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Solid state dielectric screening versus band gap trends and implications

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ABSTRACT

High-frequency (optical) and low-frequency (static) dielectric constant versus band gap trends, as well as index of refraction versus band gap trends are plotted for 107 inorganic semiconductors and insulators. These plots are describable via power-law fitting. Dielectric screening trends that emerge from this analysis have important optical and electronic implications. For example, barrier lowering during Schottky emission, phonon-assisted or Fowler-Nordheim tunneling, or Frenkel-Poole emission from a trap is found to be significantly more pronounced with increasing band gap due to a reduction in the optical dielectric constant with increasing band gap. The decrease in the interface state density with increasing band gap is another optical dielectric constant trend. The tendency for a material with a wider band gap to be more difficult to dope is attributed to an increase in the ionization energy of the donor or acceptor dopant, which in turn, depends on the optical dielectric constant and the effective mass. Since the effective mass for holes is almost always larger than that for electrons, p-type doping is more challenging than n-type doping in a wide band gap material. Finally, the polar optical phonon-limited mobility depends critically upon the reciprocal difference of the optical and the static dielectric constant. Consequently, electron and hole mobility tend to decrease with increasing band gap in a polar material.

1. Introduction

Dielectric constant is a fundamental property of a solid-state material. It accounts for a reduction (screening) of the electric field within a material due do an internal rearrangement of charge (polarization) upon application of an external electric field. Screening is often classified as either static or dynamic, as characterized by a low-frequency (static) or a high-frequency (optical) relative dielectric constant denoted herein as ε_{SR} or $\varepsilon_{\infty R}$, respectively. Many optical and electronic phenomena intimately depend upon dielectric screening.

In the development of our atomic solid-state energy (SSE) scale [1–3], we have discovered several interesting dielectric constant versus band gap trends exhibited by a large number of semiconductors and insulators in the SSE data base [2]. The goal of the work reported herein is to (i) discuss these trends by data mining the SSE data base, and (ii) explore how these trends can be gainfully employed in optical and electronic assessment of solid state semiconductor and insulator materials.

2. Index of refraction trends

Formulation of refractive index versus band gap (n-E_G) relationships has a long and rich history [4–12], as has been periodically reviewed [13–15]. Table 1 highlights four proposed two-parameter n-E_G relations. These relations are used to fit 107 n-E_G pairs obtained from the SSE data base (see Supporting Information), as shown in Fig. 1. Using the SSE dielectric constant data base, we approximate the index of refraction using $n \approx [\varepsilon_{\infty R}]^{1/2}$ instead of employing the more precise expression $n = [\varepsilon_{\infty R} + \kappa^2]^{1/2}$, where κ is the extinction coefficient. This approximation is of questionable viability only for small band gap semiconductors. However, we find that the n-E_G regression fitting parameters are almost identical regardless of whether or not the extinction coefficient correction is employed.

Returning to Fig. 1, it is clear that the power-law, hyperbolic, and logarithmic models are all capable of reasonably describing the n-E_G trend, while the linear model is a poor descriptor of the data. From a coefficient of determination (R^2) perspective, the power-law

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Table 1
Two-parameter index of refraction versus band gap (n-E_G) relations.

Relation	a	b	Reference
Power Law $n = a\,E_G^b$	3.12 eV^{-1}	−0.25	4,5
	3.22 eV^{-1}	−0.25	6
	3.3668 eV^{-1}	−0.32234	7
	3.33 eV^{-1}	−0.34	$R^2 = 0.90$
Hyperbolic $n = \sqrt{1 + \left(\frac{a}{E_G + b}\right)^2}$	13 eV	2.7 eV	8
	13.6 eV	3.4 eV	9
	15.2 eV	3.9 eV	$R^2 = 0.89$
Logarithmic $n = a\ln(E_G) + b$	−1	3.59	10
	−0.99	3.55	$R^2 = 0.82$
Linear $n = a + b\,E_G$	4.084	−0.62 eV^{-1}	11,12
	3.47	−0.24 eV^{-1}	$R^2 = 0.48$

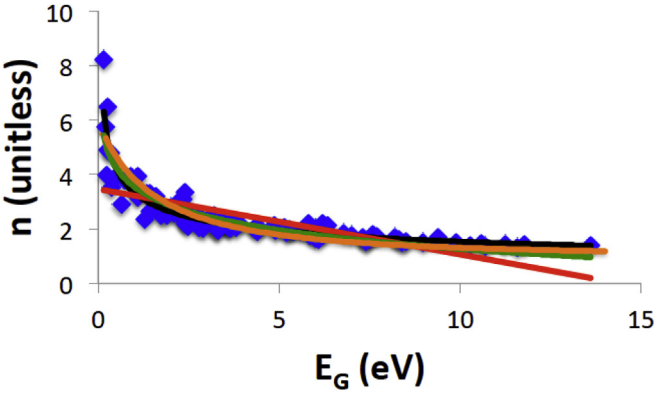

Fig. 1. Index of refraction versus band gap (n-E_G) plot for 107 inorganic semiconductors and insulators. Data is fit using a power-law (black), hyperbolic (orange), logarithmic (green), or linear (red) model. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

model ($R^2 = 0.90$) is slightly better than the hyperbolic model ($R^2 = 0.89$) and is somewhat better than the logarithmic model ($R^2 = 0.82$), at least for the data set used to construct Fig. 1.

In selecting between use of the power-law or the hyperbolic n-E_G model, a compelling attribute of the hyperbolic model is its physical basis since it derives from the Penn model [8,9,16]. Penn asserts that the dielectric properties of a semiconductor or insulator can be envisaged as arising from two isotropic bands (valence and conduction) separated in energy by an average band gap, E_{Penn}, such that

$$n \approx \sqrt{\varepsilon_{\infty R}} = \sqrt{1 + \left(\frac{\hbar\omega_p}{E_{Penn}}\right)^2} \quad (1)$$

where $\hbar\omega_p$ is the valence electron plasma energy. Comparing Eq. (1) to the hyperbolic model included in Table 1, $a = \hbar\omega_p = 15.2$ eV, and $b = E_{Penn} - E_G = 3.9$ eV. Moreover,

$$\omega_p = \sqrt{\frac{q^2 N_V}{m_0 \varepsilon_0}} \quad (2)$$

where q is electronic charge, N_V is the valence electron density, m_0 is the electron rest mass, and ε_0 is the free space dielectric constant. Using Eq. (2) in conjunction with $\hbar\omega_p = 15.2$ eV yields $N_V = 1.7 \times 10^{23}$ cm^{-3}.

Thus, the hyperbolic fit to the n-E_G data shown in Fig. 1 and summarized in Table 1 indicates that the n-E_G trend is consistent with a simple two-band Penn model in which $N_V = 1.7 \times 10^{23}$ cm^{-3} and $E_{Penn} - E_G = 3.9$ eV. If $E_{Penn} - E_G$ is equally partitioned between the valence and conduction bands, then the Penn gap is positioned ~1.95 eV below or above the valence band maximum or conduction band minimum, respectively. This constant positioning trend suggests that the Penn gap is established by energies sufficiently removed from the band edges that an appreciable density of states is reached so that an adequately large joint density of states is achieved for strong optical absorption. This interpretation differs somewhat from the perspective of Penn and others [17] who consider the Penn gap to be an average band gap essentially establishing the centroid of the valence and conduction band joint density of states.

Although the physical foundation upon which the hyperbolic model rests makes it an attractive n-E_G data fitting model option, we typically employ the power-law model to describe n-E_G and other trends in the remainder of this contribution. We do this since (i) the power-law model provides an accurate description of n-E_G and other trends considered herein, and (ii) power-law fitting can be accomplished directly without having to precondition the data for linear regression (e.g., linear regression fitting of the index of refraction to the Penn model requires plotting $[n^2 - 1]^{-0.5}$ versus E_G).

3. Dielectric constant trends and implications

A power-law fit to a plot of the high-frequency (optical) relative dielectric constant as a function of band gap ($\varepsilon_{\infty R}$-E_G) is given in Fig. 2. Since the index of refraction, n, is taken to be equal to the square root of $\varepsilon_{\infty R}$, the power-law fit included in Fig. 1 is simply a square-root version of Fig. 2. Thus, $R^2 = 0.90$ for both of the power-law fits shown in Figs. 1 and 2. The insert included in Fig. 2 displays a log-log plot of the data. A straight-line fit to a log-log plot is supporting evidence for the viability of the power-law. Additionally, a log-log plot is useful for visualizing the variability of the data.

A power-law fit to a plot of the low-frequency (static) relative dielectric constant as a function of band gap (ε_{SR}-E_G) is indicated in Fig. 3. The much smaller $R^2 = 0.48$ in Fig. 3 compared to $R^2 = 0.90$ in Fig. 2 reveals that ε_{SR} exhibits much more variability with respect to E_G than does $\varepsilon_{\infty R}$. Nevertheless, Fig. 3 demonstrates a clear tendency for ε_{SR} to decrease with increasing E_G. Comparing the log-log plot insert of Fig. 3 to the insert of Fig. 2 confirms that the variability of ε_{SR} is indeed much greater than the variability of $\varepsilon_{\infty R}$.

Next we discuss implications of these $\varepsilon_{\infty R}$-E_G and ε_{SR}-E_G trends. We begin with barrier lowering. A variety of electronic phenomena involve the reduction of an energetic barrier upon application of an electric field (see insert of Fig. 4 for an example involving electron injection from a metal into the conduction band of an insulator)

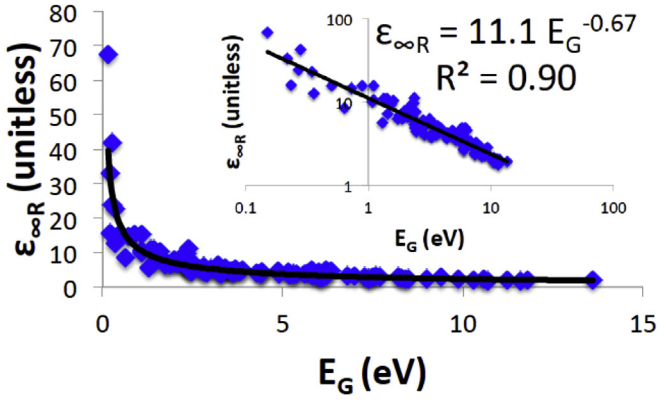

Fig. 2. High-frequency (optical) relative dielectric constant versus band gap ($\varepsilon_{\infty R}$-E_G) plot for 107 inorganic semiconductors and insulators. Insert is a log-log plot.