Modeling the optical constants of $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 crystals

M. León, R. Serna, S. Levchenko, A. Nateprov, A. Nicorici et al.

Citation: *J. Appl. Phys.* **101**, 013524 (2007); doi: 10.1063/1.2409608

View online: <http://dx.doi.org/10.1063/1.2409608>

View Table of Contents: <http://jap.aip.org/resource/1/JAPIAU/v101/i1>

Published by the [American Institute of Physics](#).

Related Articles

Optical conductivity of highly mismatched GaP alloys

Appl. Phys. Lett. **102**, 023901 (2013)

Electrical and optical properties of p-type $\text{CuFe}_{1-x}\text{Sn}_x\text{O}_2$ ($x = 0.03, 0.05$) delafossite-oxide

J. Appl. Phys. **113**, 023103 (2013)

Stoichiometry dependence of resistance drift phenomena in amorphous GeSnTe phase-change alloys

J. Appl. Phys. **113**, 023704 (2013)

Negative refraction and subwavelength imaging in a hexagonal two-dimensional annular photonic crystal

J. Appl. Phys. **113**, 013109 (2013)

The vibrational spectrum of CaCO_3 aragonite: A combined experimental and quantum-mechanical investigation

J. Chem. Phys. **138**, 014201 (2013)

Additional information on *J. Appl. Phys.*

Journal Homepage: <http://jap.aip.org/>

Journal Information: http://jap.aip.org/about/about_the_journal

Top downloads: http://jap.aip.org/features/most_downloaded

Information for Authors: <http://jap.aip.org/authors>

ADVERTISEMENT

AIPAdvances

Now Indexed in
Thomson Reuters
Databases

Explore AIP's open access journal:

- Rapid publication
- Article-level metrics
- Post-publication rating and commenting

Modeling the optical constants of $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 crystals

M. León^{a)}*Departamento Física Aplicada, Universidad Autónoma de Madrid, C-XII, 28049 Madrid, Spain*

R. Serna

Instituto de Optica, CSIC, Serrano 121, 28006 Madrid, Spain

S. Levchenko, A. Nateprov, and A. Nicorici

Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau MD 2028, Moldova

J. M. Merino

Departamento Física Aplicada, Universidad Autónoma de Madrid, C-XII, 28049 Madrid, Spain

E. Arushanov

Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau MD 2028, Moldova and Departamento Física Aplicada, Universidad Autónoma de Madrid, C-XII, 28049 Madrid, Spain

(Received 23 June 2006; accepted 31 October 2006; published online 12 January 2007)

Spectral dependence of the pseudodielectric function $\varepsilon(E) = \varepsilon_1(E) + i\varepsilon_2(E)$ as well as of the complex refractive index, extinction coefficient, absorption coefficient, and normal-incidence reflectivity of $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 ordered vacancy compound crystals are modeled in the 0.8–4.4 eV photon energy range using a modification of Adachi's model [T. Kawashima *et al.* J. Appl. Phys. **84**, 5202 (1998)] for optical properties of semiconductors. Model parameters are determined using the acceptance-probability-controlled simulated annealing method. Excellent agreement with experimental data is obtained; the relative errors for the real ε_1 and for imaginary ε_2 part of the dielectric function are equal to 0.9%–1.5% and 3.2%–4.1% for the studied compounds. © 2007 American Institute of Physics. [DOI: [10.1063/1.2409608](https://doi.org/10.1063/1.2409608)]

I. INTRODUCTION

Chalcopyrite-type semiconductor compounds are superior materials for thin film photovoltaic cells. Laboratory cells based on $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ have demonstrated an efficiency up to 19.3%.¹ Recent studies showed the existence of CuIn_3Se_5 as a segregated secondary phase at the surface of the In-rich CuInSe_2 thin films. Such layer is expected to play an important role in the performance of the high efficiency $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ -based solar cells.^{2,3} The $\text{Cu}_2\text{In}_4\text{Se}_7$ (I247) and CuGa_3Se_5 (G35) belong to the I-III-VI family of Cu-deficient defect ternary semiconductor compounds with ordered vacancies. These compounds, called ordered vacancy compounds (OVCs) or ordered defect compounds, attract a lot of attention as the perspective materials for application both in high efficiency photovoltaic devices and in nonlinear optics. Therefore a detailed study of their various physical properties is necessary in order to develop efficient devices. However, so far most of the characteristics of OVC have not been studied in depth. Only some optical properties, mainly the band gaps E_g of $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 thin films^{4,5} and bulk samples^{6–10} have been reported so far.

Spectroscopic ellipsometry (SE) is recognized as a highly suitable method to determine dielectric functions of semiconductors over a wide energy range. These functions are related to the electronic band structure and can be used as a powerful source of the experimental information on the latter.¹¹ Recently, ellipsometric investigations of $\text{Cu}_2\text{In}_4\text{Se}_7$

and CuGa_3Se_5 crystals have been reported.¹² The main aim of this work is to model the optical constants of $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 .

$\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 have been grown by the Bridgman (*B*) method. Compositional measurements were carried out by energy dispersive x-ray microanalysis (EDAX). Samples used for the optical study show some deviation from stoichiometry (Table I). Experimental details concerning the structural analysis and SE measurements are given in Ref. 12.

II. THEORETICAL MODEL

Two different methods are usually used to analyze in detail the observed structures of the dielectric function, namely, fitting the numerically differentiated experimental spectrum to analytical line shapes^{11,13} and modeling of measured $\varepsilon(E)$ spectra, using interband transitions models.^{14–16} In our paper main attention is paid to the latter. The former has been used for our compounds in Ref. 12 and the obtained values of the transition energies will be presented to compare the results of both methods.

TABLE I. Data on compositional measurements of samples studied carried out by EDAX.

Samples ^{a)}	Cu (at. %)	In (or Ga) (at. %)	Se (at. %)	In/Cu (or Ga/Cu)	Se/Cu
$\text{Cu}_2\text{In}_4\text{Se}_7$ (I247/B)	16.6	31.1	52.3	1.9	3.1
CuGa_3Se_5 (G35T/B)	13.1	34.55	52.35	2.6	4.0
CuGa_3Se_5 (G35B/B)	12.7	35.08	52.22	2.8	4.1

^{a)}Electronic mail: maximo.leon@uam.es

Adachi's model dielectric function has been successfully applied to model the dielectric function as well as the optical constants of III-V and I-II-VI₂ compounds.^{14–16} The complex dielectric function as a function of energy $E = \hbar\omega$ is described by the sum of terms corresponding to one-electron contributions at critical points $E_{0\alpha}$ ($\alpha=A, B, C$) and $E_{1\beta}$ ($\beta=A, B$), $\varepsilon_0(E)$ and $\varepsilon_1(E)$, and an additive constant a ,

$$\varepsilon(E) = \varepsilon_0(E) + \varepsilon_1(E) + a. \quad (1)$$

The $E_{0\alpha}$ ($\alpha=A, B$, and C) gaps in chalcopyrite crystals were assigned to the three-dimensional (3D) M_0 critical point. Assuming that the valence and conduction bands are parabolic and using the Kramers-Kronig transformation, the contribution of these gaps to $\varepsilon_0(E)$ can be written as

$$\varepsilon_0(E) = \sum_{\alpha=A,B,C} A_{0\alpha} E_{0\alpha}^{-3/2} f(\chi_{0\alpha}),$$

with

$$A_{0\alpha} = (4/3)(3/2\mu_{0\alpha})^{3/2} P_{0\alpha}^2,$$

$$f(\chi_{0\alpha}) = \chi_{0\alpha}^{-2} [2 - (1 + \chi_{0\alpha})^{1/2} - (1 - \chi_{0\alpha})^{1/2}], \quad (2)$$

$$\chi_{0\alpha} = (E + i\Gamma)/E_{0\alpha}.$$

In Eq. (2) $\mu_{0\alpha}$ is the combined density-of-states mass, $P_{0\alpha}^2$ is the squared momentum-matrix element, and Γ is the damping energy of the $E_{0\alpha}$ gap. It is worth mentioning that normally, one should calculate the separate contributions from $E_{0\alpha}$ ($\alpha=A, B$, and C) critical points according to Eq. (2), but in our case, splitting among these critical points is not observed, and $E_{0\alpha}$ has been treated as a single degenerate one. Contributions of the two-dimensional (2D) M_0 critical points $E_{1\beta}$ are given by Adachi's model,¹⁵

$$\varepsilon_1(E) = - \sum_{\beta=A,B} B_{1\beta} \chi_{1\beta}^{-2} \ln(1 - \chi_{1\beta}^2),$$

with

$$\chi_{1\beta} = (E + i\Gamma_{1\beta})/E_{1\beta}, \quad (3)$$

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

Djurisic *et al.*¹⁷ have proposed the acceptance-probability-controlled simulated annealing (APCSA) algorithm to obtain the model parameters. It is known that all fitting routines based on classical optimization algorithms, such as Levenberg-Marquardt or simplex algorithms, require initial parameter values close to the final ones to provide a meaningful solution and it is usually hard to provide good initial values for adjustable parameters of the model. Therefore, to determine accurately the model parameters, one should employ a global optimization routine, such as a simulated annealing algorithm employed in Ref. 17. Djurisic and Li¹⁶ have modeled the optical constants of hexagonal GaN, InN, and AlN using Adachi's model and obtained good agreement with experimental data. Model parameters are determined using the APCS algorithm through minimizing the following objective function:

FIG. 1. Real (ε_1) and imaginary (ε_2) parts of the dielectric function vs energy for (a) $\text{Cu}_2\text{In}_4\text{Se}_7$ (I247/B) and (b) CuGa_3Se_5 (G35B/B and G35T/B) crystals.

$$F = \sum_{i=1}^N \left(\left| \frac{\varepsilon_1(E_i)}{\varepsilon_1^{\text{expt}}(E_i)} - 1 \right| + \left| \frac{\varepsilon_2(E_i)}{\varepsilon_2^{\text{expt}}(E_i)} - 1 \right| \right)^2, \quad (4)$$

where the summation is performed over the available experimental points and $\varepsilon_1^{\text{expt}}(E_i)$, $\varepsilon_1(E_i)$, $\varepsilon_2^{\text{expt}}(E_i)$, and $\varepsilon_2(E_i)$ are, respectively, the experimental and calculated values of the real and imaginary parts of complex dielectric function at point E_i .

III. RESULTS AND DISCUSSIONS

The real $\varepsilon_1(E)$ and imaginary parts $\varepsilon_2(E)$ of the pseudodielectric function $\varepsilon(E) = \varepsilon_1(E) + i\varepsilon_2(E)$ for $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 crystals are shown in Figs. 1(a) and 1(b). The structures observed in the $\varepsilon(E)$ spectra are attributed to interband critical points (CP's), related to regions of the band structure with large or singular point electronic density of states.

We have applied Adachi's model and APCS algorithm to our SE data analysis. Figures 1(a) and 1(b) show the real and imaginary parts of the dielectric functions of I247/B, G35B/B, and G35T/B as a function of the energy. The solid circles represent our experimental data,¹² while the solid lines show the dielectric function calculated using Adachi's model. Excellent agreement between our calculations and experimental data can be observed. As an indication of accuracy with respect to experimental values, the relative errors have been calculated. These values are, respectively, about 0.9%–1.5% and 3.2%–4.1% for the real and imaginary parts of the dielectric functions for the studied compounds.

The model parameters A , B , E_0 , E_{1A} , E_{1B} , and Γ calculated using APCS algorithm are given in Table II. The values of E_0 , E_{1A} , and E_{1B} are in a good agreement with those obtained from an analysis of the numerically derived $d^2\varepsilon(E)/d\omega^2$ (Table II).¹² The lowest value of $E_{0\alpha}$, observed in the region below 2 eV of CuIn_3Se_5 , corresponds to its fundamental energy gap $E_0 = E_g$. A second $E_1(A)$ and third energy thresholds $E_1(B)$ appear in the region between 2 and 4.5 eV. The fit-determined E_0 and E_1 values, together with their related strength and broadening parameters, are listed in Table II. The resulting analytical lines from the fits of the experimental data in Figs. 1(a) and 1(b) have been obtained considering CP's of the three-dimensional-type 3D in the E_g region and of the type 2D in the E_1 region. It is worth mentioning that reasonable agreement can be achieved between experimental data and calculated curves.

TABLE II. Model parameter values.

Parameter	Samples					
	G35B/B		G35T/B		I247/B	
A (eV ^{1.5})	7.71		7.9		5.15	
E_0 (eV)	1.85 (1.88) ^a		1.86 (1.88)		1.125 (1.15)	
Γ (eV)	0.057		0.049		0.03	
B_{1A}	2.33		2.42		2.38	
E_{1A} (eV)	2.89 (2.87)		2.9 (2.94)		2.55 (2.60)	
Γ_{1A} (eV)	0.31		0.305		0.31	
B_{1B}	3.59		3.31		3.28	
E_{1B} (eV)	4.14 (3.97)		4.12 (3.94)		4.01	
Γ_{1B} (eV)	0.75		0.61		0.73	
a	0.54		0.72		0.88	
error	ε_1	ε_2	ε_1	ε_2	ε_1	ε_2
	1.2%	3.8%	0.9%	4.1%	1.5%	3.2%

^aValues of E_0 and E_1 calculated by fitting the numerically differentiated experimental spectrum to analytical line shapes are in brackets.

Band structure calculation needed to perform identifications of the observed energy transitions is not available for $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 . Identifications of the observed energy have been done taking into account the CuInSe_2 and CuGaSe_2 band structure calculations. As it has been established for such compounds, the main transitions contributing to $\varepsilon(E)$ occur at the Brillouin zone (BZ) center (fundamental gap at Γ) and at the N and T points in the BZ edge (predominant upper transitions).¹⁹ The energy threshold of the fundamental absorption edge $E_0 = E_g$ corresponds to direct transition from the valence band maximum to the conduction band minimum at the center of the BZ (Γ point). Our obtained values of $E_g = 1.125$ for I247 and 1.85 eV for and G35 at room temperature (Table II) are in a reasonable agreement with those obtained from the optical measurements.^{4–10} The variation in the reported values of the band gap of OVC can be attributed to the compositional change. The chalcopyrites and OVCs usually exhibit high tolerance to deviations in stoichiometry. In fact, CuInSe_2 shows band gap values ranging from 0.94 to 1.04 eV. In the region of 2.5–4.6 eV two transitions for I247 and G35 named as $E_1(A)$ and $E_1(B)$ have been observed. They can be attributed to transitions at the N point in the BZ following Refs. 18 and 19, where ellipsometric data on CuInSe_2 and CuGaSe_2 were analyzed. The energy separation between these two transitions corresponds to the crystal-field splitting of the valence band at the N point. The differences in energy $E_1(A) - E_1(B)$ are about 1.25 and 1.45 eV for G35 and I247, respectively. The value of about 0.8 eV was reported for CuInSe_2 and CuGaSe_2 crystals.^{18,19}

Optical parameters, namely, the complex refractive index $n^* = n + ik$, normal-incidence reflectivity R and the absorption coefficient α , can be obtained from the present study in the form of practical functions, since they are directly related to the complex dielectric function $\varepsilon(E) = \varepsilon_1(E) + i\varepsilon_2(E)$.

The real refractive index n and extinction coefficient k are given by

FIG. 2. Spectral dependence of the real refractive index n and the extension coefficient k for (a) $\text{Cu}_2\text{In}_4\text{Se}_7$ (I247/B) and (b) CuGa_3Se_5 (G35B/B and G35T/B) crystals.

$$n(E) = \left(\frac{[\varepsilon_1(E)^2 + \varepsilon_2(E)^2]^{1/2} + \varepsilon_1(E)}{2} \right)^{1/2}, \quad (5)$$

$$k(E) = \left(\frac{[\varepsilon_1(E)^2 + \varepsilon_2(E)^2]^{1/2} - \varepsilon_1(E)}{2} \right)^{1/2}. \quad (6)$$

The absorption coefficient α and normal-incidence reflectivity R can be written as

$$\alpha(E) = \frac{4\pi}{\lambda} k(E), \quad (7)$$

$$R(E) = \frac{[n(E) - 1]^2 + k(E)^2}{[n(E) + 1]^2 + k(E)^2}, \quad (8)$$

where λ is the wavelength of light in the vacuum.

Figures 2(a) and 2(b) show the real and imaginary parts of the complex refractive index as a function of energy for $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 crystals, respectively. Figures 3(a) and 3(b) show the spectral dependence of the absorption coefficient α and normal-incidence reflectivity R for $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 crystals, respectively. The solid circles represent the experimental data; the solid line is the theoretical dispersion calculated using Adachi's model and APCSA algorithm. A good agreement is observed for the samples studied and especially for G35B/B. All these spectra are found to reveal distinct structures at the CP's in the BZ. It is worth mentioning that the studied samples show a small absorption tail below the fundamental gap edge. The tail may result from defects and grain boundary in polycrystalline material and/or deviation from stoichiometry.¹⁸

The obtained values of the interband CP parameters (strength, threshold energy and broadening) are given in Table II. It is worth mentioning that the broadening factor decreases as the gallium concentration (Ga/Cu) decreases (Table II). This result following to Ref. 20, where a similar

FIG. 3. Spectral dependence of the absorption coefficient α and normal-incidence reflectivity R for (a) $\text{Cu}_2\text{In}_4\text{Se}_7$ (I247/B) and (b) CuGa_3Se_5 (G35B/B and G35T/B) crystals.

FIG. 4. n vs photon energy for $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 crystals. The solid line shows the calculated result of Eq. (9).

effect has been observed in CuInSe_2 and GaAs indicates that the characteristic structures of dielectric function of CuGa_3Se_5 crystals slowly vanish as the concentration of gallium increases.

The experimental n data are analyzed using a simple theoretical model, namely, the first-order Sellmeier equation,¹⁵

$$n^2(\lambda) = A + \frac{\lambda^2}{\lambda^2 - B}, \quad (9)$$

where A and B are the fitting parameters. The solid line in Fig. 4 shows the fitted result of Eq. (9) to the experimental data. Values of the fitting parameters A , B are equal to 6.6, 0.61 and 6.23, 0.285 for CuIn_3Se_5 and CuGa_3Se_5 , respectively. As $\lambda \rightarrow \infty$, the electronic contribution to the dielectric function approaches a limiting value ε_∞ , the high-frequency dielectric constant. The value of ε_∞ which is equal to $\varepsilon_\infty = n^2(\lambda \rightarrow \infty) = A + 1$ is about 7.6 and 7.2 for $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 , respectively. The ε_∞ values reported for CuInSe_2 and CuGaSe_2 are about 6–6.9 and 4.2–5.1, respectively.²¹ Therefore, the ε_∞ values for $\text{Cu}(\text{Ga}/\text{In})_3\text{Se}_5$ OVC are higher than those for the $\text{Cu}(\text{Ga}/\text{In})\text{Se}_2$ chalcopyrites. This is especially for the case of the Ga-based compound.

We have analyzed the SE data for $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 . Zhang *et al.*²² reported the existence of ordered defect compounds CuM_3Se_8 , CuM_5Se_8 , $\text{Cu}_3\text{M}_7\text{Se}_{12}$, and $\text{Cu}_3\text{M}_5\text{Se}_9$ with $M = \text{In}$ or Ga . The EDAX data in Table I suggest that the present G35 crystals may also be $\text{Cu}_3\text{Ga}_7\text{Se}_{12}$. We concluded that the Ga-based compound is CuGa_3Se_5 taking into account both the EDAX data and the structural data and the E_g data. No possibility to compare our data with $\text{Cu}_3\text{Ga}_7\text{Se}_{12}$. Neither the structural nor the E_g data are available at present for $\text{Cu}_3\text{Ga}_7\text{Se}_{12}$.

IV. CONCLUSIONS

Spectral dependence of the real part $\varepsilon_1(E)$ and imaginary part $\varepsilon_2(E)$ of the pseudodielectric function $\varepsilon(E) = \varepsilon_1(E) + i\varepsilon_2(E)$ as well as of the complex refractive index, extinction coefficient, absorption coefficient, and normal-incidence reflectivity of $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 crystals are modeled in the 0.8–4.4 eV photon energy range using Adachi's model

of optical properties of semiconductors and APCSA algorithm. For the studied compounds, no previous attempts were made to model the experimental data. The excellent agreement with experimental data is obtained over the entire range of photon energy. Model parameters (strength, threshold energy, and broadening) are determined using the APCSA method. The values of the lowest direct gap (E_0) and higher energy CP's are in a good agreement with those obtained from the numerically differentiated experimental spectra of $\varepsilon(E)$. The present results offer a valuable set of data for $\text{Cu}_2\text{In}_4\text{Se}_7$ and CuGa_3Se_5 that can be useful for the design of solar cells based on these compounds.

ACKNOWLEDGMENTS

Financial supports from INTAS program (Project 03-51-6314), Comunidad de Madrid (Project FOTOFLEX S-0505/ENE/0123), and from Spanish government MEC (Projects ENE 2004-07446-C02-01 and MAT2003-01490) are acknowledged. One of the authors (S.L.) would like to thank the World Federation of Scientists for financial support.

- ¹K. Ramanathan, G. Teeter, J. Keane, and R. Noufi, *Thin Solid Films* **480–481**, 499 (2005).
- ²D. Schmid, M. Ruckh, F. Granwald, and H. W. Schock, *J. Appl. Phys.* **73**, 2902 (1993); J. Kessler, D. Schmid, R. Schafner, H. W. Schock, and S. Menezes, *Proceedings of the 23rd IEEE Photovoltaic Conference (Louisville)* (IEEE, New York, 1993), p. 549.
- ³H. Z. Xiao, L. Y. Chung, and A. Rockett, *J. Appl. Phys.* **76**, 1503 (1994).
- ⁴Y. B. K. Reddy and V. S. Raja, *Mater. Lett.* **58**, 1839 (2004).
- ⁵T. Negami, N. Kohara, M. Nishitani, T. Wada, and T. Hirao, *Appl. Phys. Lett.* **67**, 825 (1995).
- ⁶C. Rincon, S. M. Wasim, G. Marin, and G. Sanchez Perez, *J. Appl. Phys.* **93**, 8939 (2003).
- ⁷S. Mahanty, J. M. Merino, R. Diaz, F. Rueda, J. L. Martin de Vidales, and M. Leon, *Inst. Phys. Conf. Ser.* **152**, 499 (1998).
- ⁸S. Shirakata, S. Chichibu, H. Miyake, S. Isomura, H. Nakanishi, and K. Sugiyama, *Inst. Phys. Conf. Ser.* **152**, 598 (1998).
- ⁹C. Rincon, S. M. Wasim, G. Marin, and I. Molina, *J. Appl. Phys.* **93**, 780 (2003).
- ¹⁰G. Marin, C. Rincon, S. M. Wasim, G. Sanches Perez, and I. Molina, *J. Alloys Compd.* **283**, 1 (1999).
- ¹¹P. Lautenschlager, M. Garriga, S. Logothetidis, and M. Cardona, *Phys. Rev. B* **35**, 9174 (1987); M. Cardona, *Modulation spectroscopy* (Academic, New York, 1969).
- ¹²M. León, R. Serna, S. Levchenko, A. Nateprov, A. Nicorici, J. M. Merino, and E. Arushanov, *Phys. Status Solidi A* **203**, 2913 (2006).
- ¹³J. G. Albornoz, R. Serna, and M. Leon, *J. Appl. Phys.* **97**, 103515 (2005).
- ¹⁴T. Kawashima, S. Adachi, H. Miyake, and K. Sugiyama, *J. Appl. Phys.* **84**, 5202 (1998).
- ¹⁵T. Kawashima, H. Yoshikawa, S. Adachi, S. Fuke, and K. Ohtsuka, *J. Appl. Phys.* **82**, 3528 (1997).
- ¹⁶A. B. Djuricic and E. H. Li, *J. Appl. Phys.* **85**, 2848 (1999).
- ¹⁷A. B. Djuricic, A. D. Rakic, and J. M. Elazar, *Phys. Rev. E* **55**, 4797 (1997).
- ¹⁸M. I. Alonso, M. Garriga, C. A. Durante Rincon, and M. Leon, *J. Appl. Phys.* **88**, 5796 (2000).
- ¹⁹M. I. Alonso, K. Wakita, J. Pascual, M. Garriga, and N. Yamamoto, *Phys. Rev. B* **63**, 075203 (2001).
- ²⁰K. Zeaiter, A. Yanuar, and C. Llinares, *Sol. Energy Mater. Sol. Cells* **70**, 213 (2001).
- ²¹N. N. Syrbu, M. Bogdanash, V. E. Tezlevan, and I. Mushcutariu, *Physica B* **229**, 199 (1997).
- ²²N. Zhang, S.-U. Wei, A. Zunger, and H. Katayama-Yoshida, *Phys. Rev. B* **57**, 9642 (1998).