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Empirical formula for the dielectric constant of cubic semiconductors

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Empirical formulae are presented relating the dielectric constants of cubic semiconductors with the average atomic number of the constituent atoms. The inverses of the constants are found to be linearly related to the average atomic number with a square foot mean percentage error of less than 0.25% for elemental semiconductors, 1.3% for gallium and indium compounds, 3.4% for aluminium compounds, 1.4% for II-VI compounds, and 1.2% for lead compounds. Usefulness of the formulae is also illustrated for identifying incorrect values and for estimating unknown values.
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Experimental values of the dielectric constants of cubic semiconductors have a large amount of scatter. For example, the reported values of the static dielectric constant, K_s, of gallium arsenide[1] range between 11.6 and 13.3 and those of indium antimonide[2] range between 16.8 and 18. Such figures are not available for other materials as relatively few directly measured values have been reported. Values of K_s have been obtained for most of the semiconductors from the high-frequency dielectric constant, K_∞, by using the Lyddane–Sachs–Teller (LST) relation.[3] The scatter in the values of K_∞, is comparatively smaller. One possible reason is that the data[4–11] are taken mostly from a single experiment in each case. But, the samples in such experiments were often multigrained,[4] which may make the results different from those for single crystals. Experimental results are also considerably affected by the surface conditions[4] of the sample, which is difficult to control for some materials. For example, aluminium compounds are hygroscopic, react readily with air, and may even decompose.[6] Furthermore, the high-frequency value of the dielectric constant has to be extracted from the dispersion curves[4] by adjusting the oscillator strengths and damping constants and by using the data on critical energies of the energy bands. Experiments with the required precision have not been done on all the materials. The presence of free carriers, bound carriers, and lattice absorption also makes it difficult to ascertain the correct value.

It should be evident that a relation between the dielectric constants and an accurately known physical constant, if available, would be useful in fixing an acceptable value from among those reported. Such a relation may be used in addition, to predict the values for ternaries and quaternaries.

The dielectric constants are determined by the polarizability of the atoms and are expected to increase with the atomic number.[12] It is in fact, as seen from the collected values of the constants given in Table I, that the values increase monotonically, as expected, with the average atomic number of the constituent atoms. The values for all the semiconductors cannot, however, be fitted to a simple relation. Such relations are obtained if the semiconductors are grouped separately.

The dielectric constant, K, of a solid may be expressed in terms of the polarizability of the constituent atoms, α, as follows:[13]

$$K = 1 + (N\alpha/\epsilon_0)/(1 - \gamma N\alpha/\epsilon_0), \qquad (1)$$

where N is the number of atoms per unit volume, ϵ_0 is the free-space permittivity, and γ is the Lorentz factor. It is seen that if the Lorentz factor be taken as unity, then the inverse of K varies linearly with α and since α may be considered to be linearly related with the atomic number Z, we may expect a linear relation between $1/K$ and Z. Interestingly, it is found that $1/K$ varies linearly for each group almost exactly with the average atomic number, Z_{av} (defined as the mean of the atomic numbers of the constituent atoms), as shown in Figs. 1 and 2.

The dielectric constant, K, may, therefore, be expressed as

$$K = (a - bZ_{av})^{-1}, \qquad (2)$$

where K indicates either K_∞ or K_s, a and b are constant for each group. Values of the constants for the different groups

TABLE I. Dielectric constants of semiconductors at 300 K. Values are taken from Ref. 5, unless otherwise indicated. Numbers within parenthesis indicate values obtained from the empirical relations.

| Semiconductor	Average atomic number	Dielectric constant	
		High-frequency	Static
Si	14	⋯	11.9 (11.93)
Ge	32	⋯	16.0 (15.94)
α-Sn	50	⋯	24.0 (24.02)
A1P	14	7.54 (7.37)	9.8 (9.56)
A1As	23	8.16 (8.51)	10.06 (10.57)
A1Sb	32	10.24 (10.07)	12.04 (11.80)
GaP	23	9.11 (9.02)	11.11 (11.06)
GaAs[a]	32	10.88 (11.07)	12.85 (12.96)
GaSb	41	14.44 (14.34)	15.69 (15.63)
InP	32	9.61 (9.72)	12.55 (12.69)
InAs	41	12.25 (12.03)	15.16 (14.89)
InSb[b]	50	15.68 (15.79)	17.88 (18.01)
ZnS[c]	23	5.13 (5.19)	8.32 (8.40)
ZnSe[c]	32	6.2 (6.08)	9.2 (9.04)
ZnTe[c]	41	7.28 (7.34)	9.67 (9.78)
CdTe[c]	50	7.21	10.76 (10.65)
PbS	49	17.6[d] (17.69)	175[e] (177)
PbSe	58	23.1[d] (22.93)	250[e] (245)
PbTe	67	32.5[d] (32.59)	400[e] (402)

[a]Ref. 11.
[b]Ref. 8.
[c]Ref. 7.
[d]Ref. 9.
[e]Ref. 10.
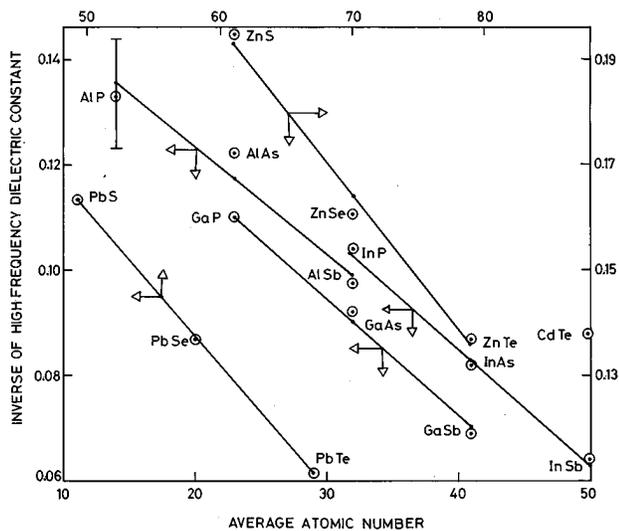
FIG. 1. Inverse of the high-frequency dielectric constant, K_∞, vs the average atomic number, Z_{av}, of the constituent atoms. Arrows indicate the relevant scales. The ordinate gives values of $2/K_\infty$ in place of $1/K_\infty$ for lead compounds.

are given in Table II. A measure of the agreement of the empirical relation with the experiment is given by the square root of the mean square percentage error (SRMSPE), values of which are also given in Table II.

The low values of SRMSPE indicate that the formulae, though empirical, should be considered to have a firm basis. On accepting the formulae, it is found that the value of the static dielectric constant of indium antimonide is more likely to be 17.88[8] rather than 16.8.[2] It is also found that the values for the ternaries and quaternaries would be obtained more accurately from the linearly interpolated values of the inverse of the dielectric constants, rather than from the interpolated values of the constants themselves.

The differences for aluminium compounds are much larger than those for the other compounds. It is suspected that the reported values for the aluminium compounds may
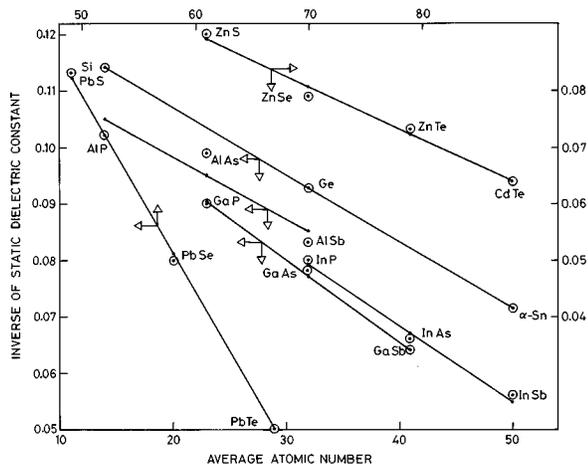
TABLE II. Constants for the empirical relations for dielectric constants.

Semiconductor	High-frequency		SRMSPE (%)	Static		SRMSPE (%)
	a	$b \times 10^3$		a	$b \times 10^3$	
Elemental	0.1	1.17	0.25	-	-	-
Gallium compounds	0.164	2.29	1.24	0.124	1.47	0.57
Indium compounds	0.173	2.20	1.28	0.120	1.30	1.28
Aluminium compounds	0.164	2.02	2.9	0.120	1.10	3.4
II-VI compounds	0.265	3.134	1.38	0.140	0.935	1.15
Lead compounds	0.127	1.436	0.5	0.0142	0.175	1.2

not be accurate enough. In fact, the error limits in the refractive index for aluminium phosphide[6] were mentioned as ± 0.1, which give values of K_∞ lying between 7.02 and 8.12 as indicated by the error bar in Fig. 1. The value for aluminium antimonide[12] was also found to be anomalous in the plot of ionic charge against the difference in the polarizability of the constituent atoms. Values for aluminium arsenide are also reported to show considerable scatter.[14] It may be concluded that new experiments for checking the values for the aluminium compounds would be worthwhile.

It should be mentioned also that K_∞ for cadmium telluride (CdTe) does not fit the line fitting K_∞'s for zinc compounds, although values of K_s of all the four II-VI compounds may be fitted to the same line. A fit for K_∞ of CdTe requires a value of 9.0 which appears very unlikely as the value[15] reported by different workers lies within 7.03 and 7.2. This discrepancy may be explained by assuming that CdTe belongs to a different group even though its K_s may be fitted to the line for the zinc compounds.

In conclusion, the inverse of the dielectric constant of semiconductors is found to be linearly related to the average atomic number of the constituent atoms. This linear relation may be used to obtain the values for the mixed compounds and also to judge the acceptability of the reported values.

FIG. 2. Inverse of the static dielectric constant, K_s, vs the average atomic number, Z_{av}, of the constituent atoms. Arrows indicate the relevant scales. The ordinate gives values of $20/K_s$ in place of $1/K_s$ for lead compounds.

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