

Modeling the optical properties of hexagonal GaN

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An adjustable broadening function instead of the conventional Lorentzian one is incorporated in the dielectric function model for hexagonal GaN. One-electron contributions at E_1 critical points and higher-state ($m > 1$) exciton terms, which were incorrectly disregarded in the previous study, are taken into account. Model parameters were determined using the acceptance-probability-controlled simulated annealing. As a result, excellent agreement with experimental data for both real and imaginary parts in the range from 1.5 to 10 eV is obtained. Average discrepancy between experimental and calculated data for the real part of the index of refraction equals 2.75×10^{-4} , and for the imaginary part is 1.66×10^{-3} . © 1998 American Institute of Physics. [S0003-6951(98)03533-5]

GaN is a promising material for the fabrication of optoelectronic devices which operate in the near ultraviolet region, since it has a direct band gap at around 3.4 eV. It is resistant to radiation damage and can form solid solutions with InN and AlN, which enables fabrication of electroluminescence devices emitting light from orange to ultraviolet.¹ Therefore, understanding of optical properties of this material is important from both an application and a fundamental point of view. There have been extensive studies on the optical properties of hexagonal GaN. However, these studies are mostly limited to photoreflectance and photoluminescence studies which are useful for estimating the fundamental band gap, while studies of optical properties in the wide spectral range²⁻⁴ are scarce.

It is well known that the optical properties of solids can be described in terms of the complex dielectric function $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$. In the design of optoelectronic devices, for instance lasers and waveguide devices, interplay between the physical dimensions of the device, and the index of refraction requires the index of refraction to be known as a function of the wavelength as precisely as possible. The model for the index of refraction should be simple and concise, but complex enough to account for all relevant features of the index of refraction over the wide energy range. There have been several attempts to model the dielectric function of hexagonal GaN, in the narrow spectral range^{3,5,6} as well as in the wide spectral range.^{2,7,8} However, in the wide spectral range both the semiempirical tight-binding approach in calculating the dielectric function^{7,8} and Adachi's model dielectric function (MDF)² agree with experimental data only in terms of positions of absorption peaks corresponding to major critical points, while significant discrepancies exist between the calculated and experimental values of the dielectric function and index of refraction.

Here, we propose a modification of MDF giving significant improvement on accuracy. Our model departs from the MDF employed in the previous study of Kawashima *et al.*² in three important points. First, we take into account the one-electron contribution at $E_{1\beta}$, where $\beta = A, B, C$ denotes

the critical points, which were disregarded in the previous study² under the weak argument that excitonic transitions in hexagonal GaN are more pronounced than in other semiconductors, and therefore, that they are much stronger than one-electron contributions. Second, summation in the equations describing exciton contributions is performed until the contribution to the sum becomes less than 10^{-4} , while in the previous study only the ground state exciton term ($m = 1$) was taken into account. And, finally, we employ frequency dependant damping instead of the damping constant. In such a manner, broadening of the spectral lines is not restricted to the conventional Lorentzian one. It varies over a range of broadening functions, enabling greater flexibility of the model.

We shall briefly describe the employed model. The dielectric function is given by the sum of one-electron contributions at E_0 , E_{1A} , E_{1B} and E_{1C} critical points, excitonic contributions and additive constant ϵ_∞

$$\epsilon(E) = \epsilon_0(E) + \epsilon_{0E}(E) + \epsilon_1(E) + \epsilon_{1E}(E) + \epsilon_\infty. \quad (1)$$

Under the parabolic band assumption, contribution of three-dimensional (3D) M_0 critical point E_0 is given by

$$\epsilon_0(E) = AE_0^{-3/2} \chi_0^{-2} [2 - (1 + \chi_0)^{1/2} - (1 - \chi_0)^{1/2}], \quad (2)$$

where

$$\chi_0 = \frac{E + i\Gamma_0}{E_0}, \quad (3)$$

TABLE I. Model parameter values.

ϵ_∞	0.426	A (eV ^{1.5})	41.251		
Γ_0 (eV)	0.287	α_0	1.241	E_0 (eV)	3.550
B_{1A} (eV)	0.778	B_{1B} (eV)	0.103	B_{1C} (eV)	0.920
B_{1A}^X (eV)	2.042	B_{1B}^X (eV)	1.024	B_{1C}^X (eV)	1.997
Γ_{1A} (eV)	0.743	Γ_{1B} (eV)	0.428	Γ_{1C} (eV)	0.440
α_{1A}	0.240	α_{1B}	0.011	α_{1C}	0.005
G_{1A}^{2D} (eV)	0.0003	G_{1B}^{2D} (eV)	0.356	G_{1C}^{2D} (eV)	1.962
E_{1A} (eV)	6.010	E_{1B} (eV)	8.182	E_{1C} (eV)	8.761
A_0^{ex} (eV)	0.249	G_0^{3D} (eV)	0.030		

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while A and Γ_0 are the strength and damping constant of the E_0 transition, respectively. Actually, one should calculate separate contributions from E_{0A} , E_{0B} and E_{0C} critical points, but due to very small splitting energies between these critical points, $E_{0\beta}$ can be treated as a single degenerate one.²

Exciton contributions at E_0 critical points are given by

$$\epsilon_{0E}(E) = \sum_{m=1}^{\infty} \frac{A_0^{\text{ex}}}{m^3} \frac{1}{E_0 - (G_0^{3D}/m^2) - E - i\Gamma_0}, \quad (4)$$

where A_0^{ex} is the 3D exciton strength parameter, and G_0^{3D} is the 3D exciton binding energy.

Contributions of the two-dimensional (2D) M_0 critical points $E_{1\beta}$ are given by

$$\epsilon_{1E}(E) = \sum_{\beta=A,B,C} \sum_{m=1}^{\infty} \frac{B_{1\beta}^X}{(2m-1)^3} \frac{1}{E_{1\beta} - [G_{1\beta}^{2D}/(2m-1)^2] - E - i\Gamma_{1\beta}}, \quad (7)$$

where $B_{1\beta}^X$ and $G_{1\beta}^{2D}$, are the strengths and binding energies of the excitons at $E_{1\beta}$, respectively.

One of the major shortcomings of the above described model is that it was based on the assumption of Lorentzian broadening. The fact that Lorentzian broadening does not accurately describe absorption processes, especially in the E_0 critical point region, has already been recognized.^{9,10} Kim *et al.*⁹ have replaced the damping constant Γ_j ($j=0,1A,1B,1C$) in their model with frequency dependant damping constant Γ'_j given by

$$\Gamma'_j(E) = \Gamma_j \exp\left[-\alpha_j \left(\frac{E - E_j}{\Gamma_j}\right)^2\right]. \quad (8)$$

They have shown that using this variable line shape, where the type of broadening is determined by the ratio of parameters α_j and Γ_j (for example, $\alpha_j/\Gamma_j < 0.1$ for Lorentzian and $\alpha_j/\Gamma_j \approx 0.3$ for Gaussian), better agreement with experiment can be obtained. However, their model is rather complicated, with a large number of parameters, and the equations are material dependent, which prevents it from being widely accepted and used. On the other hand, Rakić *et al.* have shown that frequency dependent damping applies equally well to Adachi's model of the dielectric function of zinc-blende semiconductors, for example, of GaAs and AlAs. Therefore, we have incorporated the described modification into MDF for hexagonal semiconductors, by replacing damping constants Γ_j in Eqs. (2)–(7) with the expression given by Eq. (8).

The model parameters, obtained by the acceptance-probability-controlled simulated annealing algorithm,¹¹ are given in Table I. The parameters were obtained by minimizing the following objective function:

$$F = \sum_{i=1}^N \left(\left| \frac{n(\omega_i)}{n^{\text{expt}}(\omega_i)} - 1 \right| + \left| \frac{k(\omega_i)}{k^{\text{expt}}(\omega_i)} - 1 \right| \right)^2, \quad (9)$$

where the summation is performed over available experimental points at frequency ω_i , while $n^{\text{expt}}(\omega_i)$, $n(\omega_i)$,

$$\epsilon_1(E) = - \sum_{\beta=A,B,C} B_{1\beta} \chi_{1\beta}^{-2} \ln(1 - \chi_{1\beta}^2), \quad (5)$$

where

$$\chi_{1\beta} = \frac{E + i\Gamma_{1\beta}}{E_{1\beta}}, \quad (6)$$

$B_{1\beta}$ and $\Gamma_{1\beta}$ are the strengths and damping constants of the $E_{1\beta}$ transitions, respectively.

Contribution of the Wannier type 2D excitons (discrete series of exciton lines at the $E_{1\beta}$ critical points) is given by

$k^{\text{expt}}(\omega_i)$, $k(\omega_i)$ are the experimental and calculated values of the real and imaginary part of the index of refraction at point ω_i , respectively.

Figure 1 shows the real and imaginary parts of the dielectric function of hexagonal GaN as a function of energy. The open circles represent experimental data,² the solid line is the dielectric function calculated in this work, while the broken line represents results of the Kawashima *et al.*² Figure 2 shows the real and imaginary part of the index of refraction of GaN versus energy. The inset shows relative errors for the real and imaginary part of the index of refraction

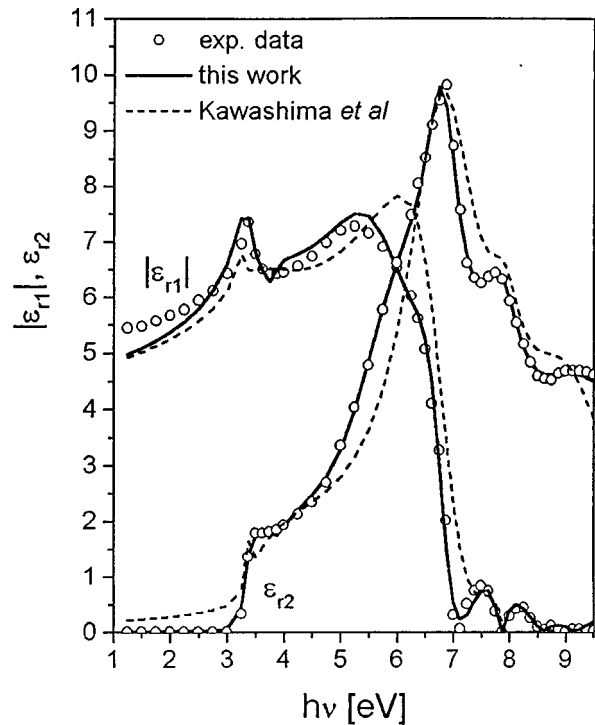


FIG. 1. Real and imaginary part of the dielectric function of GaN vs energy: circles, experimental data; solid line, this work; and broken line, model of Kawashima *et al.* (Ref. 2).

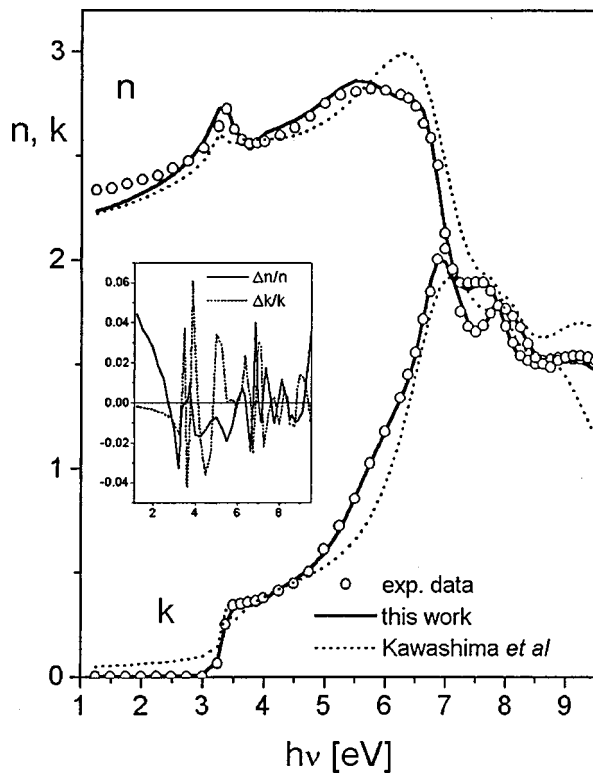


FIG. 2. Real and imaginary part of the index of refraction of GaN vs energy: open circles, experimental data; solid line, this work; and broken line, model of Kawashima *et al.* (Ref. 2). Inset shows relative errors for the real and imaginary parts of the index of refraction.

tion (in the region where k equals 0, absolute error is given). Excellent agreement between our calculations and experimental data can be observed. As an indication of accuracy with respect to experimental values, we have calculated relative rms (root-mean-square) errors, which are, in our case, 1.7% for n and 4.1% for k , while for the results of Kawashima *et al.*² they equal 7.4% for n and even 22.8% for k .

In conclusion, we have modeled the optical dielectric function of hexagonal nitride with the average relative error between the experimental and calculated data for the real

part of the index of refraction n is 2.75×10^{-4} , and for the imaginary part k is 1.66×10^{-3} . For comparison, the average relative error between calculated and experimental data in the study of Kawashima *et al.*² equaled 5.42×10^{-3} for n and 0.051 for k . There are several reasons for the significant improvement of the accuracy of our calculations. First, the type of broadening at each critical point is variable and it represents an adjustable parameter of the model. Second, higher-state excitons ($m > 1$) are taken into account. And, finally, our calculations include one-electron contributions at E_{1B} critical points. From the parameters given in Table I, we can deduce the ratio of strengths of excitonic to strengths of one-electron contributions, which equals 2.6 at E_{1A} , 9.9 at E_{1B} and 2.2 at E_{1C} . Since the strength of the excitonic contribution is only about two times larger than that of the one-electron contributions at E_{1A} and E_{1C} , it is obvious that the disregarding of one-electron contributions would be entirely unjustified.

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