

Calculation of the orientation of the optical indicatrix in monoclinic and triclinic crystals: The point-dipole model

RICHARD N. ABBOTT, JR.

Department of Geology, Appalachian State University, Boone, North Carolina 28608, U.S.A.

ABSTRACT

Using point-dipole theory, the orientation of the optical indicatrix in monoclinic and triclinic crystals is calculated from structure data and electronic polarizabilities. Calculations were performed for kyanite, wollastonite, sanidine, orthoclase, microcline, and plagioclases of compositions An_0 , An_{48} , An_{63} , An_{64} , An_{66} , An_{67} , and An_{100} . On the basis of these calculations it is concluded that (1) the calculated orientation of the optical indicatrix depends mainly on the geometry of the structure and only to a lesser extent on the electronic polarizabilities of the species (atoms or groups of atoms) occupying the sites; and (2) magnitudes of calculated refractive indices depend mainly on the electronic polarizabilities and to a lesser extent on the geometry of the structure.

INTRODUCTION

Among the fundamental objectives of the theory of optical crystallography are the prediction of refractive indices and the prediction of the orientation of the optical indicatrix for homogeneous crystals of low symmetry. Convincing results have been presented with regard to the first objective, from the earliest efforts of Bragg (1924) to recent efforts of Lager et al. (1987). The present effort addresses the second objective, which seems not to have commanded much attention. Hauser and Wenk (1976) calculated variations in the orientation of the optical indicatrix, but only for heterogeneous crystals, as volume-weight averages of the respective properties of sub-microscopic domains. In contrast, as applied to such heterogeneous crystals, the present research addresses directly the problem of the orientation of the optical indicatrix in an individual domain as a function of the internal structure of the domain and its electronic properties. The research builds upon point-dipole theory as advanced by Cummins et al. (1976) and implemented by Pohl and coworkers (Pohl, 1978; Pohl et al., 1978; Pohl and Rath, 1979; Lager et al., 1987). The purpose is to develop a method for calculating not only refractive indices (e.g., Lager et al., 1987), but also the orientation of the optical indicatrix for nontrivial cases of homogenous monoclinic and triclinic crystals. The focus is on low-symmetry structures where the orientation of the optical indicatrix is not constrained by symmetry; i.e., the indicatrix is subject to one (monoclinic) or two (triclinic) degrees of freedom with respect to rotation. The method provides a crucial test of the point-dipole theoretical model.

THEORY AND METHOD

In principle, for a given frequency of light, the wavelength in an anisotropic crystalline substance (hence a

refractive index) is calculable from a knowledge of the structure and the electronic polarizabilities of the species making up the structure (Pohl, 1978; Lager et al., 1987). The species are usually, but not necessarily, defined as individual atoms. The relationship among structure, electronic polarizability, and refractive index can be summarized in four equations. The first equation (Cummins et al., 1976; Pohl, 1978) gives the local electric field at site k , $F(k)$, as a function of the local electric fields at all sites, k' , in the unit cell,

$$F(k) = E + (1/V) \sum_{k'} L(kk') \alpha(k') F(k') \quad (1)$$

where E is the macroscopic (externally applied) electric field, $L(kk')$ is the Lorentz factor tensor for the pair $k-k'$, $\alpha(k')$ is the electronic polarizability of species k' , and V is the volume of the unit cell. The macroscopic electric field is a vector equated with the vibration direction (hence the plane of polarization) of the incident light and having a magnitude which, for the present purpose, is most conveniently identified with the wavenumber (i.e., $1/\lambda$). The Lorentz factor tensors, $L(kk')$, depend only on the geometry of the structure and were calculated using the method of Cummins et al. (1976). The polarizabilities, $\alpha(k')$, are empirical quantities taken from Lasaga and Cygan (1982) but are readily obtainable elsewhere (see Jaffe, 1988). Equation 1 forms a system of linear equations solvable for the individual local electric fields, $F(k)$.

The dielectric susceptibility tensor, χ , is obtained from the local electric fields from

$$\chi E = (1/V) \sum_k \alpha(k) F(k) \quad (2)$$

(Pohl, 1978). Referred to a Cartesian base, $x^T = [x, y, z]$, the coefficients of the dielectric susceptibility tensor describe the surface of an ellipsoid,

$$x^T \chi x = 1. \quad (3)$$

TABLE 1. Electronic polarizabilities

		For ions*
$\alpha(\text{Si})$	=	0.08 Å ³
$\alpha(\text{O})$	=	1.31 Å ³
$\alpha(\text{K})$	=	1.98 Å ³
$\alpha(\text{Na})$	=	1.11 Å ³
$\alpha(\text{Ca})$	=	1.66 Å ³
Measured**† for minerals		
$\alpha(\text{KAlSi}_3\text{O}_8, \text{ orthoclase})$	=	13.11 Å ³
$\alpha(\text{KAlSi}_3\text{O}_8, \text{ microcline})$	=	13.23 Å ³
$\alpha(\text{NaAlSi}_3\text{O}_8, \text{ albite})$	=	12.25 Å ³
$\alpha(\text{CaAl}_2\text{Si}_2\text{O}_8, \text{ anorthite})$	=	13.35 Å ³
$\alpha(\text{KAlSi}_2\text{O}_6, \text{ leucite})$	=	10.46 Å ³
$\alpha(\text{NaAlSiO}_4, \text{ nepheline})$	=	6.71 Å ³
$\alpha(\text{Al}_2\text{SiO}_5, \text{ kyanite})$	=	7.05 Å ³
Polarizability of SiO₂		
$\alpha(\text{SiO}_2)$	= $\alpha(\text{Si}) + 2\alpha(\text{O})$	= 2.70 Å ³
Polarizability of ⁱAlO₂		
$\alpha(\text{AlO}_2)$	= $\alpha(\text{KAlSi}_3\text{O}_8, \text{ orthoclase}) - \alpha(\text{K}) - 3\alpha(\text{SiO}_2)$	= 3.03 Å ³
$\alpha(\text{AlO}_2)$	= $\alpha(\text{KAlSi}_3\text{O}_8, \text{ microcline}) - \alpha(\text{K}) - 3\alpha(\text{SiO}_2)$	= 3.15 Å ³
$\alpha(\text{AlO}_2)$	= $\alpha(\text{NaAlSi}_3\text{O}_8, \text{ albite}) - \alpha(\text{Na}) - 3\alpha(\text{SiO}_2)$	= 3.01 Å ³
$\alpha(\text{AlO}_2)$	= $[\alpha(\text{CaAl}_2\text{Si}_2\text{O}_8, \text{ anorthite}) - \alpha(\text{Ca}) - 2\alpha(\text{SiO}_2)]/2$	= 3.15 Å ³
$\alpha(\text{AlO}_2)$	= $\alpha(\text{KAlSi}_2\text{O}_6, \text{ leucite}) - \alpha(\text{K}) - 2\alpha(\text{SiO}_2)$	= 3.08 Å ³
$\alpha(\text{AlO}_2)$	= $\alpha(\text{NaAlSiO}_4, \text{ nepheline}) - \alpha(\text{Na}) - \alpha(\text{SiO}_2)$	= 2.87 Å ³
Average $\alpha(\text{AlO}_2) \pm$ standard deviation		= 3.05 ± 0.11 Å ³
Polarizability of ⁱAlO_{1.5} in kyanite		
$\alpha(\text{AlO}_{1.5})$	= $[\alpha(\text{Al}_2\text{SiO}_5, \text{ kyanite}) - \alpha(\text{SiO}_2)]/2$	= 2.175 Å ³
Polarizability of CaO in wollastonite		
$\alpha(\text{CaO})$	= $\alpha(\text{Ca}) + \alpha(\text{O})$	= 2.97 Å ³

Note: the italicized species and polarizabilities were used in the calculations.

* Table 3 in Lasaga and Cygan (1982).

** Orthoclase, microcline, albite, anorthite, leucite, nepheline from Table 2 in Lasaga and Cygan (1982).

† Kyanite, calculated from Deer et al. (1985).

The principal axes of the ellipsoid are parallel to the principal axes of the optical indicatrix. The directions of the principal axes (eigenvectors) and their magnitudes (eigenvalues) are found by diagonalizing the dielectric susceptibility tensor (e.g., Julian and Bloss, 1987). The principal refractive indices are then simply related to the eigenvalues, χ_{ii} , by

$$n_i = (\chi_{ii} + 1)^{1/2}. \tag{4}$$

The quantity, $\chi_{ii} + 1$, is the familiar dielectric constant.

In addition to the formalism of Cummins et al. (1976), the computer program written to perform the calculations relies on subroutines and methods documented by Cooper (1981) and Boisen and Gibbs (1985). The program was coded in Pascal and is available from the author.

Calculating Lorentz factor tensors consumes most of the computing time, and storing them for rapid retrieval can require large amounts of memory. The present PC version of the program is limited to a maximum of 28 sites in the unit cell. This limitation is imposed by the memory allocation of the Pascal compiler. For large structures, useful results can be obtained by taking advantage of the additivity of electronic polarizabilities (Lasaga and Cygan, 1982), and defining some species as groups of atoms (e.g., Lager et al., 1987). For the applications given below, the species and polarizabilities (for $\lambda_D = 5893 \text{ \AA}$) used in the calculations (Table 1) were

from, or derived from, Lasaga and Cygan (1982). In effect the structures were described only in terms of the positions of the cations. The contribution by the anions to the overall polarizability was distributed over the cations. This compromise was tested on wollastonite, albite, and microcline by repeating the calculations with just the Ca, K, Na, and O sites and distributing the small polarizabilities of Al and Si (Table 1) over the O sites. The results showed no significant improvement in the calculated orientation of the indicatrix and showed only minor improvement in the magnitudes of the calculated refractive indices. Thus, distributing the polarizability of the O atoms over the cation sites cannot be directly responsible for discrepancies between calculated and observed orientations of the indicatrix. Furthermore, regardless of how a structure is described for the purpose of the calculation, the electronic polarizability of a selected species (e.g., SiO₂, AlO₂, K, Na, or Ca in the feldspars) can be varied sympathetically relative to other species in the structure (such that the sum of the polarizabilities for one chemical formula is constant) by >50% without causing any significant change in the calculated orientation of the optical indicatrix. Quite clearly, the orientation of the indicatrix depends mainly on the Lorentz factor tensors, hence on the geometry of the structure, and not so much on the electronic polarizabilities.

As implemented by Lager et al. (1987) for the sole pur-

TABLE 2. Calculated and observed refractive indices

Mineral	Struct. ref.	Refractive indices			R.I. Ref.
		n_1	n_2	n_3	
Kyanite	1	1.705 (1.710–1.718)	1.743 (1.719–1.724)	1.808 (1.724–1.734)	11
Wollastonite	2	1.611 (1.615–1.646)	1.657 (1.629–1.662)	1.659 (1.627–1.659)	12
Low sanidine	3	1.513 (1.518)	1.535 (1.522)	1.551 (1.522)	11
Orthoclase	4	1.510 (1.518)	1.532 (1.522)	1.553 (1.522)	11
Microcline	5	1.507 (1.518)	1.540 (1.522)	1.548 (1.524)	13
Plagioclase					
An ₀	6	1.516 (1.529)	1.539 (1.533)	1.569 (1.539)	13
An ₀	7	1.516	1.539	1.568	
An ₄₈	8	1.532 (1.554)	1.546 (1.557)	1.579 (1.561)	11
An ₆₃	9	1.541 (1.561)	1.554 (1.565)	1.586 (1.570)	11
An ₆₄	9	1.540	1.553	1.585	
An ₆₆	9	1.542 (1.563)	1.556 (1.568)	1.589 (1.572)	11
An ₆₇	9	1.547	1.560	1.593	
An ₁₀₀	10	1.560 (1.577)	1.576 (1.585)	1.609 (1.590)	11

Note: observed indices are in parentheses. References are numbered as follows: 1 = Winter and Ghose (1979); 2 = Ohashi (1984); 3 = Phillips and Ribbe (1973); 4 = Prince et al. (1973); 5 = Blasi et al. (1987); 6 = Armbruster et al. (1990); 7 = Harlow and Brown (1980); 8 = Fitzgerald et al. (1986); 9 = Wenk et al. (1980); 10 = Angel (1988); 11 = Deer et al. (1985); 12 = Phillips and Griffen (1981); 13 = Su et al. (1986).

pose of predicting magnitudes of refractive indices, point-dipole theory (Eqs. 1 and 2) can give rather stunning agreement with observed refractive indices. Discrepancies can be ascribed at least partly to the use of isotropic electronic polarizabilities. In reality, the polarizability of a species (an atom or a group of atoms) can be expected to vary depending on the direction. Given this limitation, the following examples test the theory with regard to prediction of the orientation of the optical indicatrix. Relevant cases are thus restricted to monoclinic and triclinic minerals. Of course, the most compelling test cases are triclinic minerals because the orientation of the optical indicatrix is not constrained in any way by symmetry.

APPLICATIONS

Minerals used in the calculations are listed in Table 2, along with calculated and observed refractive indices. Two of the minerals, sanidine and orthoclase, are monoclinic; the rest are triclinic.

In order to reduce the number of species per unit cell in the feldspars, lattice parameters and atomic coordinates were expressed in terms of a primitive unit cell consistent with the transformation

$$\begin{pmatrix} \mathbf{a}' \\ \mathbf{b}' \\ \mathbf{c}' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -0.5 & 0.5 & -1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix} \quad (5)$$

for C-centered feldspars (alkali feldspars and all plagioclases except anorthite), and consistent with the transformation

$$\begin{pmatrix} \mathbf{a}' \\ \mathbf{b}' \\ \mathbf{c}' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -0.5 & 0.5 & -0.5 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix} \quad (6)$$

for body-centered plagioclase (anorthite). This greatly reduces the computing time by decreasing the number of species per unit cell by one-half. The results were then

referred back to the standard C-centered or body-centered unit-cell geometry.

Polarizabilities for the tetrahedral sites in the feldspars were weighted according to the observed $\text{Al}_x\text{Si}_{1-x}$ site occupancy. Also, in all of the plagioclase structures, except for the albite structure, Ca and Na are disordered, with an equal number of vacancies over two sites that are close together. Disordering of this sort can be treated neither readily nor realistically in the calculations. As a compromise, the average of the two sites was used, so that vacant sites could be ignored. The polarizability for the average Ca-Na site was then weighted according to the composition in terms of $\text{Na}_x\text{Ca}_{1-x}$.

Except for wollastonite, the agreement between observed and calculated refractive indices is not altogether satisfactory (Table 2), presumably for reasons already acknowledged (Lager et al., 1987) having to do with the use of isotropic polarizabilities and polyatomic species. The calculated and observed refractive indices for wollastonite are very close.

With the exceptions of wollastonite and microcline, the calculated refractive indices (Table 2) are correctly correlated according to general vibration direction with the observed refractive indices. For wollastonite the vibration directions for the calculated n_2 and n_3 refractive indices correspond respectively with the observed vibration directions for n_γ and n_β . The observed difference $n_\gamma - n_\beta = 0.003$ is small for wollastonite, and close to the difference between the calculated refractive indices $n_3 - n_2 = 0.002$. Of course, taking the vibration directions as the frame of reference, the sign of the birefringence is different. Adjusting the polarizabilities of SiO_2 and CaO produced neither a change in the sign nor the magnitude of the discrepancy.

For microcline, the calculated vibration direction for n_2 correlates correctly with the observed vibration direction for n_β . Thus the calculated and observed orientations

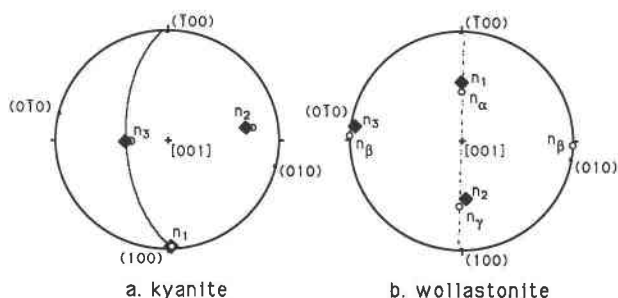


Fig. 1. Cyclographic projections of calculated and observed vibration directions in (a) kyanite and (b) wollastonite. Calculated directions, solid diamonds; observed directions, open circles. Observed relationships from Troger (1982).

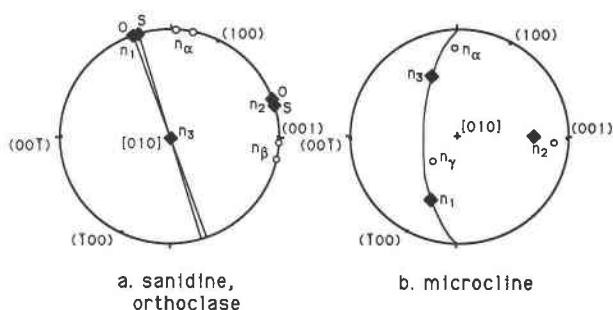


Fig. 2. Cyclographic projections of calculated and observed vibration directions. (a) Sanidine (S), orthoclase (O). (b) Microcline. Calculated directions, solid diamonds; observed directions, open circles. Observed relationships from Troger (1982).

for the optic axial plane are similar, but within the optic axial plane the calculated n_1 and n_3 vibration directions do not correlate uniquely with the appropriate observed vibration directions.

Figures 1, 2, and 3 are cyclographic projections of calculated and observed vibration directions for kyanite, wollastonite, alkali feldspars, and plagioclases. For kyanite (Fig. 1a), the calculated orientation of the optical indicatrix faithfully reproduces the observed orientation. Also for wollastonite (Fig. 1b), the calculated orientation very closely approximates the observed orientation, except that the calculated vibration directions for n_3 and n_2 are transposed relative to the observed vibration directions for n_3 and n_2 . As noted above, the difference between the calculated n_2 and n_3 is small, so the shape of the indicatrix is quite well approximated.

Figure 2 shows results of the calculations on the potassium feldspars. The calculated vibration direction for n_3 is correctly aligned parallel to [010] for the monoclinic feldspars and reasonably close to [010] for the microcline. The calculated vibration direction for n_1 is correctly predicted to be close to [100], although the calculated $[100] \angle n_1$ (15° for sanidine, 22° for orthoclase) is somewhat exaggerated (5° observed, Deer et al., 1985), and on the wrong side of [100] relative to [001]. The $[001] \angle n_3$ is likewise exaggerated. As noted above, the calculated orientation for the optic axial plane in microcline is close to the observed orientation, but the calculated n_1 and n_3 vibration directions are not aligned very well with the corresponding observed vibration directions. Except for these deficiencies, the general orientation of the calculated optical indicatrix is reasonable for all of the alkali feldspars. Changing the assigned polarizabilities within the constraints of a fixed sum for one formula unit has little or no effect on the calculated orientation of the optical indicatrix.

The calculations on plagioclase provide further insight into the structural control on the orientation of the optical indicatrix. As with the alkali feldspars, the calculated vibration direction for n_3 is correctly situated close to [010] for all compositions. For albite the calculated vibration direction for n_1 is close to the [100] direction. For

more calcic compositions the vibration direction for n_1 is close to the [100] direction. For more calcic compositions the vibration direction for n_1 is close to the observed trend (Fig. 3b). Similarly, the calculated vibration direction for n_2 is close to the (001) pole for albite, and for more calcic compositions the calculated vibration direction for n_2 is close to the observed trend. Thus calculated orientations for the optical indicatrix agree in a general way with observed orientations. However, while the calculated orientations for the optical indicatrix are generally consistent with those observed for intermediate plagioclase, on closer inspection the compositions corresponding to the calculated orientations do not vary systematically along the calculated trend. For instance, along the trend defined by the calculated n_1 the order of the compositions is $An_0, An_{48}, An_{64}, An_{100}, An_{63}, An_{66}, An_{67}$. The misordering of the An_{64} composition may well be accommodated by experimental uncertainty in the structure determination or may have to do with averaging the otherwise split Ca-Na sites. The reason for the more conspicuous problem of the An_{100} composition is not so clear. By analogy with the intermediate compositions, the problem may have to do with averaging the split Ca sites. Alternatively, the problem may have to do with leaving the O sites out of the calculation or representing the actual $P\bar{1}$ structure as an average in space group $I\bar{1}$.

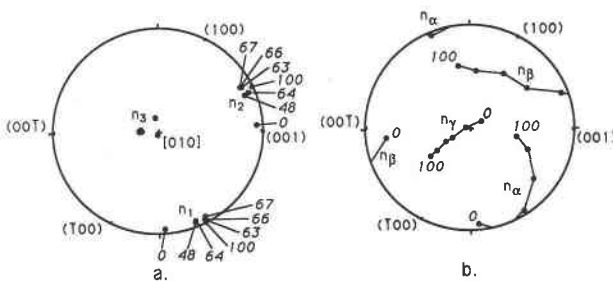


Fig. 3. Cyclographic projections of (a) calculated and (b) observed vibration directions in plagioclase. Italic numbers give the percent of An component ($An = CaAl_2Si_2O_8$). Observed relationships from Winchell and Winchell (1951).

CONCLUSIONS

Using point-dipole theory, the orientation of the optical indicatrix in monoclinic and triclinic minerals can be calculated reasonably well from crystallographic data and electronic polarizabilities. In fact, for a given mineral, a good orientation can be calculated without including all of the different kinds of atomic sites in the structure. However, good crystal chemical sense cautions that a calculation must include at the very least those sites of the lowest point symmetry. The calculations provide a crucial test of the general validity of the point-dipole theory, while highlighting certain deficiencies.

The calculations show the following: (1) The calculated orientation of the optical indicatrix is not influenced much by the way the total electronic polarizability is distributed over the species making up a structure. The calculated orientation of the optical indicatrix depends mainly on the Lorentz factor tensors, hence on the geometry of the structure. (2) Magnitudes of calculated refractive indices depend mainly on the electronic polarizabilities. Discrepancies between observed and calculated refractive indices are presumably due to the use of isotropic polarizabilities and polyatomic species.

Anisotropic polarizabilities are not yet available in the correct tensorial form for individual species but may be obtainable empirically for some structures (e.g., Armbruster and Bloss, 1982; Bloss et al., 1983). However, being inherently structure dependent, anisotropic, electronic polarizabilities cannot be transferred to other structures, thereby greatly limiting their general applicability.

One promising application of the approach might involve an analysis of the relationship between strain and optical properties. If strain in a structure can be modeled, the optical properties can be calculated for comparison with observed strain effects.

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