COMMUNICATIONS

Sellmeier parameters for $ZnGaP_2$ and GaP

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Sellmeier parameters are determined for the birefringent material $ZnGaP_2$ and the singly refractive material GaP by the minimization of chi-square employing the Levenberg–Marquardt method. The distinguishing feature of the present work is that all five Sellmeier parameters are treated as adjustable. In previous work the Sellmeier parameter related to the restrahlen frequency was fixed and set equal for both ordinary and extraordinary waves in the birefringent material. The fitted results show there is approximately an 8% difference between the two. Taking this parameter as adjustable allows for a better fit on all other parameters. © *2000 American Institute of Physics.* [S0021-8979(00)00103-1]

Chalcopyrite semiconductors are promising for optical frequency conversion applications in solid state laser systems, such as optic parametric oscillators OPOs and frequency doubling devices.[1,2] $ZnGeP_2$ is an excellent nonlinear optical material that exhibits good optical transparency over the 0.7–12 mm wavelength region, and is therefore well suited for producing tunable laser output in the near infrared.[3–8] The feasibility of constructing $ZnGeP_2$–GaP heterostructures with appropriate refractive index profiles for waveguiding was reported several years back.[9]

Materials characterization and device performance modeling are critically dependent on an accurate knowledge of the ordinary and extraordinary indices of refraction as a function wavelength. Indeed, accurate measurements of these quantities have been carried out and reported in the literature for sometime.[4,10] The utility of these data is facilitated by its fit to the Sellmeier equation given by

$$n_{o,e}^2 = A_{o,e} + \frac{B_{o,e}}{1-(C_{o,e}/\lambda^2)} + \frac{D_{o,e}}{1-(E_{o,e}/\lambda^2)}. \qquad (1)$$

Here, n is the index of refraction, λ is the wavelength, A, B, C, D, and E are the fitting parameters, and the subscripts o and e stand for the ordinary and extraordinary propagation, respectively. The first and second terms on the right-hand side of the equation are the contributions due to the higher and lower energy band gaps, respectively. The third term is due to resonant absorption by the lattice vibrations. The coefficients A, B, and D are related to the oscillator strengths of the corresponding terms, while C and E fix the locale on the n^2 vs λ plot where the associated mechanisms are most relevant.

Previous fits to experimental data have always had the parameter E preset and fixed while determining the other four parameters.[11–13] Moreover, for the birefringent material it was assumed that $E_o = E_e$. While the justification for doing so is physically reasonable[11–13] it is absolutely unnecessary, especially if a numerical algorithm for the minimization of a statistical quantity such as chi-square is used. In this communication we fit all five parameters for both the ordinary and extraordinary optical data on $ZnGaP_2$ as well as that for the singly refracting GaP.

An excellent goodness-of-fit merit function for multidimensional fits is the χ^2 (chi-square). When fitting a model which depends nonlinearly on a set of unknown parameters the minimization of χ^2 is readily effected via the Levenberg–Marquardt method.[14] This is the fitting approach we took. The experimental data we fit came from several sources. The $ZnGaP_2$ data were taken from Boyd *et al.*[4] The data were taken over wavelengths ranging from $0.7\ \mu\text{m} \leq \lambda \leq 12\ \mu\text{m}$ at room temperature. The GaP data for the wavelengths $0.2066\ \mu\text{m} \leq \lambda \leq 0.8267\ \mu\text{m}$ were taken from Parson.[15] Longer wavelength data, $1\ \mu\text{m} \leq \lambda \leq 22\ \mu\text{m}$, came from Borghesi and Guizzetti.[16] Both sets of the GaP data were taken at room temperature. The results of our fits are shown in Table I. The fractional difference between the fitted

TABLE I. Sellemeier parameters for $ZnGaP_2$ and GaP. The parameters were determined with wavelengths in units of microns.

ZGP ordinary	ZGP extraordinary	GaP
$A_o = 4.4746$	$A_e = 4.6346$	$A = 4.1705$
$B_o = 5.2659$	$B_e = 5.3410$	$B = 4.9113$
$C_o = 0.1336$	$C_e = 0.1424$	$C = 0.1174$
$D_o = 1.7755$	$D_e = 1.5923$	$D = 1.9928$
$E_o = 762.58$	$E_e = 704.34$	$E = 756.46$

data and the experimental data was, in all cases, a few thousandths or smaller.

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