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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 6*H* SiC.

For both cubic[1] and 6*H* polytypes[2] 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-Teller[5] (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 6*H* SiC.

The static dielectric constant can be written

$$\epsilon_s = \epsilon_{\text{el}} + \epsilon_{\text{lat}} \quad , \tag{1}$$

where the electronic contribution ϵ_{el} 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 $n^2 = \epsilon_{\text{el}}$ 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

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

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]

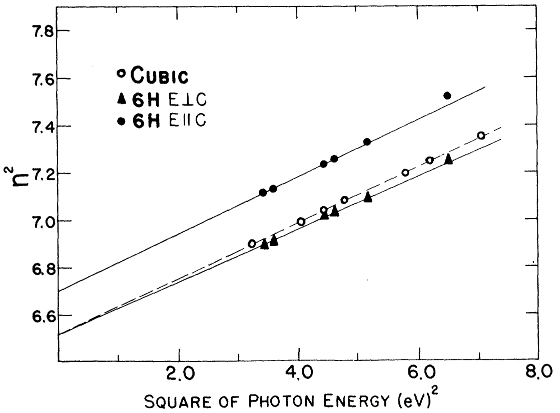

FIG. 1. Extrapolation of optical dielectric constant n^2 to zero photon energy to obtain ϵ_∞. Refractive index values are from Ref. 1 for cubic SiC, and from Ref. 2 for both ordinary ($\vec{E} \perp c$) and extraordinary ($\vec{E} \parallel c$) rays of 6*H* SiC.

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 6*H* 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 6*H* SiC, additional index measurements have been reported[6] 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.,

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

We need to explain our use of a single ratio of phonon energies in the LST formula for 6*H* 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 terms[7] 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 detected[9] in Raman scattering,[3] and

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 6*H* SiC.

Polytype	ϵ_∞	$\hbar\omega_L$ (cm^{-1})	$\hbar\omega_T$ (cm^{-1})	ϵ_s
Cubic	6.52	972	796	9.72
6*H*(⊥)	6.52	970	797	9.66
6*H*(∥)	6.70	964	788	10.03

Hodges[10] estimates the weak-mode infrared strengths to be $\approx 10^{-3}$ of the strong mode. Their combined contribution to ϵ_s (i.e., to $\epsilon_{1\text{at}} \approx 3.2$) is therefore likely to be of order $4\times10^{-3}\times 3.2 \approx 0.01$.

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 6*H*, 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 6*H* and 15*R* 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 6*H* (33% *h*) and 15*R* (40% *h*) than between 6*H* 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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