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Estimates of the dielectric and optical characteristics for the IV group 3D- and 2D-binary compounds

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Received September 30, 2022
Revised October 15, 2022
Accepted October 20, 2022

Using the Harrison's bond orbital model for the IV group 3D- and 2D-compounds analytical expressions of the high- and low-frequency dielectric suscepti-bilities and dielectric constants, linear electrooptical coefficient, photoelastic con-stants and pressure dependences of the dielectric constants are obtained.

Keywords:: dielectric susceptibility and permittivitiy, photoelectric coefficient.

DOI: 10.21883/PSS.2023.02.55398.491

1. The interest to investigate the possibility of existence of three-dimensional (3D) single-crystals of GeC and SnC and their properties arose in the beginning of the century [1–3]. With the emergence of graphene and subsequent search for new multilayer (2D)-materials, studies were published on two-dimensional (2D) carbides of germanium and tin [4–7]. In [8] we have considered elastic properties of carbides of group IV elements using Harrison's bond orbital model for this purpose [9–11]. The comparison between the results obtained in [8] and numerical calculations of other authors and available experimental data has shown applicability of the model to describe the elasticity of 3D- and 2D-compounds of SiC, GeC, and SnC.

In this study we shall consider the whole range of A_4B_4 binary compounds. In this range only the silicone carbide is sufficiently well studied [12]. As for other 3D-compounds of A_4B_4 type, they only exist in the form of alloys and epitaxial structures so far [13–16]. Here we shall consider dielectric and optic characteristics of three-dimensional and graphene-like A_4B_4 compounds, again using Harrison's bond orbital model. Some evaluations of these characteristics for cubic single-crystals of SiC, GeC, and SnC are reported in [17].

2. Let us start with the description of dielectric properties of 3D-compounds with a sphalerite structure. Let us determine linear $\chi^{(1)}$ and quadratic $\chi^{(2)}$ dielectric susceptibilities from the expansion of crystal polarization **P** on the basis of the electric field strength **E**:

$$P_i = \sum_j \chi_{ij}^{(1)} E_j + \sum_{jk} \chi_{ijk}^{(2)} E_j E_k + \dots \text{ [18, 19].}$$

Then, within the bond orbital model it can be shown [20,21][1], that contributions of the electron subsystem to these characteristics are:

$$\chi_1^{el} = \frac{n_e(e\gamma d)^2\alpha_c^3}{12V_2}, \quad \chi_{14}^{el} = \frac{\sqrt{3}n_e(e\gamma d)^3\alpha_c^4\alpha_p}{48V_2^2}, \tag{1}$$

while ionic (lattice) contributions are as follows:

$$\chi_1^{ion} = \frac{n_e(e\gamma d)^2\alpha_p^2(1+2\alpha_c^2)}{24\alpha_c V_2},$$

$$\chi_{14}^{ion} = \frac{\sqrt{3}n_e(e\gamma d)^3\alpha_c^2\alpha_p(1-2\alpha_p^2)}{48V_2^2}. \tag{2}$$

The following expressions are obtained for sum values of linear and quadratic susceptibilities:

$$\chi_1 = \chi_1^{el}(1+\vartheta), \quad \vartheta = \frac{\alpha_p^2(1+2\alpha_c^2)}{2\alpha_c^4},$$

$$\chi_{14} = \frac{\sqrt{3}n_e(e\gamma d)^3\alpha_c^4\alpha_p^3}{48V_2^2}. \tag{3}$$

Here $V_2 = 3.22(\hbar^2/md^2)$ — covalent energy of σ-bond of sp^3-orbitals of A and B atoms, where $\hbar$ — reduced Planck constant, m — mass of free electron, $d = a\sqrt{3}/4$ — distance between the nearest neighbors in the sphalerite structure with lattice constant a and, as opposed to [20,21], we assume $V_2 > 0$; $\alpha_c = V_2/\sqrt{V_2^2+V_3^2}$ and $\alpha_p = \sqrt{1-\alpha_c^2}$ — covalency and polarity of the bond, $V_3 = |\varepsilon_h^A - \varepsilon_h^B|/2$ — polar energy of the bond, where $\varepsilon_h^{A(B)} = (\varepsilon_s^{A(B)} + 3\varepsilon_p^{A(B)})/4$ — energy of sp^3-orbitals and $\varepsilon_{s(p)}^{A(B)}$ — energy of $s(p)$-state of $A(B)$ atom; $n_e = 32/a^3$ — density of electrons, e — elementary charge, γ — scaling factor that takes into account corrections for the local field and is used as an adjustable parameter [9,20,21]. For high-frequency ε_∞ and static dielectric permittivity, we have the following:

$$\varepsilon_\infty = 1 + 4\pi\chi_1^{ei}, \quad \varepsilon_0 = 1 + 4\pi\chi_1. \tag{4}$$

Let us now turn to the determination of problem parameters by assuming $a = 4.36, 4.59$, and 5.11 Å respectively for cubic compounds of SiC, GeC, and SnC [3]. Since

[1] In [21], in the last term on the right part of formula (12) the $2\alpha_c^2$ must be replaced with the $2\alpha_p^2$.

Table 1. Initial parameters for cubic crystals of A_4B_4: distance between the nearest neighbors d, covalent V_2 and polar V_3 energies, covalency α_c and polarity α_P of the $A-B$ bond. The top row of values is the calculation as per Mann tables [11], the lower row is the calculation as per Herman–Skillman tables [9]

Parameter	SiC	GeC	SnC	SiGe	SiSn	GeSn
d, Å	1.89	1.99	2.21	2.42	2.60	2.80
V_2, eV	6.87	6.20	5.02	4.19	3.63	3.13
V_3, eV	1.88 1.42	1.93 1.37	2.41 1.77	0.05 0.04	0.53 0.35	0.48 0.39
α_c	0.96 0.98	0.95 0.98	0.90 0.94	1.0 1.0	0.99 1.0	0.99 0.99
α_P	0.26 0.20	0.30 0.22	0.44 0.33	0.01 0.01	0.14 0.10	0.15 0.12

values of a foe other compounds are unknown, let us determine them on the basis of atomic radii r_a, but taking into account that $a(AB) < r_a(A) + r_a(B)$. By taking r_a from [22] and evaluating the mean ratio for carbides as $a(XC)/\big(r_a(X) + r_a(C)\big) \approx 0.94$ $(X = \text{Si, Ge, Sn})$, we get values of d for SiGe, SiSn, and GeSn listed in Table 1. To calculate polar energy V_3, we shall use tables of atomic terms $\varepsilon_{s(p)}^{A(B)}$ of Mann [11] and Herman–Skillman [9]. From the consideration of parameter values determined in this way (see Table 1) it follows, that first, in the SiC$\to$GeSn series the interatomic bond length d increases. Second, all the compounds of A_4B_4 type can be split between group I, that includes carbides XC, and group II, that includes SiGe, SiSn, and GeSn. In both groups, when moving from the first compound to the last compound the polarity of bond α_p increases, although compounds of group II can be considered almost homopolar. And finally the scaling factor γ can be evaluated on the basis of experimental data [23] for 3C-SiC: $\varepsilon_\infty = 6.52$ and $\varepsilon_0 = 9.72$. By choosing ε_∞ for fitting, we get the value of $\gamma = 1.44$, which will be used for all other 3C-A_4B_4 compounds.

For the further analysis, it is convenient to re-write expressions for χ_1^{el} and χ_{14} in the following form: $\chi_1^{el} \approx 0.26(d\alpha_c^3)$ and $\chi_{14} \approx 2.01(d^4\alpha_c^2\alpha_p^3)\cdot 10^{-8}\,\text{CGSE}$ (or $\chi_{14} \approx$ $\approx 0.67(d^4\alpha_c^2\alpha_p^3)\cdot 10^{-12}\,\text{m/V}$ in SI measurement units), where d is measured in Å. The calculation results are given in Table 2. Values of χ_1^{el}, χ_1 and ε_∞ for carbides have a little difference, because a decrease in covalency α_c in the series of SiC$\to$SnC is compensated by an increase in d. The increase in ε_0 in the same series is related to the increase in the multiplier ϑ. It should be noted that the obtained values of ε_0 are presumably conservative. At least, this is the case for 3C-SiC.

The low level of quadratic susceptibilities χ_{14}^{el} and χ_{14} of A_4B_4 compounds as compared to semiconductors A_3B_5 and A_2B_6 (see, for example, Table 5.1 in [9]) is explained by the low polarity of bonds α_p. The growth of χ_{14}^{el} and χ_{14} in groups I and II (when moving from the first to the last compound) is related to increase in both α_p and d. Among the considered compounds, the highest values of χ_{14}^{el} and χ_{14} correspond to 3C-SnC. This is easy to explain, because the maximum value of χ_{14}^{el} takes place at $\alpha_c^* = \sqrt{4/5}$ and $\alpha_p^* = \sqrt{1/5}$, which is almost coincides with characteristics of the Sn$-$C bond. Maximum of the sum (low-frequency) susceptibility χ_{14} is realized at $\bar{\alpha}_c^* = \sqrt{2/5}$ and $\bar{\alpha}_p^* = \sqrt{3/5}$.

It should be stressed that when the formulae includes high exponents of α_c and α_p, the results of calculations based on Mann and Herman–Skillman tables have noticeable differences. It must be noted that this study ignores the metallicity of interatomic bonds [9,10], consideration of which, generally speaking, can considerably affect the calculation results [20,21].

3. Now let us turn to the consideration of optical properties of cubic crystals. The linear electrooptical coefficient r_{41}, which describes the change in the refraction index$n = \sqrt{\varepsilon_\infty}$ of noncentrosymmetric crystals in a low-frequency electric field is determined according to [18–21] as

$$r_{41} = -4\pi\chi_{14}/n^4. \tag{5}$$

The calculation results presented in Table 3 show that the behavior of change in coefficients $r_{41}^{el} = -4\pi\chi_{14}^{el}/n^4$ and r_{41} in the A_4B_4 series is defined by quadratic susceptibilities χ_{14}^{el} and χ_{14}. It's worth noting that values of $|r_{41}^{el}|$ and $|r_{41}|$ of cubic crystals A_4B_4 are extremely low as compared with other materials (see, for example, Table 77.2 in [19]).

Photoelastic constants p_{ij} for cubic 3D-compounds, that define the impact of mechanical stresses on the light

Table 2. Values of linear susceptibilities χ_1^{el}, χ_1, high-frequency ε_∞ and static ε_0 dielectric permittivities, multiplier ϑ and quadratic dielectric susceptibilities $\chi_{14}^{el}, \chi_{14}$, for A_4B_4 cubic crystals. The top row of values is the calculation as per Mann tables [11], the lower row is the calculation as per Herman–Skillman tables [9]

Parameter	SiC	GeC	SnC	SiGe	SiSn	GeSn
χ_1^{el}	0.43 0.46	0.44 0.49	0.42 0.48	0.63 0.63	0.66 0.68	0.71 0.71
χ_1	0.48 0.49	0.51 0.53	0.58 0.57	0.63 0.63	0.68 0.69	0.73 0.73
ε_∞	6.46 6.81	6.57 7.11	6.28 7.00	8.55 8.55	9.24 9.49	9.48 9.48
ϑ	0.11 0.06	0.15 0.08	0.39 0.19	0 0	0.03 0.015	0.03 0.02
ε_0	7.00 7.13	7.39 7.63	8.29 8.18	8.55 8.55	9.54 9.67	10.23 10.12
χ_{14}^{el}, 10^{-12} m/V	1.86 1.60	2.54 2.12	4.59 4.08	0 0	3.00 2.33	5.95 4.76
χ_{14}, 10^{-12} m/V	0.14 0.07	0.25 0.10	1.10 0.50	0 0	0.06 0.02	0.14 0.07

propagation in a crystalline medium [20,21], have the following form:

$$p_{11} = \xi\left(1 + \frac{8\lambda}{8+\lambda}\right), \quad p_{12} = \xi\left(1 - \frac{4\lambda}{8+\lambda}\right),$$

$$p_{44} = \frac{99\xi\lambda}{(8+\lambda)(8+3\lambda)}, \qquad (6)$$

where $\xi = -2\eta(\varepsilon_\infty - 1)/3\varepsilon_\infty^2$, $\eta = 2(1-3\alpha_p^2)$, $\lambda = 0.85$ [24]. The values of p_{ij} resulted from the calculation (Table 3) are close to diamond photoelastic constants $p_{11} = -0.31$, $p_{12} = -0.09$, and $p_{44} = -0.12$ (see Table 77.1 in [19]). The insignificant decrease in the values of $|p_{ij}|$ in the SiC $\rightarrow$ SnC and SiGe $\rightarrow$ GeSn series is due to the increasing bond polarity.

4. Now let us turn to the dependencies of dielectric permittivities ε_∞ and ε_0 of cubic crystals on the pressure P. In [25] it is shown that

$$\frac{\partial\varepsilon_\infty}{\partial P} = -\eta\frac{\varepsilon_\infty - 1}{3B}, \quad \frac{\partial\varepsilon_0}{\partial P} = (\varepsilon_\infty - 1)\frac{\partial\vartheta}{\partial P} + (1+\vartheta)\frac{\partial\varepsilon_\infty}{\partial P},$$

$$\frac{\partial\vartheta}{\partial P} = -\frac{2\alpha_p^2}{\alpha_c^2 B}\left(1 + \frac{2\alpha_p^2}{3\alpha_c^2}\right), \qquad (7)$$

where B is the compression bulk modulus. In the Harrison's bond orbital model $B = 2\alpha_c^3 V_2/\sqrt{3}d^3$ [9]. The calculation results are given in Table 3. It should be emphasized that the values of $|\partial\varepsilon_\infty/\partial P|$ and $|\partial\varepsilon_0/\partial P|$ given in Table 3 are the maximum estimates, since the calculation variant used in [8] (exclusive of short-range repulsion) underestimates the value of compression bulk modulus. Indeed, for 3C-SiC according to the data of [26] (see Table 4.6), we have $B = 246$ GPa, which is ~ 1.5 times greater than our result. Therefore, we have added to Table 3 the results of calculation of dimensionless derivatives $(\partial\varepsilon_\infty/\partial P)B$ and $(\partial\varepsilon_0/\partial P)B$, which allow for determining the values of $\partial\varepsilon_\infty/\partial P$ and $\partial\varepsilon_0/\partial P$ on the basis of known (from experiment or ab initio calculations) values of the compression bulk modulus.

5. Let us turn to the description of properties of 2D-compounds A_4B_4. For the electron $\bar{\chi}_1^{el}$ and lattice $\bar{\chi}_1^{ion}$ contributions to the linear dielectric susceptibility $\bar{\chi}_1$ of graphene-like structures (in-plane contributions) the following expressions were obtained in [29]:

$$\bar{\chi}_1^{el} = \frac{(e\bar{\gamma})^2\bar{\alpha}_c^3}{\sqrt{3}\bar{V}_2\bar{h}}, \quad \bar{\chi}_1^{ion} = \frac{2(e\bar{\gamma})^2\bar{\alpha}_p^2(1+2\bar{\alpha}_c^2)}{\sqrt{3}\bar{k}_0\bar{d}^2\bar{h}}, \qquad (8)$$

where force constant of the central-force interaction of the closest neighbors is:

$$\bar{k}_0 = \frac{4\bar{\alpha}_c\bar{V}_2(2\bar{\alpha}_c^2 - 1)}{\bar{d}^2} \qquad (9)$$

and again we have ignored the metallicity of bonds. In these formulae the overscribed bar of symbol indicates that we deal with a 2D-structure, $\bar{h}$ — „thickness" of

Table 3. Values of linear electrooptical coefficients r_{14}^{el}, r_{41}, elasto-optical constants p_{ij}, parameters $(\partial\varepsilon_\infty/\partial P)B$ and $(\partial\varepsilon_0/\partial P)B$, compression bulk moduli B, and derivatives of dielectric susceptibilities with respect to pressure $\partial\varepsilon_\infty/\partial P$ and $\partial\varepsilon_0/\partial P$ for cubic crystals A_4B_4. The top row of values is the calculation as per Mann tables [11], the lower row is the calculation as per Herman–Skillman tables [9]

Parameter	SiC	GeC	SnC	SiGe	SiSn	GeSn
$-r_{14}^{el}$, 10^{-12} m/V	0.55 0.40	0.74 0.53	1.46 1.05	0 0	0.50 0.33	0.87 0.68
$-r_{41}$, 10^{-12} m/V	0.04 0.02	0.07 0.02	0.35 0.13	0 0	0.01 0	0.02 0.01
$-p_{11}$	0.25 0.26	0.22 0.24	0.14 0.19	0.24 0.24	0.21 0.21	0.21 0.21
$-p_{12}$	0.08 0.08	0.07 0.08	0.04 0.06	0.08 0.08	0.07 0.07	0.07 0.07
$-p_{44}$	0.13 0.13	0.11 0.12	0.07 0.10	0.12 0.12	0.11 0.11	0.11 0.11
$-(\partial\varepsilon_\infty/\partial P)B$	2.89 3.41	2.71 3.48	1.36 2.70	5.03 5.03	5.16 5.49	5.25 5.40
$-(\partial\varepsilon_0/\partial P)B$	4.03 4.41	4.29 4.37	4.56 4.83	5.03 5.03	5.64 5.74	5.83 5.76
B, GPa	166 177	124 137	64 72	132 132	96 99	72 72
$-\partial\varepsilon_\infty/\partial P$, 10^{-2} GPa^{-1}	1.74 1.93	2.19 2.55	2.13 3.75	3.81 3.81	5.38 5.55	7.29 7.50
$-\partial\varepsilon_0/\partial P$, 10^{-2} GPa^{-1}	2.43 2.49	3.46 3.19	7.13 6.71	3.81 3.81	5.88 5.61	10.1 10.4

monolayer[2]. In the calculations of [29] we assumed $\bar{h} = \bar{d}$ and $\bar{\gamma} = 1$. In recent years it has become nearly common to assume $\bar{h}$ equal to the interplanar spacing in graphite which is 3.35 Å [23]. Let us assume, for simplicity, that $\bar{h}/\bar{\gamma}^2 = \bar{d}$. By assuming for 2D SiC : $\bar{d} = 1.79$ Å [29], we get $\bar{\gamma} = 1.37$, which is very close to the value of $\gamma = 1.44$ for 3C-SiC. For the sp^2-hybridization the covalent energy is equal to $\bar{V}_2 = 3.26(\hbar^2/m\bar{d}^2)$ [10], while the polar energy is $\bar{V}_3 = |\bar{\varepsilon}_h^X - \bar{\varepsilon}_h^C|/2$, where $\bar{\varepsilon}_h^{X(C)} = (\varepsilon_s^{X(C)} + 2\varepsilon_p^{X(C)})/3$. Numerical values of interatomic distances $\bar{d}$ [9], energies $\bar{V}_2$, $\bar{V}_3$, force constant $\bar{k}_0$, covalencies $\bar{\alpha}_c$ and polarities of bonds $\bar{\alpha}_p$ are given in Table 4, while values of characteristics (8), (9), $\bar{\varepsilon}_\infty = 1 + 4\pi\bar{\chi}_1^{el}$ and $\bar{\varepsilon}_0 = 1 + 4\pi(\bar{\chi}_1^{el} + \bar{\chi}_1^{ion})$ are given in Table 5. From Table 5 it follows that for mean values of

[2] Parameter $\bar{h}$ is introduced to have the same dimensionalities of physically identical characteristics for 3D- and 2D-structures, which is convenient first of all for the purpose of comparison. To the author's knowledge, the „thickness" has been introduced for the first time in the consideration of graphene elasticity, from where the turned-to-common statement appeared that its Young modulus is ~ 1 TPa (without the introduction of $\bar{h}$ the dimension of elasticity moduli of 2D-structures is N/m).

dielectric permittivities of carbides we have $\bar{\varepsilon}_\infty \sim 8$ and $\bar{\varepsilon}_0 \sim 9$, for compounds of group II $\bar{\varepsilon}_\infty \sim \bar{\varepsilon}_0 \sim 11-12$.

Since there is no any information on dielectric characteristics of 2D-compounds of A_4B_4 type, we provide here the data for other materials. Thus, for example, according to various authors (see [30,31]), values for graphene are in the range of 2−15. For hexagonal 2D-boron nitride (h-BN) we have $\bar{\varepsilon}_\infty = 4.96, 4.97$ and $\bar{\varepsilon}_0 = 6.82, 6.86$, while for 3D samples $\varepsilon_\infty = 4.98$ and $\varepsilon_0 = 6.93$ [32]. The data for chalcogenides of transition metal is in [32]: for example, for 2D WS_2 we have $\bar{\varepsilon}_\infty = 123.6$ and $\bar{\varepsilon}_0 = 13.7$, for 3D WS_2 — $\varepsilon_\infty = 14.5$ and $\varepsilon_0 = 124.6$; for 2D WSe_2 we have $\bar{\varepsilon}_\infty = 15.1$ and $\bar{\varepsilon}_0 = 15.3$, for 3D WSe_2 — $\varepsilon_\infty = 15.7$ and $\varepsilon_0 = 16.0$. From the data presented in [32], it follows that first, in terms of the order of magnitude our estimates of dielectric characteristics of 3D and monolayer A_4B_4 compounds are quite reasonable. Second, according to the data of [32], values of high-frequency and static dielectric permittivities have little differences both in the case of 2D and the case of 3D. We have obtained the same result as well (see Tables 2 and 5). Third, according to the data of [32], we have $\varepsilon_\infty > \bar{\varepsilon}_\infty$ and $\varepsilon_0 > \bar{\varepsilon}_0$, while according to our estimates the inequality should be the opposite. In this context it should be noted, that methods we used to determine the lattice contributions in cases of 3D [20] and 2D [29] were slightly different from each other. However, since $\chi_1^{ion} \ll \chi_1^{el}$ and $\bar{\chi}_1^{ion} \ll \bar{\chi}_1^{el}$, then without experimental information, in our opinion it is premature to unify the calculation procedures.

Now let us turn to photoelastic constants of graphene-like compounds, expressions for which were derived for the first time in [33] and have the following form:

$$\bar{p}_{11} = -\frac{1}{1+\bar{\sigma}}\,\frac{\bar{\varepsilon}_\infty - 1}{2\bar{\varepsilon}_\infty^2}, \quad \bar{p}_{12} = \bar{\sigma}\bar{p}_{11}, \tag{10}$$

where $\bar{\sigma}$ being Poisson's ratio. By borrowing values of $\bar{\sigma}$ from [4] and substituting into (10) the values of $\bar{\varepsilon}_\infty$ calculated by us, we get the results shown in Table 5. For mean values of $\bar{p}_{ij}$ of carbides we have $\bar{p}_{11} \sim -0.04$ and $\bar{p}_{12} \sim -0.015$, for compounds of group II $\bar{p}_{11} \sim -0.03$ and $\bar{p}_{12} \sim -0.01$. Unfortunately, we failed to find in literature any experimental data or results of numerical calculations of photoelastic constants for 2D-structures. Since $|\bar{p}_{ij}| \sim 10^{-2}$ (the same result is obtained in [33,34]), we have $|\bar{p}_{ij}| < |p_{ij}|$. However, it should be noted here that there is a difference between the procedures of photoelastic constants calculations for 3D [20,21] and 2D [33,34] structures.

6. So, in this work we have found that all A_4B_4 compounds (both 3D and 2D) can be split into carbide group I and group II, that includes SiGe, SiSn, and GeSn. Carbides are heteropolar compounds because they have a noticeable polarity of bonds, compounds of group II are almost homopolar.

Here and in [8], where elasticity of group IV carbides was considered, we did not detect any qualitative differences in properties of 3D- and 2D-compounds. According to some data (see, for example [4,35,36]), the character of bandgap (direct, indirect) for 3D- and 2D-structures of the same compound can be different. This fact, along with dielectric and optical properties of 2D-compounds is of a real interest for the optoelectronics (see, for example, reviews in [37–39]). Also, the application of 2D-GeC in lithium batteries [40,41] and 3D-carbides to create superlattices of GeC/SiC, SnC/SiC, SnC/GeC [42] and GeC/GaN [43] should be noted.

Table 4. Initial parameters for graphene-like compounds A_4B_4: distance between the closest neighbors $\bar{d}$, covalent $\bar{V}_2$ and polar $\bar{V}_3$ energies, force constant of the central-force interaction $\bar{k}_0$, covalency $\bar{\alpha}_c$ of the $A-B$ bond. The top row of values is the calculation as per Mann tables [11], the lower row is the calculation as per Herman–Skillman tables [9]

Parameter	SiC	GeC	SnC	SiGe	SiSn	GeSn
$\bar{d}$, Å	1.77	1.86	2.05	2.31	2.52	2.57
$\bar{V}_2$, eV	7.93	7.18	5.91	4.66	3.91	3.76
$\bar{V}_3$, eV	1.93 1.48	1.95 1.39	2.24 1.85	0.025 0.07	0.57 0.365	0.55 0.45
$\bar{\alpha}_c$	0.97 0.99	0.97 0.99	0.93 0.95	1.0 1.0	0.99 1.0	0.99 0.99
$\bar{k}_0$, eV/Å^2	8.66 9.62	7.10 7.89	3.92 4.30	3.49 3.49	2.36 3.46	2.19 2.19

Table 5. Values of electron $\bar{\chi}_1^{el}$ and lattice χ_1^{ion} contributions to linear susceptibilities χ_1, high-frequency ε_∞ and static ε_0 dielectric permittivities, Poisson's ratios [4] and photoelastic constants $\bar{p}_{ij}$ for graphene-like compounds A_4B_4. The top row of values is the calculation as per Mann tables [11], the lower row is the calculation as per Herman–Skillman tables [9]

Parameter	SiC	GeC	SnC	SiGe	SiSn	GeSn
$\bar{\chi}_1^{el}$	0.54 0.57	0.57 0.60	0.55 0.59	0.77 0.77	0.82 0.84	0.83 0.83
$\bar{\varepsilon}_\infty$	7.78 8.16	8.16 8.54	7.94 8.39	10.7 10.7	11.3 11.6	11.5 11.5
$\bar{\chi}_0^{ion}$	0.06 0.02	0.06 0.02	0.18 0.12	0 0	0.03 0	0.03 0.03
$\bar{\varepsilon}_0$	8.52 8.39	8.94 8.78	10.2 9.93	10.7 10.7	11.6 11.6	11.8 11.8
$\bar{\sigma}$	0.29	0.33	0.41	0.32	0.37	0.38
$-\bar{p}_{11}\cdot 10^2$	4.34 4.17	4.04 3.89	3.90 3.72	3.21 3.21	2.94 2.88	2.88 2.88
$-\bar{p}_{12}\cdot 10^2$	1.26 1.21	1.33 1.28	1.60 1.53	1.03 1.03	1.10 1.06	1.09 1.09

Conflict of interest

The author declares that he has no conflict of interest.

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