is selected in order to obtain realistic structures of title materials [14].

Results and Discussion

Structural Parameters

It is known that III-nitride semiconductors are inclined to crystallize in hexagonal structure [15]. The wurtzite structure of hexagonal GaN is characterized by two lattice constants, namely, a=0.319nm, c=0.519nm [16,17]. In order to improve the physical properties of wurtzite GaN crystal, indium with different proportions is introduced into GaN, forming InGaN solid solution.

At first, geometrical optimizations of supercell of wurtzite GaN with indium was executed so as to gain the stable crystal structure. The lattice parameters of wurtzite $In_xGa_{1-x}N$, with x set at 0, 0.25, 0.5, 0.75 and 1, respectively, have been computed and Table 1 has listed relevant data. It can be seen in the table that lattice parameters (a and c) change monotonously.

Table 1: Computed Lattice Constants of Wurtzite **$In_xGa_{1-x}N$** in the Most Stable State, With the Experimental Values Denoted in Brackets.

Lattice constants/ Materials	a(nm)	c(nm)
GaN	0.320(0.319[16,17])	0.522(0.519[16,17])
$In_{0.25}Ga_{0.75}N$	0.331	0.536
$In_{0.5}Ga_{0.5}N$	0.342	0.546
$In_{0.75}Ga_{0.25}N$	0.349	0.565
InN	0.358(0.35[18,19])	0.58(0.57[18,19])

Both a and c increase with the rise of indium's composition, which is due to larger volume of indium atom than that of gallium atom. It has become InN when x=1. Lattice constants of InN crystal are optimized to be a=0.358nm, c=0.58nm, c/a=1.62, which are in excellent agreement with previous data reported in the literature [18,19]. Based on these things, we can firmly believe that the computational methods adopted in this work have enough accuracy and can be used for further investigations.

Electronic Properties

Is there any change in density of states (DOS) of GaN when doping with indium? Figure 1 compares the density of states (DOS) of GaN and $In_{0.5}Ga_{0.5}N$ in order to have a clear understanding about doping effects on electronic properties.

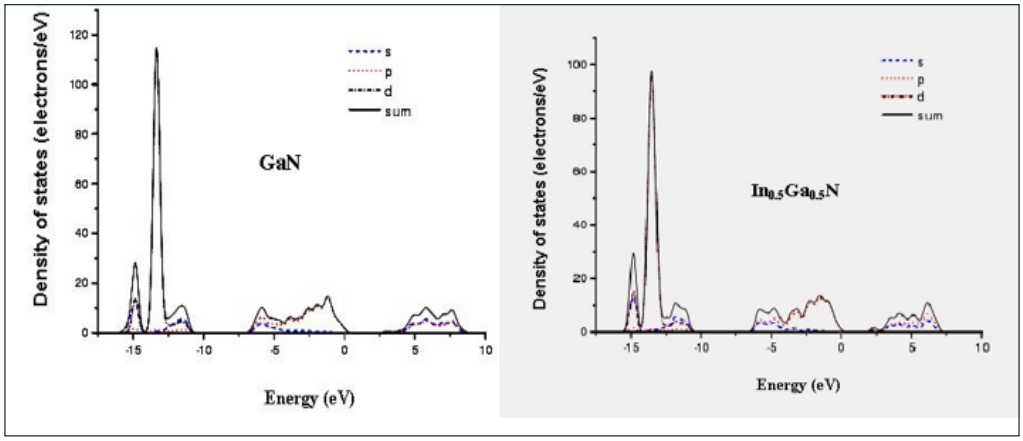

Figure 1: A comparison of Density of States between GaN and $In_{0.5}Ga_{0.5}N$ with Wurtzite Structure

It can be seen that the valence band of $In_{0.5}Ga_{0.5}N$ can be divided into two regions. The upper valence band lies between -6.57eV and 0eV, which is formed by N-2p. The lower valence band locates between -15.67 and -10.87eV. Although the region from -15.64eV to 14.22eV and the region from -13.56eV to -10.56eV are mainly formed by N-2s, the DOS peak at -13.51eV is dominated by d state from indium and gallium. Moreover, the position and intensity of the valence band in $In_{0.5}Ga_{0.5}N$ remain the same no matter whether doping indium or not.

The conduction band has the width of 5.24eV and spreads the region between 1.93eV and 7.17eV, in which most electrons are distributed in Ga-4s orbital and a few electrons occupy N-2p orbital and Ga-4p orbital. Compared with GaN, the intensity of the conduction band in $In_{0.5}Ga_{0.5}N$ remain unchanged, but the position of the conduction band shifts about 1.52eV towards lower energy, which results in narrowed optical band gap. Additionally, there is a new peak at 2.33eV, which is composed of In-5s and In-5p.

Optical Properties

Optical properties can provide a great deal of information regarding physical properties of materials, such as electronic properties and defects. The dielectric function and the absorption spectrum of $In_xGa_{1-x}N$ have been investigated in the present work. The imaginary part of dielectric function can be got as a function of photon energy from first-principles calculations, and the real part of the dielectric function can be obtained from the imaginary part by the Kramer–Kronig relationship [20]. As a matter of fact, the complex dielectric function is the starting point of calculating various optical properties [21].The imaginary part of dielectric function is very successful in deducing the optical transition between the conduction band and valence band for undoped and doped GaN, as presented in Figure 2. It can be seen that there are five curves with different colors, which correspond to x=0, 0.25, 0.5, 0.75 and 1, respectively.

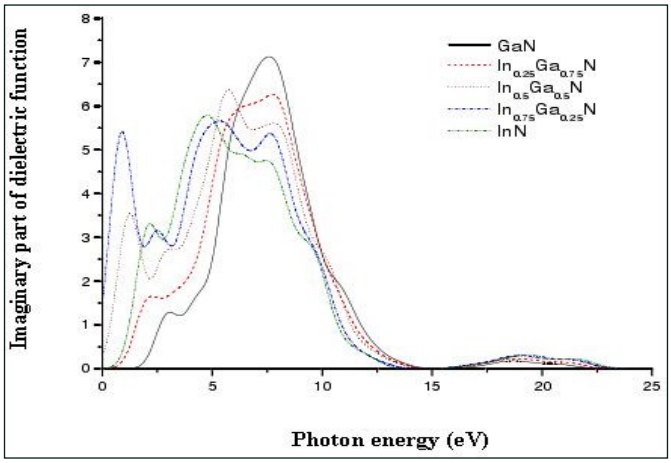

Figure 2: Imaginary Part of Dielectric Function of $In_xGa_{1-x}N$ as a Function of the Photon Energy, with x=0,

0.25, 0.5, 0.75 and 1, Respectively

There are three separate dielectric function peaks for GaN at 2.63eV, 7.51eV and 18.58eV. The peak at 2.63eV corresponds to the direct transition from top of valence band to bottom of conduction band, which is mainly originated from electrons in Ga-3p orbital. The dielectric peak at 7.51eV may correspond to the transition from lower valence band to upper valence band, which results from electrons of Ga-3d orbital or N-2s orbital in lower valence band. Moreover, the weak peak at 18.58eV corresponds to the transition between lower valence band and conduction band, which is caused by electrons in Ga-3d of lower valence band. We can also find that almost all the peaks of $In_xGa_{1-x}N$ shift towards low energy direction once the composition of indium hikes, which can be attributed to narrowed optical band gap. Quantitatively, the peak position will move about 0.5eV once the proportion of indium increases by 25%. However, the dielectric peaks can shift toward higher energies if $In_{0.75}Ga_{0.25}N$ is transformed to InN. There are six dielectric peaks at 2.19eV, 4.77eV, 6.43eV, 7.56eV, 9.50eV and 19.63eV for InN when x=1, as is marked in green color in Figure 2. Overall, a series of visible light with different colors can be realized through the participation of indium into GaN with different proportions.

Absorption spectrum of $In_xGa_{1-x}N$ is presented in Figure 3. It can be seen that there are two prominent peaks, which locate at 8.9eV and 10.5eV, respectively.

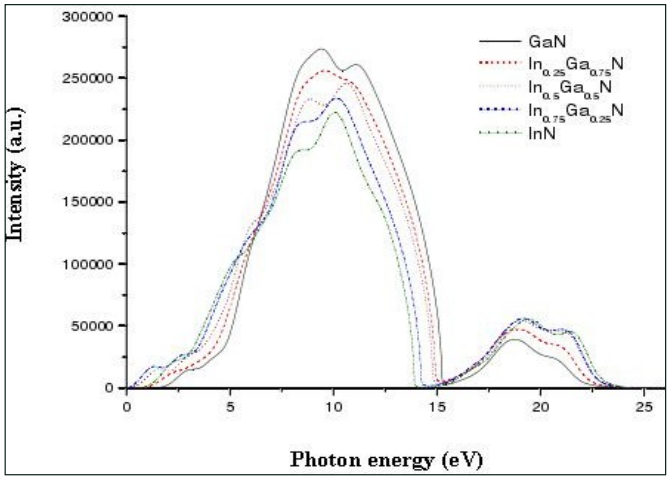

Figure 3: Absorption Spectrum of $In_xGa_{1-x}N$, with x=0, 0.25, 0.5, 0.75 and 1, Respectively

The absorption intensity at 8.9eV is the largest when the proportion of indium is less than 25%. However, the intensity at 8.9eV drop dramatically when the proportion of indium is in the range of $0.25 \leq x \leq 1$. We can see that the intensity at 10.5eV can surpass the intensity at 8.9eV and become the highest peak in the case of $In_{0.5}Ga_{0.5}N$. As can be seen in the figure, the position of each absorption peak moves toward lower energy direction with the rise of indium's content. Additionally, there are five absorption peaks for InN, which are located at 2.36eV, 8.33eV, 10.09eV, 19.49eV and 21.53eV, respectively. These optical results have wide technological applications, for instance, fabricating new electronic devices.

Epilogue

Nowadays, nearly all electronic and optoelectronic devices have been fabricated utilizing alloys of the III–V nitrides, such as gallium nitride (GaN). In the present work, structural parameters of wurtzite $In_xGa_{1-x}N$, with x=0, 0.25, 0.5, 0.75 and 1, have been computed by means of the ab initio pseudopotential plane-wave method. Then, we look into the optical properties, including the dielectric function and absorption. We also discuss the electronic structures, which have a close connection with the optical properties. It has been found that the optical wavelength range of GaN has been enlarged when doped with indium. The absorption peak position of host material can move towards the lower energy direction once the proportion of indium is introduced. That is to say,

a series of visible lights with different colors can be tuned if different indium proportions are incorporated into GaN. Therefore, good performances of InGaN solid solution can be anticipated in the future.

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