

Static Dielectric Constant of SiC

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Using the Lyddane-Sachs-Teller relation, published data, and a simple analysis, we find the static dielectric constant of cubic SiC to be $\epsilon_s = 9.72$. The same method yields $\epsilon_s(\perp) = 9.66$ and $\epsilon_s(\parallel) = 10.03$ for 6H SiC.

For both cubic¹ and 6H polytypes² of SiC, data are available on the refractive indices and their dispersion, and on phonon energies obtained in Raman scattering.^{3,4} It is therefore possible to use the Lyddane-Sachs-Teller⁵ (LST) relation with extrapolated index measurements to obtain the static dielectric constants ϵ_s , i. e., one ϵ_s for cubic and two constants $\epsilon_s(\perp)$ and $\epsilon_s(\parallel)$ for the uniaxial positive 6H SiC.

The static dielectric constant can be written

$$\epsilon_s = \epsilon_{e1} + \epsilon_{lat} \quad , \quad (1)$$

where the electronic contribution ϵ_{e1} is to be evaluated at zero frequency, and the lattice contribution ϵ_{lat} is related to the ratio of phonon energies that enter into the LST formula. We shall use ϵ_∞ to denote the extrapolation of $n^2 = \epsilon_{e1}$ to zero frequency. This somewhat contradictory notation arose because ϵ_∞ , the "optical" dielectric constant, was often set equal to n^2 at a frequency much higher than the lattice frequency, but low compared with electronic transition frequencies. In many substances no suitable frequency exists, and it is preferable to extrapolate optical data to zero frequency, using a convenient model, such

as the one-oscillator model. We therefore write

$$n^2 = 1 + \frac{\epsilon_g}{1 - (h\nu/E_g)^2} \approx \epsilon_\infty + \epsilon_g \left(\frac{h\nu}{E_g} \right)^2, \quad (2)$$

where $h\nu$ is the photon energy, E_g is a parameter that can be interpreted as an average band gap, and ϵ_g is proportional to the oscillator strength. The second form, with $\epsilon_\infty = 1 + \epsilon_g$, is a good approximation if $h\nu \ll E_g$. For SiC the appropriate values of E_g are close to 8 eV.⁶

In Fig. 1, we plot the measured n^2 against $(h\nu)^2$ for cubic SiC, using the data of Shaffer and Naum,¹ and we plot the squares of both ordinary and extraordinary indices for 6H SiC, using Thibault's data.² The zero photon-energy intercepts are the values of ϵ_∞ we need, and they are listed in Table I. For 6H SiC, additional index measurements have been reported⁸ for the ordinary ray at both larger and smaller photon energies than shown in Fig. 1. However, our approximation is not suitable for the higher energies, and the lattice bands make an undesired contribution to the index for the smaller photon energies. For cubic SiC, our approximation is asymptotically equivalent to the Cauchy formula employed by Shaffer and Naum, and our extrapolated $\epsilon_\infty = 6.52$ corresponds to their extrapolated $n = 2.55378$.

In Table I we also show the longitudinal- and transverse-phonon energies $\hbar\omega_L$ and $\hbar\omega_T$ obtained in Raman measurements.^{3,4} These values are used in the LST formula to give us the final column of Table I, i. e.,

$$\epsilon_s = \epsilon_\infty (\hbar\omega_L / \hbar\omega_T)^2 \quad . \quad (3)$$

We need to explain our use of a single ratio of phonon energies in the LST formula for 6H SiC, for there are five infrared-allowed transitions contributing to $\epsilon_s(\perp)$, and five to $\epsilon_s(\parallel)$, and a general expression would show the product of five phonon terms⁷ in Eq. (3) for either $\epsilon_s(\perp)$ or $\epsilon_s(\parallel)$. However, only one of the five transitions has appreciable infrared strength.⁸ For the other four transitions no effect of the longitudinal electric field could be detected⁹ in Raman scattering,³ and

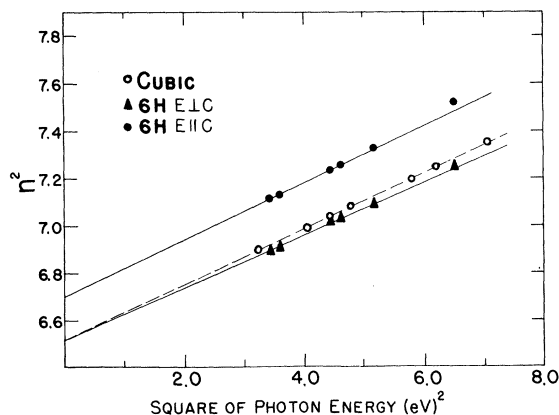


FIG. 1. Extrapolation of optical dielectric constant n^2 to zero photon energy to obtain ϵ_∞ . Refractive index values are from Ref. 1 for cubic SiC, and from Ref. 2 for both ordinary ($\vec{E} \perp c$) and extraordinary ($\vec{E} \parallel c$) rays of 6H SiC.

TABLE I. Extrapolated ϵ_∞ from Fig. 1, Raman phonon energies from Refs. 3 and 4, and calculated static dielectric constant ϵ_s for cubic and 6H SiC.

Polytype	ϵ_∞	$\hbar\omega_L$ (cm ⁻¹)	$\hbar\omega_T$ (cm ⁻¹)	ϵ_s
Cubic	6.52	972	796	9.72
6H(L)	6.52	970	797	9.66
6H(II)	6.70	964	788	10.03

Hodges¹⁰ estimates the weak-mode infrared strengths to be $\approx 10^{-3}$ of the strong mode. Their combined contribution to ϵ_s (i. e., to $\epsilon_{1at} \approx 3.2$) is therefore likely to be of order $4 \times 10^{-3} \times 3.2 \approx 0.01$.

The low-frequency value $\epsilon_s = 10.2 \pm 0.2$ reported by Hofman *et al.* was obtained by a bridge measurement in which the dielectric loss was a troublesome factor.¹¹ The SiC polytype was not stated, but probably was 6H, the most common polytype. Presumably, the experiment measured $\epsilon_s(\parallel)$, for the common growth habit yields platelets perpendicular to the *c* axis. Thus, our value of $\epsilon_s(\parallel) = 10.03$ falls just within the error limits estimated in Ref. 11.

The refractive indices and Raman data quoted above were all measured at room temperature. We have analyzed luminescence spectra due to donor-acceptor pairs in cubic SiC,¹² with the crystal held at 1.8 °K. The fitting of the spectrum yielded a low-temperature value of $\epsilon_s = 9.7 \pm 0.1$, very little reduced from the room-temperature value. This contrasts with the observed 3.3% reduction for GaP in the same temperature interval,¹³ and the 2.5 and 4.2% reductions found for Si and Ge respectively.¹⁴ The small temperature dependence of ϵ_s for SiC may be attributed to its relatively large direct energy gaps, and its large phonon energies.

Thibault was unable to find significant differences between the refractive indices of 6H and 15R polytypes.² Many SiC polytype properties have a linear dependence on hexagonality, or percent "h."¹⁵ If refractive indices follow this rule, one would predict much smaller differences between 6H (33% *h*) and 15R (40% *h*) than between 6H and cubic (0% *h*). In ZnS polytypes, which are like SiC polytypes in many respects, the birefringence is proportional to the hexagonality.¹⁶

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⁴D. W. Feldman, J. H. Parker, Jr., W. J. Choyke, and L. Patrick, *Phys. Rev.* **173**, 787 (1968), for cubic SiC.

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⁹What one looks for is an angular dependence of A_1

modes or a splitting of E_1 modes. The latter is not to be confused with the small observed discontinuities that separate two distinct A_1 or E_1 modes at boundaries within the large zone.

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