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Elasticity of 3D and 2D XC ($X=$Si, Ge, Sn) compounds: Keating and Harrison models

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For the bulk and monolayer IV group carbides in the scope of Keating and/or Harrison models analytical expressions are obtained for second order elastic constants c_{ij}, sound velocities v, third order elastic constants c_{ijk}, pressure dependencies of c_{ij} and v, Grüneisen constant, thermal expansion coefficient and temperature dependence of bulk moduli. It is shown that in the row of SiC−GeC−SnC values of all considered characteristics decrease while thermal expansion coefficient increases. All the model estimations are compared with experimental data and calculating results of other authors.

Keywords: force constants, elastic constants, sound velocities, anharmonic characteristics.

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1. Introduction

Unlike germanium and tin carbides, the silicon carbide has been intensely studied for a long time [1], whereas there is no information on GeC and SnC even in a reference book [2] for promising semiconductor materials. The theoretical interest in the properties and the possible existence of the bulk (3D) single crystals of these compounds has arisen only in the beginning of the current century [3–8]. Special attention was paid to stability of some or other crystal structures, a band spectrum and elasticity. After the advent of graphene topics and search of new monolayer materials occurred thereafter, there were studies for two-dimensional (2D) compounds XC, where $X=$ Si, Ge and Sn [9–12]. All the cited papers are numerical calculations. Here, we will consider elastic properties of the 3D and 2D compounds XC using the models of Keating [13–15] and Harrison [16,17], which are well proven for description of the semiconductors.

2. Keating's model of force constants

2.1. 3D structures

For description of the elastic constants of the bulk crystals with a diamond structure, Keating proposed a simple model [13], containing two „force constants" α and β.[1] The first constant describes the central interaction of the adjacent neighbors, while the second one — non-central interaction of the second neighbors. The second-order elastic constants take the following form:

$$c_{11}=\frac{\alpha+3\beta}{4},\quad c_{12}=\frac{\alpha-\beta}{4},\quad c_{44}=\frac{\alpha\beta}{\alpha+\beta}. \qquad (1)$$

From the expressions (1) the identity follows:

$$R=\frac{c_{44}(c_{11}+c_{12})}{c_s(c_{11}+3c_{12})}=1, \qquad (2)$$

where $c_s=(c_{11}-c_{12})/2$ is the shear modulus. The Kleinman's parameter of internal displacements is $\xi=(\alpha-\beta)/(\alpha+\beta)$. The Martin's study [15] generalized the model [13] on a sphalerite structure and applied it to describe the crystal elasticity of A_NB_{8-N}. Therefore , the model exhibits effective charges of the atoms A and B and corresponding interatomic Coulomb forces to be neglected here by us due to small polarity of the bonds $X-C$ (see Section 3.1). Thus, the formulas (1) and (2) can be applied to the calculation of elasticity of the cubic ($3C$) compounds XC.

The relationships between the elastic constants of the structures of sphalerite and wurtzite were proposed in the paper [18] and applied to the Keating's model in the paper [19], in accordance with which we have for wurtzite:

$$c_{11}=\frac{\alpha+\beta}{4}+\frac{\alpha\beta}{\alpha+\beta}-D,\quad c_{33}=\frac{3\alpha+\beta}{12}+\frac{4\alpha\beta}{3(\alpha+\beta)},$$

$$c_{44}=\beta\,\frac{2\alpha+\beta}{3(\alpha+\beta)}-\beta\,\frac{(\alpha-\beta)^2}{3(\alpha+\beta)(5\alpha+\beta)},$$

$$c_{66}=\beta\,\frac{5\alpha+\beta}{6(\alpha+\beta)}-D,$$

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[1] Here we use quotes, as in this study the constants α and β are given in units of GPa, while the units N/m are usually used.

$$c_{12} = \frac{3\alpha-\beta}{12} - \frac{\alpha\beta}{3(\alpha+\beta)} + D,\; c_{13} = \frac{3\alpha+\beta}{12} - \frac{2\alpha\beta}{3(\alpha+\beta)},$$

$$D = \beta\,\frac{(\alpha-\beta)^2}{6(\alpha+\beta)(2\alpha+\beta)}. \qquad (3)$$

Note that $c_{66} = (c_{11} - c_{12})/2$. Further on, in order to determine the constants α and β, we will use experimentally measured elastic constants c_{11} and c_{12} of the cubic crystals or elastic constants numerically calculated by other authors, so that $\alpha = c_{11} + 3c_{12}$ and $\beta = c_{11} - c_{12}$. Values of „force constants" and elastic constants of the cubic crystals XC, as determined in this way, are given in Table 1. It also contains the values of the bulk moduli $B = (c_{11} + 2c_{12})/3$ and the anisotropy factors $A' = (c_{11} + 2c_{12})/c_{11}$ [7] and $A = c_s/c_{44}$ [22].[2] The values of the elastic constants of the compounds XC with the wurtzite structure ($2H$) are given in Table 2.

Table 1. Keating's model, the sphalerite structure: values of „elastic constants" α and β, the Kleinman's parameter ξ, the elastic constants c_{ij}, the ratio R, the bulk compression modulus B and the anisotropy factors A' and A (α, β, c_{ij} and B are given in units of GPa). The upper row of the values the initial values c_{ij} from the papers specified in the extreme left column, the lower row the results of the Keating calculations, only the values different from the initial ones

Calculation option	3D XC	c_{11}	c_{12}	c_{44}	R	B	A'	A
1 [8]	SiC $\alpha = 700$ $\beta = 300$ $\xi = 0.40$	400	100	250 210	1.19 1	200	1.50	0.60 0.71
	GeC $\alpha = 600$ $\beta = 200$ $\xi = 0.50$	300	100	200 150	1.33 1	166	1.67	0.50 0.67
	SnC $\alpha = 440$ $\beta = 120$ $\xi = 0.57$	200	80	120 94	1.17 1	120	1.80	0.50 0.64
2 [5]	SiC $\alpha = 824$ $\beta = 164$ $\xi = 0.67$	329	165	163 133	1.19 1	220	2.00	0.50 0.60
	GeC $\alpha = 669$ $\beta = 173$ $\xi = 0.35$	297	124	141 137	1.03 1	188	1.84	0.61 0.63
3 [20,21]	SiC $\alpha = 790$ $\beta = 250$ $\xi = 0.52$	385	135	257 190	1.35 1	218	1.69	0.49 0.66
4 [22,21]	SiC $\alpha = 903$ $\beta = 247$ $\xi = 0.57$	411	164	194	1.00 1	246	1.80	0.64

Table 2. Keating's model, wurtzite structure: the values of the parameter D and elastic constants c_{ij} (in units of GPa). The upper row of the values results of the calculations by the formulas of the Keating's model, in brackets the calculation results of the paper [8] for option 1 and the paper [20] for option 2

Calculation option	3D XC	c_{11}	c_{33}	c_{44}	c_{66}	c_{12}	c_{13}
1 [8]	SiC $D = 5$	456 (523)	481 (558)	166 (156)	185 (215)	85 (93)	60 (44)
	GeC $D = 5$	343 (441)	365 (488)	113 (137)	132 (181)	89 (79)	65 (37)
	SnC $D = 4$	229	245	68	79	73	58
2 [5]	SiC $D = 7$	378	403	88	111	153	128
	GeC $D = 6$	343	366	85	123	112	90
3 [20,21]	SiC $D = 6$	446	474	141	162	119	91
4 [22,21]	SiC $D = 9$	471	502	141	163	149	118

Analysis of the obtained results shows that all the elastic constants of the SiC → GeC → SnC row are decreasing. The exception is the value c_{13} for $2H$-GeC when calculating as per the option 1 using the results of the paper [8] (see Table 2). Note that for this case the value $R = 1.33$, which is a considerable deviation from the value $R = 1$ of the Keating's model. The seems strange result is $c_{12} > c_{44}$ obtained for $3C$-SiC in [5] (Table 1, option 2), as in all other studied cases $c_{12} < c_{44}$. It is also necessary to indicate significant spread of values of the elastic characteristics for fairly well studied silicon carbide (except for the values c_{ij} given in Tables 1 and 2, see, for example, [2,23]). Despite the mentioned spread of the absolute values c_{ij}, their relative values $c^*_{ij} = c_{ij}/c_{11}$, shown in the Figures 1 and 2, exhibit common features for all the compounds XC and all the calculation options. The exclusions are correlated again to the according to the calculation option 2. Variations of the anisotropy factors A' and A are insignificant for all the calculation options. Note that the experimental values c_{ij}

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[2] All the values of the elastic constants and the bulk moduli (including those from the papers of other authors) were rounded by us to integer values. For the elastic constant c_{11} of the paper [8] we (fairly arbitrarily) accepted the value of 300 GPa (Table 1). The thing is that according to [8] there is an approximate equality $c_{11} \approx c_{44} \approx 200$ GPa. This result seems erroneous to us, as the equality of these elastic constants can not be found anywhere else (as far as we know).

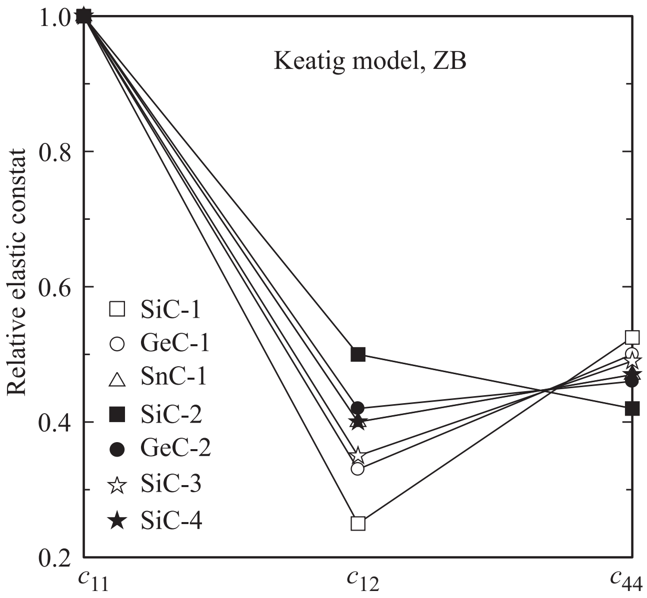

Figure 1. Keating's model, the sphalerite structure, or that of zinc blende (ZB): values of the relative elastic constants $c^*_{ij} = c_{ij}/c_{11}$, calculated by the formulas (1). The designations are shown in the figure, the digit near the chemical formula corresponds to the calculation option of Table 1. The thin straight lines are used for clarity.

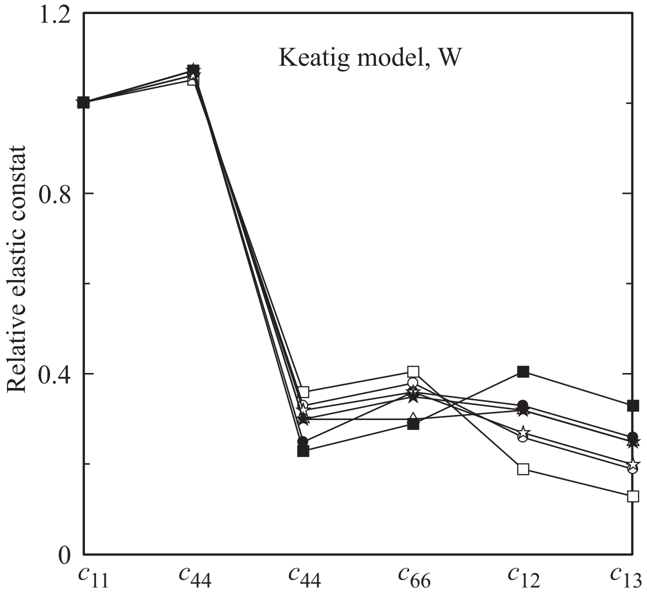

Figure 2. Keating's model, the wurtzite structure (W): values of the relative elastic constants $c^*_{ij} = c_{ij}/c_{11}$, calculated by the formulas (3). Designations are the same as in the Fig. 1. The thin straight lines are used for clarity.

for 3C-SiC, used in the option 4 and given in Table 4.6 of the paper [22], are almost exactly described by the Keating's model.

In the paper [15] (see also [22]) Martin showed that in the cubic crystals of the A_NB_{8-N} compounds the ratio $x = \beta/\alpha$ tends to decrease with increase in ionicity f_i as per Philips [24]. From the calculation as per the option 1 for SiC, GeC and SnC, we obtain $x = 0.42$, 0.33 and 0.27, respectively; in the calculation as per the option 2, for SiC and GeC we have $x = 0.20$ and 0.26, thereby doubting results of the study [5]. An issue of the ionicity of the compounds XC will be studied by us in Section 3.1.

Now, we study the dependences of the elastic constants on the pressure p, by replacing, as in [21], α and β with $\tilde\alpha = \alpha + ap$ and $\tilde\beta = \beta + bp$, where a and b dimensionless coefficients (hereinafter the tilde indicates that the corresponding value depends on the pressure). Then, instead of (1) we get:

$$\tilde c_{11} = c_{11} + [(a+3b)/4]p, \quad \tilde c_{12} = c_{12} + [(a-b)/4]p,$$

$$\tilde c_{44} \approx c_{44} + \frac{\alpha b + a\beta - \alpha\beta(a+b)/(\alpha+\beta)}{\alpha+\beta}\, p, \qquad (4)$$

where the expression for $\tilde c_{44}$ (in contrast to [21]) is linearized by p. From (4) for the bulk compression modulus we find $\tilde B = B + (a+b)p/6$. The expressions (3) can be converted similarly.

As per data of the paper [3], for the cubic crystals SiC, GeC and SnC we have $B = 206$, 181, 119 GPa and $\tilde B' \equiv \partial\tilde B/\partial p = 5.3$, 4.2 and 4.3. As per data of the paper [5], for 3C-SiC and 3C-GeC we have $B' = 3.90$ and 3.45, respectively. Analysis of the dependences $\tilde c_{ij}$ on p, shown in the Fig. 4–6 of the paper [7], for 3C–XC provides $\tilde c'_{11} \sim \tilde c'_{12} \sim 4$, $\tilde B' \sim 4$ and $\tilde c'_{44} \sim 1$, where $\tilde c'_{ij} \equiv \partial\tilde c_{ij}/\partial p$, so that $a \sim 5b \sim 10$. Based on the results of the paper [20], for 3C-SiC in [21] we have $\tilde c'_{11} = 3.49$, $\tilde c'_{12} = 4.06$, wherefrom $B' = 3.87$, $a = 15.7$, $b = -0.6$. To obtain order evaluations, we assume that $a = 16$ and $b = 0$. Then,

$$\tilde c'_{11} \approx 4\left(1 + \frac{4x}{1+x}\right), \quad \tilde c'_{33} \approx 4\left(1 + \frac{16x}{3(1+x)}\right),$$

$$\tilde c'_{12} \approx 4\left(1 - \frac{4x}{3(1+x)}\right), \quad \tilde c'_{13} \approx 4\left(1 - \frac{8x}{3(1+x)}\right),$$

$$\tilde c'_{44} \approx 0, \quad \tilde c'_{66} \approx 0,$$

where, as above, $x = \beta/\alpha$. It is easy to see that all the derivatives $\tilde c'_{ij}$ are smooth functions of the parameter x. The results of the order evaluations $\tilde c'_{ij}$ are given in Table 3.

Let us come to evaluations of the sound velocities $v_{\boldsymbol\sigma}(\mathbf{q}) = \sqrt{C_i(\mathbf{q})/\rho_{AB}}$, where the index $\boldsymbol\sigma$ corresponds to polarization of the acoustic wave propagating in the direction $\mathbf{q}$ in the crystal AB with the density ρ_{AB}, $C_{\boldsymbol\sigma}(\mathbf{q})$ a combination of the relevant elastic constants. In case of the cubic crystals we have [20,21]: for the three longitudinal acoustic waves (LA)

$$C_{[100]}([100]) = c_{11}, \quad C_{[110]}([110]) = (c_{11} + 2c_{12} + 2c_{44})/2,$$

$$C_{[111]}([111]) = (c_{11} + 2c_{12} + 4c_{44})/3; \qquad (6)$$

Table 3. Keating's model, the wurtzite structure: the order evaluations of the dependence of the elastic constants on the pressure ($\tilde{c}'_{ij} = \partial\tilde{c}_{ij}/\partial p$)

Calculation option	3D XC	$\tilde{c}'_{11}$	$\tilde{c}'_{33}$	$\tilde{c}'_{12}$	$\tilde{c}'_{13}$
1 [8]	SiC $x = 0.43$	9.1	10.8	2.3	0.6
	GeC $x = 0.33$	8.0	9.3	2.6	1.35
	SnC $x = 0.27$	7.4	8.5	2.9	1.7
2 [5]	SiC $x = 0.20$	6.7	7.6	3.1	2.2
	GeC $x = 0.26$	7.3	8.4	2.9	1.8
3 [20,21]	SiC $x = 0.32$	7.9	9.2	2.7	1.4
4 [21,22]	SiC $x = 0.27$	7.4	8.5	2.9	1.7

Table 4. Keating's model, the sphalerite structure: sound velocities $v^{[ijk]}_{L(T)A}$ (in units of km/s)

Calculation option	3D XC	$v^{[100]}_{LA}$	$v^{[110]}_{LA}$	$v^{[111]}_{LA}$	$v^{[100]}_{TA}$	$v^{[110]}_{TA}$	$v^{[111]}_{TA}$
1	SiC	11.2	12.6	12.2	8.1	6.8	7.3
[8]	GeC	7.2	8.3	8.0	5.1	4.2	4.5
	SnC	5.6	6.5	6.2	3.8	3.0	3.3
2	SiC	10.1	11.8	11.6	6.4	5.1	5.6
[5]	GeC	7.2	8.4	7.9	4.9	3.9	4.2

Table 5. Keating's model, the sphalerite structure: the order evaluations of the parameter $\eta_{\sigma}(\mathbf{q})$ (in units of GPa^{-1})

Calculation option	3D XC	$\eta^{[100]}_{LA}$	$\eta^{[110]}_{LA}$	$\eta^{[111]}_{LA}$	$\eta^{[100]}_{TA}$	$\eta^{[110]}_{TA}$	$\eta^{[111]}_{TA}$
[5,7]	SiC	4	5	4	1	−2	−2
	GeC	4	5	4	0	−3	−2

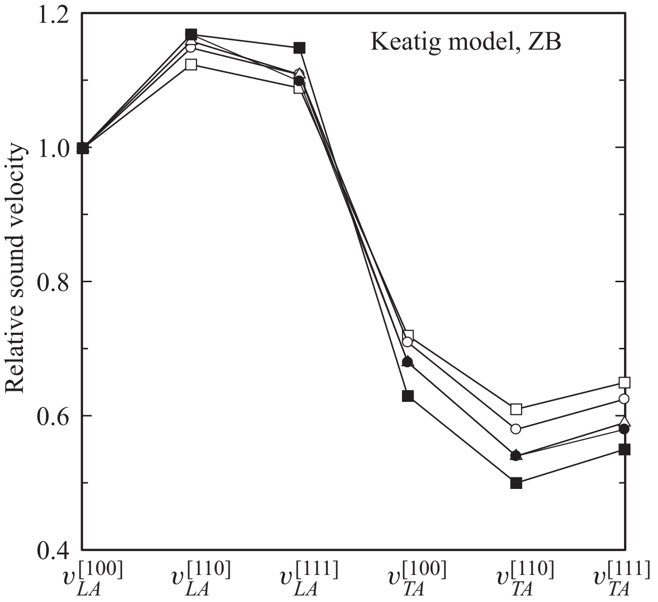

Figure 3. Keating's model, the sphalerite structure or that of zinc blende (ZB): values of the relative elastic constants $(v^{[ijk]}_{L(T)A})^* = v^{[ijk]}_{L(T)A}/v^{[100]}_{LA}$, calculated by the formulas (6) and (7). Designations are the same as in the Fig. 1. The thin straight lines are used for clarity.

for the three transverse acoustic waves (TA)

$$C_{[010]}([100]) = C_{[001]}([100]) = C_{[001]}([110]) = c_{44},$$
$$C_{[1\bar{1}0]}([110]) = c_s,$$
$$C_{[1\bar{1}0]}([111]) = C_{[11\bar{2}]}([111]) = (2c_s + c_{44})/3, \qquad (7)$$

where, as above, the shear modulus $c_s = (c_{11}-c_{12})/2$. Taking into account that the constants of the cubic lattices SiC, GeC and SnC are equal to 4.36, 4.59 and 5.11 Å [7], respectively, so that $\rho_{\mathrm{SiC}} = 3.21\,\mathrm{g/cm^3}$, $\rho_{\mathrm{GeC}} = 5.77\,\mathrm{g/cm^3}$ and $\rho_{\mathrm{SnC}} = 6.47\,\mathrm{g/cm^3}$, and using the values c_{ij} calculated by us (Table 1), we will get the results of Table 4, which quite satisfactorily agree with available experimental data [2]. It is obvious that the sound velocity diminishes when transferring from 3*C*-SiC to 3*C*-SnC. The Fig. 3 shows the relative sound velocities $(v^{[ijk]}_{L(T)A})^* = v^{[ijk]}_{L(T)A}/v^{[100]}_{LA}$. As in the case of elastic constants (Figures 1 and 2), the values $(v^{[ijk]}_{L(T)A})^*$ show the relatively weak dependence on the X element and the calculation method.

Influence of the pressure on the sound velocity $\eta_{\sigma}(\mathbf{q}) = \partial v_{\sigma}(\mathbf{q})/\partial p$ may be presented as:

$$\frac{\partial v_{\sigma}(\mathbf{q})}{\partial p} = v_{\sigma}(\mathbf{q})\eta_{\sigma}(\mathbf{q}), \ \ \eta_{\sigma}(\mathbf{q}) = \frac{1}{2}\left(\frac{C'_{\sigma}(\mathbf{q})}{C_{\sigma}(\mathbf{q})} - \frac{1}{B}\right), \qquad (8)$$

where $C'_{\sigma}(\mathbf{q}) = \partial C_{\sigma}(\mathbf{q})/\partial p$ [20]. For the cubic carbides of silicon and germanium, the values of the parameter $\eta_{\sigma}(\mathbf{q})$ are shown in Table 5. Since, in doing so c_{ij} were taken from data processing of the paper [5], and c'_{ij} — from data processing of the paper [7], the given values $\eta_{\sigma}(\mathbf{q})$ should be considered to be order evaluations.

2.2. 2D structures

For graphene, the expressions for the elastic constants of the second $\bar{c}_{ij}$ and third $\bar{c}_{ijk}$ orders, as well as the dependences $\tilde{\bar{c}}_{ij}$ on the two-dimensional pressure $\bar{p}$ were obtained in the papers [25–27], respectively, and take the

Table 6. Keating's model, 2D: values of the elastic constants of the second $\bar{c}_{ij}$ and third $\bar{c}_{ijk}$ orders (in units of N/m), the sound velocities (in units of km/s) and the pressure derivatives of the elastic constants of the second order $\bar{c}'_{ij}$

2D XC	$\bar{c}_{11}$	$\bar{c}_{12}$	$-\bar{c}_{111}$	$-\bar{c}_{222}$	$-\bar{c}_{112}$	v_p	v_s	$\tilde{\bar{c}}'_{11}$	$\tilde{\bar{c}}'_{22}$	$\tilde{\bar{c}}'_{12}$
SiC	184	53	1748	1827	331	16.5	8.1	8.7	7.6	1.4
GeC	158	53	929	971	176	15.6	5.8	5.2	4.6	0.8
SnC	117	48	628	657	119	10.7	4.9	4.5	4.0	0.7
[27]										
SiC [11]	177	56	1391	1181	392	16.6	8.3	7.6	5.1	1.68
GeC [10]	156	44	1413	1186	155	13.9	5.3	7.8	5.9	0.8

following form:

$$\bar{c}_{11} = \frac{1}{\sqrt{3}}\left(4\bar{\alpha} + \bar{\beta} + 18\,\frac{\bar{\alpha}\bar{\beta}}{4\bar{\alpha}+\bar{\beta}}\right),$$

$$\bar{c}_{12} = \frac{1}{\sqrt{3}}\left(4\bar{\alpha} + \bar{\beta} - 18\,\frac{\bar{\alpha}\bar{\beta}}{4\bar{\alpha}+\bar{\beta}}\right), \quad (9)$$

$$\bar{c}_{111} = (16\bar{\gamma}/\sqrt{3})[(1.5-\bar{\xi})^3 + 4\bar{\xi}^3],$$

$$\bar{c}_{222} = (16\bar{\gamma}/\sqrt{3})[(0.5+\bar{\xi})^3 + 4(1-\bar{\xi})^3],$$

$$\bar{c}_{112} = (16\bar{\gamma}/3\sqrt{3})[(1.5-\bar{\xi})^2(0.5+\bar{\xi}) + 4\bar{\xi}^2(1-\bar{\xi})], \quad (10)$$

$$\tilde{\bar{c}}_{11} = \bar{c}_{11} - (\bar{c}_{111} + \bar{c}_{112})\,\frac{1-\bar{\sigma}}{\bar{E}}\,\bar{p},$$

$$\tilde{\bar{c}}_{22} = \bar{c}_{11} - \bar{c}_{222}\,\frac{1-\bar{\sigma}}{\bar{E}}\,\bar{p}, \quad \tilde{\bar{c}}_{12} = \bar{c}_{12} - \bar{c}_{112}\,\frac{1-\bar{\sigma}}{\bar{E}}\,\bar{p}. \quad (11)$$

Here, $\bar{\alpha}$ and $\bar{\beta}$ the harmonic force constants of central and noncentral interaction, $\bar{\gamma}$ the anharmonic constant of the central interaction, $\bar{\xi} = (2\bar{\alpha} - \bar{\beta})/(4\bar{\alpha} + \bar{\beta})$ the Kleinman's parameter of internal displacements, $\bar{\sigma} = \bar{c}_{12}/\bar{c}_{11}$ the Poisson ratio, $\bar{E} = (\bar{c}_{11}^2 - \bar{c}_{12}^2)/\bar{c}_{11}$ the Young modulus. The overline of the symbol means referring to the 2D structure, for which all the elastic constants and the force constants are expressed in N/m. The paper [27] applies the expressions (9)−(11) to graphene-like compounds $A_N B_{8-N}$. For 2D compounds XC under our study, the following values of the parameters are obtained: $\bar{\alpha}, \bar{\beta}, \bar{\gamma}$ (in units of N/m), $\bar{x} = \bar{\alpha}/\bar{\beta}$ and $\bar{\xi}$: 44, 29, 63, 0.67 and 0.28 for SiC; 40, 23, 44, 0.59 and 0.31 for GeC; 32, 15, 30, 0.47 and 0.34 for SnC. The results of calculation of the elastic constants of the second and third orders and the dependences of the elastic constants of the second order on the pressure $\tilde{\bar{c}}_{ij} = \partial\bar{c}_{ij}/\partial\bar{p}$ are provided in Table 6. At this, determining the force constants $\bar{\alpha}$ and $\bar{\beta}$, we proceeded from the numerical calculations of [9], whereas for evaluation of $\bar{\gamma}$ we used graphene data and lattice constants' scaling (see [27] for more details). It follows from Table 6 that when transferring from SiC to SnC, all the values of the elastic characteristics diminish. So, does the ratio $\bar{x} = \bar{\alpha}/\bar{\beta}$.

Table 6 also shows the results of the numerical calculations [10,11]. The biggest divergence with our results is for the elastic constants $\bar{c}_{ijk}$. This is not surprising since we have determined the values $\bar{\gamma}$ quite approximately. Moreover, in order to describe the diamond structure, Keating used 3 anharmonic force constants — a central one and two noncentral ones [14], whereas we used only the central force constant. That is why we obtain $|\bar{c}_{111}| < |\bar{c}_{222}|$.

The sound velocities in the graphene-like compounds are determined by the expressions:

$$v_p = \sqrt{\frac{\bar{E}(1-\bar{\sigma})}{\bar{\rho}(1+\bar{\sigma})(1-2\bar{\sigma})}}, \quad v_s = \sqrt{\frac{\bar{c}_{12}}{\bar{\rho}}}, \quad (12)$$

where v_p the velocity of the compression wave causing the two-axis deformation, v_s the velocity of the shear wave, $\bar{\rho} = 2\bar{M}_{cell}/3\sqrt{3}\bar{d}^2$ the density of the 2D structure, $\bar{M}_{cell}$ the weight of the lattice cell atoms, $\bar{d}$ the distance between the adjacent neighbors, which is equal, for SiC, GeC and SnC, to 1.77, 1.86 and 2.05 Å, respectively [9]. From here we have: $\bar{E} = 169$ GPa, $\bar{\sigma} = 0.29$, $\bar{\rho} = 0.82 \cdot 10^{-6}$ kg/m^2 for SiC; $\bar{E} = 140$ GPa, $\bar{\sigma} = 0.335$, $\bar{\rho} = 1.55 \cdot 10^{-6}$ kg/m^2 for GeC; $\bar{E} = 97$ GPa, $\bar{\sigma} = 0.41$, $\bar{\rho} = 1.98 \cdot 10^{-6}$ kg/m^2 for SnC, which well agrees with the results of the papers [10,11]. The results of calculation of the sound velocities shown in Table 6 show decrease in the values of v_p and v_s in the SiC → SnC row. We underline that our model evaluations well agree with the results of the numerical calculations [19,11].

3. Model of Harrison's bonding orbitals

3.1. 3D structures

The Harrison's model for the tetrahedral semiconductors [16,17,28] is a simplified option of the LCAO method, wherein all the necessary matrix elements are specified by simple and physically transparent analytical expressions. As per [16,29], for the cubic crystals, the elastic constants take the following form:

$$c_{11} = \frac{2\sqrt{3}(1+\lambda)}{2}\,w, \quad c_{12} = \frac{\sqrt{3}(2-\lambda)}{3}\,w,$$

$$c_{44} = \frac{3\sqrt{3}\lambda}{3+2\lambda}\,w. \quad (13)$$

Here, $w = \alpha_c^3 V_2/d^3$, $V_2 = 3.22(\hbar^2/md^2)$ the covalence energy of the σ-bond of the sp^3-orbitals of the X and C atoms, $\hbar$ the reduced Planck constant, m the mass of free electron, $d = a_0\sqrt{3}/4$ the distance between adjacent neighbors, a_0 the lattice constant, $\lambda = 0.85$ the constant describing the change of the energy V_2 in misorientation of the sp^3-orbitals,

Table 7. Harrison's model, the sphalerite structure: the values of the covalence V_2 and polar V_3 energies (in eV), the covalence of the bonds α_c, the elastic constants c_{ij}, the bulk compression module B and the shear module c_x (all the elastic characteristics are given in units of GPa). The upper row of the values corresponds to using the tables of the Mann atomic terms [29], the lower row — using the tables of the Hermann–Skillman atomic terms [16]

3D XC	V_2	V_3	α_c	c_{11}	c_{12}	c_{44}	B	c_s
SiC	6.87	1.88	0.96	308	96	135	166	106
		1.42	0.98	328	102	144	177	113
GeC	6.20	1.93	0.95	229	71	101	124	79
		1.37	0.98	253	79	111	137	87
SnC	5.02	2.41	0.90	116	36	51	64	40
		1.77	0.94	133	41	59	72	46

forming the σ-bond, $\alpha_c = V_2/\sqrt{V_2^2 + V_3^2}$ the covalency of the $X{-}C$ bond, $V_3 = |\varepsilon_h^X - \varepsilon_h^C|/2$ the bond polar energy, $\varepsilon_h^{X(C)} = (\varepsilon_s^{X(C)} + 3\varepsilon_p^{X(C)})/4$ the energies of the sp^3-orbitals and $\varepsilon_{s(p)}^{X(C)}$ the energy of the $s(p)$-state of the $X(C)$ atom. From the expressions (13) we find:

$$c_{22}/c_{11} = (2-\lambda)/2(1+\lambda) = 0.31,$$

$$c_{44}/c_{11} = 9\lambda/2(1+\lambda)(3+2\lambda) = 0.44,$$

$$R = (4+\lambda)/(8-\lambda) = 0.68,$$

$$\xi = (1-\lambda/3)/(1+2\lambda/3) = 0.47,$$

$$A' = 3/(1+\lambda) = 1.62, \quad A = (3+2\lambda)/6 = 0.78.$$

The results of calculation of the elastic characteristics are given in Table 7, wherein we assumed that $a = 4.36$, 4.59 and 5.11 Å respectively for 3D SiC, GeC [7] and SnC and used the tables of the Mann atomic terms [28] and the Hermann–Skillman atomic terms [16]. First of all, we note a high degree of covalence of the bonds $X{-}C$. This makes it possible to apply the Keating's model [13,14], neglecting corrections [15], correlated to presence of the charge in the X and C atoms. Secondly, the covalence of the bonds α_c reduces in the SiC → SnC row, and their polarity $\alpha_p = (1-\alpha_c^2)^{1.2}$ and ionicity as per Philips $f_i = 1-\alpha_c^3$ increase. And, finally, all the elastic characteristics diminish with increase in the polarity within the SiC → SnC row. The comparison of the values of c_{ij} obtained here for 3C-SiC with results of calculation as per Keating (Table 1) show good numerical consistence for c_{11} and c_{44}, obtained by using the Hermann–Skillman tables in the calculation option 2, whereas the values c_{12} differ in 1.5 times (see Table 1). Here, we shall again doubt the results of the study [5]. Additional argument in favor of such doubts is that the universal ratio obtained as per Harrison $c_{11} : c_{12} : c_{44} = 1 : 0.31 : 0.44$ qualitatively corresponds to all the calculation options as per Keating. The only exclusion the SiC-2 curve, which is marked in the Fig. 1 by black squares and based on using the date from the paper [5]. Next, as per Harrison we have $A' = 1.62$ and $A = 0.78$, whereas as per Keating the average values of Table 1 are $A' = 1.76$ and $A = 0.65$. It also means the vicinity of the results provided by the two models under study.

Now, let us come to the hexagonal compounds. As per [18,30], the elastic constants take the following form:

$$c_{11}^W = \bar{c}_{11}^W - \Delta^2/\bar{c}_{44}^W, \quad c_{33}^W = \bar{c}_{33}^W,$$

$$c_{44}^W = \bar{c}_{44}^W - \Delta^2/\bar{c}_{66}^W, \quad c_{66}^W = \bar{c}_{66}^W - \Delta^2/\bar{c}_{44}^W,$$

$$c_{12}^W = \bar{c}_{12}^W + \Delta^2/\bar{c}_{44}^W, \quad c_{13}^W = \bar{c}_{13}^W, \tag{14}$$

where $\Delta = (1/3\sqrt{2})(c_{11} - c_{12} - 2c_{44})^{\text{ZB}}$ and

$$\bar{c}_{11}^W = (c_{11} + c_{12} + 2c_{44})^{\text{ZB}}/2,$$

$$\bar{c}_{33}^W = (c_{11} + 2c_{12} + 4c_{44})^{\text{ZB}}/3,$$

$$\bar{c}_{44}^W = (c_{11} - c_{12} + c_{44})^{\text{ZB}}/3,$$

$$\bar{c}_{66}^W = (c_{11} - c_{12} + 4c_{44})^{\text{ZB}}/6,$$

$$\bar{c}_{12}^W = (c_{11} + 5c_{12} - 2c_{44})^{\text{ZB}}/6,$$

$$\bar{c}_{13}^W = (c_{11} + 2c_{12} - 2c_{44})^{\text{ZB}}/3. \tag{15}$$

Note that the correction for the internal stresses $\Delta^2/\bar{c}_{44}^W$ is similar to the correction D in the formulas (3), while the correction $\Delta^2/\bar{c}_{66}^W$ corresponds to the second summand in the expression for c_{44} in (3). The calculation results are shown in Table 8, from which it follows, firstly, that all the elastic constants diminish in the SiC → SnC row, as in the cubic compounds. Secondly, the relationships c_{ij}^W/c_{11}^W are universal, i.e. they do not depend on a specific

Table 8. Harrison's model, the wurtzite structure: the values of the elastic constants c_{ij}^W (in units of GPa) and the relative elastic constants c_{ij}^W/c_{11}^W. The upper row of the values corresponds to using the tables of the Mann atomic terms [29], the lower row — using the tables of the Hermann–Skillman atomic terms [16]

3D XC	c_{11}^W	c_{33}^W	c_{44}^W	c_{66}^W	c_{12}^W	c_{13}^W
SiC	337	347	116	125	86	77
	359	369	123	134	92	81
GeC	251	258	86	94	64	56
	277	285	95	103	71	63
SnC	127	131	44	47	35	29
	146	150	50	55	37	32
c_{ij}^W/c_{11}^W	1	1.03	0.34	0.37	0.26	0.23

compound and the used tables of the atomic terms, (which follows from the formulas (13)–(15)). Moreover, the obtained values of c_{ij}^W/c_{11}^W quantitatively agree with the calculation results as per Keating (Fig. 2). Again, the only deviation the calculation results as per the option 2. Unfortunately, direct comparison with the experimental values c_{ij}^W is excluded even for the silicon carbide, since, as it is known to the author, the 2*H*-SiC single crystals are still not produced. In connection therewith, invariants may turn out to be useful combinations of the elastic constants, whose value does not change when transferring from the sphalerite to wurtzite, to be constant for all the hexagonal polytypes *NH*, where *N* is equal, for example, to 2, 4, 6, 8 [30]:

$$(c_{11}+c_{12})^{NH} = 2(c_{11}+2c_{12}+c_{44})^{\text{ZB}}/3,$$

$$c_{33}^{NH} = (c_{11}+2c_{12}+4c_{44})^{\text{ZB}}/3,$$

$$c_{13}^{NB} = (c_{12}+2c_{12}-2c_{44})/3. \tag{16}$$

Thus, for example, taking up the experimental values $c_{11}^{\text{ZB}} = 390$, $c_{12}^{\text{ZB}} = 142$ and $c_{44}^{\text{ZB}} = 256$ GPa [23], we obtain $(c_{11}+c_{12})^{NH} = 620$, $c_{33}^{NH} = 566$ and $c_{13}^{NH} = 54$ GPa. However, the invariants (16) are insufficient to determine a full set of the values c_{ij}^W.

The sound velocities $v_{L(T)A}^{[ijk]}$ and their relative values $v_{L(T)A}^{[ijk]}/v_{LA}^{[100]}$ calculated by the formulas (6) and (7) for the cubic crystals are given in Table 9. Comparison with the calculations as per Keating (see Table 4 and Fig. 3) shows practical identity of the results obtained.

Table 9. Harrison's model, the sphalerite structure: the sound velocities $v_{L(T)A}^{[ijk]}$ (in units of km/s) and the relative velocities $(v_{L(T)A}^{[ijk]})^* = v_{L(T)A}^{[ijk]}/v_{LA}^{[100]}$. The upper row corresponds to using the tables of the Mann atomic terms [29], the lower row — using the tables of the Hermann–Skillman atomic terms [16]

3D *XC*	$v_{LA}^{[100]}$	$v_{LA}^{[110]}$	$v_{LA}^{[111]}$	$v_{TA}^{[100]}$	$v_{TA}^{[110]}$	$v_{TA}^{[111]}$
SiC	9.8 10.1	11.0 11.3	10.4 10.7	6.5 6.7	5.7 5.9	6.0 6.2
GeC	6.3 6.6	7.0 7.4	6.7 7.0	4.2 4.4	3.7 3.9	3.9 4.1
SnC	4.2 4.5	4.7 5.1	4.5 4.8	2.8 3.0	2.5 2.7	2.6 2.8
$(v_{L(T)A}^{[ijk]})^*$	1	1.12	1.06	0.67	0.59	0.61

Table 10. Harrison's model, the sphalerite structure: the Grüneisen constant γ^*, the dependences of the compression module on the pressure $\tilde{B}' = \partial\tilde{B}/\partial p$, the linear coefficient of thermal expansion α_T (in units of $10^{-6}\,\text{K}^{-1}$) and the dependence of the bulk compression module on the temperature $\partial B(T)/\partial T$ and $B^{-1}\partial B(T)/\partial T$ (in unis of 10^{-4} GPa/K and $10^{-4}\,\text{K}^{-1}$)

3D *XC*	γ^*	$\tilde{B}'$	α_T	$-\partial B(T)/\partial T$	$-B^{-1}\partial B(T)/\partial T$
SiC	1.58 1.54	3.16 3.08	6.3 5.8	110 103	0.66 0.58
GeC	1.60 1.54	3.20 3.08	7.3 6.4	97 88	0.78 0.64
SnC	1.69 1.62	3.37 3.23	11.2 9.4	81 73	1.27 1.01

Now, let us consider the evaluations of the anharmonic properties of the cubic crystals *XC*. As it is shown in [31], the dependences of the bulk moduli on the pressure $\tilde{B}'$ and the temperature *T* and the thermal expansion coefficient α_T are specified by the following expressions:

$$\tilde{B}' = 2\gamma^*, \quad \partial B(T)/\partial T = -3\sqrt{3}k_{\text{B}}Q/32d^3,$$

$$\alpha_T = 9k_{\text{B}}\gamma^*/32V_2\alpha_c^3, \tag{17}$$

where k_{B} the Boltzmann constant, $\gamma^* = (3-\alpha_p^2-2\alpha_p^4)/2\alpha_c^2$ the Grüneisen constant and $Q = (29-6\alpha_p^2-71\alpha_p^4+44\alpha_p^6+4\alpha_p^8)/\alpha_c^4$. Note that the expressions for $\partial B(T)/\partial T$ and α_T are obtained in the high-temperature limit. Results of the calculation are summarized in Table 10. For 3*C*-SiC the evaluations [32,33] provide $\gamma^* \approx 1$, which in 1.5 times lower than our result. On the other hand, the experimental values $\tilde{B}' = 3.57$ [34] and 2.9–4.0 [33,35] for 3*C*-SiC well agree with our evaluation. The same refers to the thermal expansion, too: for the high temperatures the experiment provides $\alpha_T \sim 5\cdot10^{-6}\,\text{K}^{-1}$ [2,35–37]. As per [32] and [38], for 3*C*-SiC we have, respectively, $\partial B(T)/\partial T \sim -250$ and ~ -290 (in units of 10^{-4} GPa/K), which significantly exceeds the value obtained by us. This situation may be corrected by inputting interatomic short-range repulsion into the Harrison's model [39,40]. At this, however, the universal dependences annihilate and the formulas are somewhat complicated. That is why we have neglected this correction, so have we taking into account metallicity of the interatomic bonds [16,17].

3.2. 2D structures

The elastic properties of the graphene-like compounds in the Harrison's model are described in the paper [27]. Besides the crystallography, the 3D and 2D compounds differ in bond hybridization: the first case includes usage of the sp^3-orbitals, while the second one — the sp^2-orbitals. For the sp^2-hybridization the covalence energy is equal to $\overline{V}_2 = 3.26(\hbar^2/m\overline{d}^2)$ [17], where $\overline{d} = 1.77$, 1.86 and 2.05 Å for 2D SiC, GeC and SnC [9], while the polar energy $\overline{V}_3 = |\overline{\varepsilon}_h^X - \overline{\varepsilon}_h^C|/2$, where $\overline{\varepsilon}_h^{X(C)} = (\varepsilon_s^{X(C)} + 2\varepsilon_p^{X(C)})/3$ (as in the item 2.2, all the 2D characteristics will be provided

Table 11. Harrison's model, 2D: the covalence $\bar{V}_2$ and polar $\bar{V}_3$ energies (in units of eV), the band covalence $\bar{\alpha}_c$, $\bar{k}_0$ — the force constant of the central interaction (in units of eV/Å^2), the linear coefficient of thermal expansion α_T (in units of $10^{-6}\,\mathrm{K}^{-1}$) and the dependence of the compression module on the temperature $\partial B(T)/\partial T$ (in units of 10^{-4} GPa/K)

3D XC	$\bar{V}_2$	$\bar{V}_3$	$\bar{\alpha}_c$	$\bar{k}_0$	$\bar{k}_0$	$\bar{\alpha}_T$	$-\partial\bar{B}(T)/\partial T$
					$\alpha_c = 1$		
SiC	7.93	1.93 1.48	0.97 0.99	8.66 9.62	10.12	11	0.66
GeC	7.18	1.95 1.39	0.97 0.99	7.10 7.89	8.30	12	0.72
SnC	5.91	2.24 1.85	0.93 0.95	3.92 4.30	5.63	15	0.90

with the overline). The numerical values of the energies $\bar{V}_2, \bar{V}_3$ and the bond covalences $\bar{\alpha}_c$ are give in Table 11. By neglecting the metallicity of bonds in [27,41], we obtain the force constants of the central $\bar{k}_0$ and noncentral $\bar{k}_1$ interactions in $\bar{k}_0 = 4\bar{\alpha}_c\bar{V}_2(2\alpha_c^2-1)/d^2$, $\bar{k}_1 = \bar{\lambda}\bar{k}_0/3$, where the constant $\bar{\lambda} = 0.66$ is the 2D analog of the 3D constant λ [42]. The values $\bar{k}_0$, diminishing in the SiC → SnC row, are given in Table 11.

Turning to the evaluations of the anharmonic characteristics, we assume for all the compounds that $\bar{\alpha}_c = 1$. Such simplification is similar to usage of the Keating's model [13] instead of the Martin's model [15]. As per [41], we will obtain $\bar{\gamma}^* = 2$ and $\bar{B}' = 2\bar{\gamma}^* = 4$ for all the graphene-like compounds. Further on, we have:

$$\bar{\alpha}_T = 4k_\mathrm{B}/\bar{V}_2, \quad \bar{B}^{-1}\big(\partial\bar{B}(T)/\partial T\big) = -24k_\mathrm{B}/\bar{V}_2. \tag{18}$$

The numerical values $\bar{\alpha}_T$ and $\bar{B}^{-1}\big(\partial\bar{B}(T)/\partial T\big)$ are given in Table 11. Thus, for the 2D structure $\bar{\alpha}_T$ is in two times bigger than for 3D. According to our evaluations [41] based on the results of the paper [43], within the temperature range $900-2100\,\mathrm{K}$ for graphene the middle value $\bar{B}^{-1}\big(\partial\bar{B}(T)/\partial T\big) \sim -0.5\cdot 10^{-4}\,\mathrm{K}^{-1}$, which perfectly agrees with our results. The value $|\bar{B}^{-1}\big(\partial\bar{B}(T)/\partial T\big)|$ is growing when transferring from SiC to SnC. The same dependence is for the 3D compounds, too (see Table 10). Note the vicinity of the values $\bar{B}^{-1}\big(\partial\bar{B}(T)/\partial T\big)$ for 2D and 3D structures.

4. Concluding remarks

The Keating's model quite adequately describes the elastic properties of the tetrahedral crystals, as meant by an approximate fulfilment of the condition (2) for a number of the $A_N B_{8-N}$ semiconductor compounds. A weak side of this model is that it is necessary to determine a value of the force constants by the experimental values c_{ij} (which refers to all the models with force constants). The Harrison's model somewhat more poorly describes the $A_N B_{8-N}$ elasticity, but has only three parameters (the lattice constant and the energy terms of the s- and p-states of the A and B atoms), with neither of them being adjustable. Furthermore, the Harrison's model allows evaluating the temperature impact on the elasticity. The present study shows that both the models are quite suitable for describing the elasticity of the XC compounds.

The principle difference of the Keating and Harrison approaches is correlated to modeling the noncentral forces. In the Keating's model, the force constant β corresponds to a crystal reaction to the change of the angle between the two neighboring σ-bonds (an angular stiffness) belonging to one atom. In the Harrison's model, the angles between the neighboring sp^k-orbitals centered at the same atom, are considered to be fixes ones (a rigid tetrahedron), while the shear deformation is contributed by misorientation of the sp^k-orbitals of the neighboring atoms making up the σ-bond.

We have had to make several simplifications in the present study. Thus, for heteropolar compounds, the Keating's model is used, so not the Martin's. The Harrison's model neglects the metallicity of bonds and short-range repulsion. Such simplifications allowed us obtaining simple analytical expressions for the elastic and thermoelastic characteristics, which are convenient for usage by experimenters and technologists. By using the obtained results, it is easy, in principle, to evaluate the characteristics of the ternary semiconductor compounds $\mathrm{Si}_{1-x}\mathrm{Ge}_x\mathrm{C}$ [44].

The 3D and 2D compounds of SnC and, above all, GeC, studied by us, are of both a theoretical and application interest. Besides the elasticity, there is a study of the electron spectrum [3,4,6–9,44,45], the magnetic properties being doped by chromium [46], thermal conductivity [8], the GeC/SiC, SnC/SiC, SnC/GeC [47] and GeC/GaN [48] superlattices are created, and application of 2D GeC in lithium batteries is under consideration [49,50].

Conflict of interest

The author declares that he has no conflict of interest.

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