

# Correlations for single-crystal elastic constants of compound semiconductors and their representation in isomechanical groups

B. Derby

*School of Materials, University of Manchester, Grosvenor Street, Manchester M1 7HS, United Kingdom*

(Received 30 November 2006; revised manuscript received 18 May 2007; published 31 August 2007)

A correlation is presented for the single-crystal elastic constants ( $C_{ij}$ ) of elemental (and IV-IV), III-V, and II-VI semiconductors with the diamond cubic, sphalerite, and wurtzite crystal structures. Both experimental data and theoretical calculations based on density functional theory follow the correlation. The elastic constants can be represented by an empirical linear relation that is a simple function of melting temperature  $T_M$  and mean atomic volume  $\Omega$  with  $C_{ij}=A_{ij}+B_{ij}(k_B T_M/\Omega)$ , where  $k_B$  is Boltzmann's constant. The empirical constants  $A_{ij}$  and  $B_{ij}$  are different for each of the groupings of semiconductors considered, which are identified as isomechanical groups. This correlation is similar in form to other correlations in the literature for diffusion data of materials that indicate the significance of the melting temperature as a scaling for lattice dynamic properties of materials.

DOI: [10.1103/PhysRevB.76.054126](https://doi.org/10.1103/PhysRevB.76.054126)

PACS number(s): 81.05.Dz

## I. INTRODUCTION

The elastic properties of semiconductors are of considerable importance in determining the residual stress state in thin film structures after processing and also for optimizing growth conditions in multilayers. Single-crystal elastic properties are difficult to measure experimentally. Well developed single crystals can be difficult to fabricate, and some phases are only stabilized in thin film form by epitaxy or other geometrical constraints. Recent developments in modeling, through the use of density functional theory (DFT) and the increased availability of computational power, have made predictions of mechanical properties *ab initio* from theoretical principles relatively straightforward. Hence it is now common to see calculations for the elastic properties of compound semiconductors and semiconductor alloys. Experimental data to verify these predictions are sparse, especially for nonequilibrium systems, and it can be difficult to interpret the accuracy of published data.

In order to assess both theoretical predictions and the quality of experimental data, it can be useful to use empirical relations that enable the extrapolation of the mechanical properties of well characterized materials to the material under study. In this paper, we investigate extending correlations that have been proposed for the elastic properties of polycrystalline materials to the single-crystal elastic constants of semiconductors. Here, we present a greater collection of data than was available to many of the earlier correlations proposed, and we demonstrate that for this correlation, there is a remarkable agreement with data within a specific crystal structure and valence state.

There have been a number of reports in the past of empirical relations describing the mechanical properties of compound semiconductors. Keyes<sup>1</sup> used dimensional analysis to propose a characteristic constant with the same dimensions as the elastic modulus that scales with the electronic charge  $e$  and the interatomic nearest neighbor spacing  $r$  with the form  $e^2/r^4$ . This relation was used to normalize the elastic constants of a range of semiconductors, and it was found that the normalized elastic properties covered a very narrow range of

values for the group IV elemental semiconductors, with similar but different narrow ranges found for III-V and II-VI compound semiconductors. Martin<sup>2</sup> used this normalizing constant and proposed that the shear elastic properties of sphalerite (zinc blende) structure semiconductors are also controlled by the relative ionicity of the bonding, which is consistent with the assumption of Keyes normalization that bonding is fundamentally electrostatic in these materials. This relation was developed further by Azuhata *et al.*<sup>3</sup> who noted that both Keyes and Martin's relations were not consistent with the elastic constants of BN or BP. Hence they introduced a further empirical dependence on lattice parameter in order to generate a better fit with data. However, this ever increasing complexity of the correlation is at odds with Occam's principle and masks any underlying physical mechanism for the correlation.

Siethoff<sup>4</sup> suggested another basis for correlation of the elastic properties of materials and the activation energies of their transport properties, based on the Debye temperature, and presented data for cubic metals and compound semiconductors. However, Siethoff's empirical relations required quite dramatic changes in form for different crystal structures, which reduces their usefulness and questions whether they rest on any physical principles. Reeber and Wang also used the Debye temperature but now used it to produce an empirical correlation for the temperature dependence of elastic properties.<sup>5</sup> Correlations for elastic properties that require the Debye temperature also contain an inherent risk of circularity of argument, because many published estimates of the Debye temperature are themselves derived from measures used to determine crystal elastic properties (e.g., the speed of sound in a material).

Simple empirical methods of predicting the physical properties of materials are of interest to research communities other than that of compound semiconductors. An extensive study of the relationship between the transport properties of materials of different crystal structure and bond chemistry was undertaken by Brown and Ashby.<sup>6</sup> They found that a more reliable correlation for physical transport properties was provided by the melting temperature rather than the De-

TABLE I. Single-crystal elastic constants, melting temperature, and lattice parameter data for diamond cubic structure elemental semiconductors. Elastic properties determined by Brillouin scattering (Br), Raman scattering (Rm), ultrasound (US), surface acoustic wave (SAW), or resonance (R). Lattice constant  $a$  and melting temperatures are taken from Landolt-Börnstein series (Refs. 9 and 10) unless otherwise referenced.

Element	$C_{11}$ (GPa)	$C_{12}$ (GPa)	$C_{44}$ (GPa)	Method	$T_M$ (K)	Lattice constant,		Ref.
						$a$ (nm)	$k_B T_M / \Omega$ (GPa)	
C	1029	238	527	SAW	3800	0.3567	9.250	11
	1080	127	576	Br				12
Ge	128.5	48.3	66.8	US	1211	0.5657	0.739	13
	128.7	48.7	66.7	US				14
Si	165.8	63.9	79.6	US	1687	0.5431	1.163	15
	160.1	57.8	80.0	<sup>a</sup>				16
$\alpha$ -Sn	69	29.3	36.2	<sup>b</sup>	505	0.6490	0.204	17

<sup>a</sup>Bulk measurements.

<sup>b</sup>Neutron diffraction.

bye temperature. This was further extended by Frost and Ashby,<sup>7</sup> who presented evidence for a very strong correlation between the elastic properties of polycrystalline solids and their melting temperature  $T_M$ , with the following empirical relationships proposed for Young's modulus,  $E$  and shear modulus  $\mu$ :

$$E = \frac{100k_B T_M}{\Omega}, \quad (1a)$$

$$\mu = \frac{44k_B T_M}{\Omega}. \quad (1b)$$

Here,  $k_B$  is Boltzmann's constant and  $\Omega$  is the atomic volume. Frost and Ashby further refined these empirical relations by studying the variation of the numerical constant in the shear modulus correlation [44 in Eq. (1b)] with material class, which is determined by crystal structure and chemical bonding. This constant was found to be approximately constant for each material class and varied from 20 for alkali metals to 95 for simple oxides with the corundum ( $\alpha$ -Al<sub>2</sub>O<sub>3</sub>) crystal structure. From this they developed the concept of the isomechanical group, which is a group of materials that display identical or very similar mechanical and transport properties when described by the appropriate empirical normalization.

In this paper, we explore the applicability of the  $k_B T_M / \Omega$  normalization for the single-crystal elastic properties of elemental and compound semiconductors. We note that Yonenaga and Suzuki have already used the parameter  $\mu\Omega/k_B$  to scale temperatures in a study of the elevated temperature mechanical properties of compound semiconductors.<sup>8</sup>

## II. SINGLE-CRYSTAL ELASTIC CONSTANTS

The group IV elemental semiconductors all form the diamond cubic crystal structure under standard conditions of

temperature and pressure. Most III-V and II-VI compound semiconductors have either the sphalerite (zinc blende) or wurtzite crystal structure under normal conditions of temperature and pressure. These have cubic and hexagonal symmetries, respectively, and thus their single-crystal elastic constants can be represented in matrix form with three and five independent terms, as given in Eq. (2) below:

$$\begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{12} & 0 & 0 & 0 \\ & & C_{11} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{44} \end{pmatrix} \quad (\text{cubic}), \quad (2a)$$

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{11} & C_{13} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & (C_{11} - C_{12})/2 \end{pmatrix} \quad (\text{hexagonal}). \quad (2b)$$

There is an extensive literature on the experimental measurement of single-crystal elastic constants of semiconductors using a range of techniques including ultrasonic transmission, surface acoustic waves, and Raman or Brillouin spectroscopy, and also from the mean square displacement of atoms determined by diffraction techniques. In recent years, many groups have published theoretical predictions for the single-crystal elastic constants of compound semiconductors based on a range of methods and techniques. The theoretical approach has become increasingly more refined with the introduction of density functional theory and easily available computing power; hence theoreticians have expressed in-

creasing confidence in these predictions. Tables I–III present a compilation of experimental data and theoretical predictions obtained for the single-crystal elastic constants of elemental and compound semiconductors. The tables also display the melting temperature and lattice parameter data for these materials, which are necessary to compute the parameter  $k_B T_M / \Omega$ .

#### A. Cubic crystal structure semiconductors

The elastic property data obtained from the elemental group IV semiconductors with the diamond cubic crystal structure are plotted against  $k_B T_M / \Omega$  in Fig. 1. This plot includes the data obtained from the only IV-IV compound included,  $\beta$ -SiC. However, to distinguish these data, they are displayed shaded in yellow at  $k_B T_M / \Omega \approx 3.96$  (light gray in print) and are not used in subsequent analysis. Visual inspection of the data shows a clear linear trend for all three elastic constants with the exception of  $C_{12}$ , where there is a significant difference between the value of  $C_{12}$  for diamond obtained by Tourlog *et al.* using Rayleigh waves generated by acoustic microscopy<sup>11</sup> and the results of Vogelgesang *et al.* using Brillouin spectroscopy.<sup>12</sup> We note that the procedure for determining  $C_{12}$  from these techniques considers a difference between experimental measurements, and this could magnify errors. The value obtained by Vogelgesang *et al.* appears to be low when its ratio to  $C_{11}$  is compared with that of other materials. Thus we remove the datum for  $C_{12}$  of diamond measured by Vogelgesang *et al.* from further analysis and signify this by the yellow color of the datum in Fig. 1 (light gray in print).

Linear regression lines have been plotted for each of the elastic constants  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$ , which result in equations of the form

$$C_{ij} = A_{ij} + B_{ij}(k_B T_M / \Omega). \quad (3)$$

The constants  $A_{ij}$  and  $B_{ij}$  are given in Table IV along with the correlation coefficient ( $R$ ) obtained from the regression analysis. The significance of the regression is given as the probability  $P$  of the null hypothesis (that there is no correlation). A value of  $P > 0.05$  is conventionally taken as indicating that the null hypothesis cannot be rejected. It is clear from Fig. 1 and Table II that Eq. (3) describes well the behavior of all three elastic constants and that the correlation is appropriate.

Figure 2(a) shows a plot of the single-crystal elastic constant data as a function of  $k_B T_M / \Omega$  for III-V compound semiconductors with the sphalerite crystal structure. These materials have, by far, the greatest number of reports of their single-crystal elastic constants both by experimental measurement and from theoretical calculations. In Fig. 2(a), experimental data points are represented by filled symbols and labeled  $C_{ij}$ , and data derived from theoretical calculation are represented by open symbols and labeled  $CC_{ij}$ . On inspecting the data in Table II, it is evident that one of the values for  $C_{12}$  of BN, reported by Sokolovskii, appears to be anomalously high.<sup>27</sup> This datum is identified in yellow on the figure (light gray in print) and was omitted from subsequent regression analysis. Also marked in yellow (light gray in print) at

$k_B T_M / \Omega \approx 3.96$  are the data for  $\beta$ -SiC. These data were also excluded from regression analysis.

As with the data from the elemental semiconductors, there is a clear linear relation evident between the elastic modulus data and  $k_B T_M / \Omega$ . In the figure, the solid lines and broken lines represent the linear regression to the experimental data and the theoretical data, respectively. There is excellent agreement between both the experimental and theoretical data when represented as scatter around the regression lines with broadly similar values of both slope and intercept for the three independent elastic constants. These results support the confidence shown in the literature for density functional theory, providing a reasonable model for crystal elastic properties. The scatter about the regression line shown by the theoretically calculated elastic property data is slightly greater than that for the experimental data; despite this, it was decided to include both experimental and theoretical data sets in computing the regression constants for III-V compounds with the sphalerite structure, and these are shown in Table IV. The significance of the regression is identical to that obtained from the elemental semiconductors. Given this, we will consider experimental and theoretical data together for subsequent analyses of other compound semiconductors.

Figure 2(b) shows an identical plot for II-VI compounds with the sphalerite structure; experimental data are displayed as filled symbols and theoretical DFT calculations are shown as open symbols. There are fewer reports in the literature for theoretical predictions for the elastic constants of this class of materials. As with the III-V data, the theoretical predictions show a greater deviation from the regression line than do the experimental data points. However, for these materials, a reasonable linear fit to the variable  $k_B T_M / \Omega$  is again found.

#### B. Wurtzite crystal structure semiconductors

The single-crystal elastic constants of III-V and II-VI semiconductor compounds that form the hexagonal wurtzite structure are plotted against  $k_B T_M / \Omega$  in Fig. 3; experimental data are displayed as filled symbols and theoretical DFT calculations are shown as open symbols. There are fewer compounds that form stable phases with this crystal structure and, in general, fewer experimental measurements or theoretical calculations of the single-crystal elastic properties have been reported in the literature for each material. Figure 3(a) shows regression lines for the five independent elastic constants of these III-V semiconductors as a function of  $k_B T_M / \Omega$ . The datum for  $C_{33}$  reported by Yamaguchi *et al.* for GaN is much lower than their value for  $C_{11}$  (Ref. 70) and is also at variance with the other published data; this datum was omitted from regression analysis and is indicated in yellow in the figure (light gray in print). The data obtained for hexagonal SiC are included in this plot (the experimental elastic property data are taken from 4H and 6H polytypes although the atomic volume and melting temperature are from the 2H polytype); the SiC data were not used in the regression analysis and are also indicated in yellow in the figure (light gray in print). All the data for the II-VI plots appeared self-consistent and are used to produce the linear

TABLE II. (a) Single-crystal elastic constants, melting temperature, and lattice parameter data for sphalerite crystal structure IV-IV, III-V, and II-VI compound semiconductors. Elastic properties determined by Brillouin scattering (Br), Raman scattering (Rm), ultrasound (US), or resonance (R). Lattice constants and melting temperatures are taken from Landolt-Börnstein series (Refs. 9 and 10) unless otherwise referenced. (b) Single-crystal elastic constants and lattice constants determined by theoretical calculation using DFT for sphalerite structure III-V, and II-VI compound semiconductors. Melting temperatures are taken from Landolt-Börnstein series (Refs. 9 and 10) unless otherwise referenced.

Compound	$C_{11}$ (GPa)	$C_{12}$ (GPa)	$C_{44}$ (GPa)	Method	$T_M$ (K)	Lattice constant,		Ref.
						$a$ (nm)	$k_B T_M / \Omega$ (GPa)	
(a) IV-IV								
$\beta$ -SiC	390	142	246	<sup>a</sup>	2973	0.4360	3.963	18 and 19
	444	148	207	Rm				20 and 21
III-V								
AlAs	119.9	57.5	56.6	Br	2013	0.5661	1.226	21
AlP	121		47.4	Br	2863	0.5463	1.940	22
AlSb	87.7	43.4	40.8	US	1325	0.6135	0.634	23 and 24
BN	820	190	480	Br	3400	0.3617	7.938	25
	831	420	450	Br				26
BP	315	100	160	Br	2800	0.4543	3.299	27
GaAs	118.4	53.7	59.1	US	1511	0.5653	0.924	28
	118.8	53.7	59.4	US				29
	119.0	54.0	59.5	Br				21
GaP	141.4	64.0	70.3	US	1743	0.5452	1.188	30
	141.2	62.5	70.5	US				31
	143.6	62.5	70.5	Br				32
	145.1	61.2	71.6	US				33
GaSb	88.3	40.2	43.2	US	986	0.6096	0.481	30
	88.4	40.3	43.2	US				29
	88.5	40.4	43.3	US				34
InAs	83.3	45.3	39.6	US	1215	0.6058	0.604	35
	88.5	40.4	43.3	US				34
InP	102.2	57.6	46.0	US	1333	0.5869	0.728	36
	101.1	56.1	45.6	US				37
	103.4	58.3	41.1	US				38
InSb	66.7	36.5	30.2	US	797	0.6479	0.324	39
	64.7	32.7	30.7	R				40
	67.2	36.7	30.2	US				34
II-VI								
BeTe	89			R	1570	0.5627	0.974	41
CdTe	53.5	36.8	19.9	R	1368	0.6481	0.555	42
	53.8	37.4	20.2	US				43
	53.5	36.8	19.9	US				44
HgSe	62.2	46.4	22.7	US	1072	0.5997	0.549	45
HgTe	53.6	36.6	21.1	US	946	0.6453	0.389	46
	54.8	38.1	20.4	US				47
	53.6	36.6	21.2	US				48

TABLE II. (*Continued.*)

Compound	$C_{11}$ (GPa)	$C_{12}$ (GPa)	$C_{44}$ (GPa)	Method	$T_M$ (K)	Lattice constant,		Ref.
						$a$ (nm)	$k_B T_M / \Omega$ (GPa)	
ZnS	104.6	65.3	46.1	R	1991	0.5405	1.393	42
	97.6	59.0	45.1	US				49
	103.2	64.6	46.2	US				50
	98.3	62.7	44.8	R				46
ZnSe	81.0	48.1	44.3	R	1799	0.5667	1.092	42
	85.9	50.6	40.6	Rm				51
	86.4			Rm				41
	88.8	52.7	41.4	US				51
ZnTe	71.3	40.7	31.2	R	1573	0.6088	0.770	42
	71.1	40.7	31.3	Rm				41
	72.2	40.9	30.3	Br				52
	73.7	42.3	32.1	US				51
(b) IV-IV								
SiC-3C	390	134	253	DFT	2973	0.4345	4.004	53
	420	126	287	DFT				19
III-V								
AIP	134	68	70	DFT	2823 <sup>b</sup>	0.5400	1.981	54
AlN	298	164	187	DFT	3023 <sup>c</sup>	0.4320	4.143	56 and 57
	313	168	192	DFT		0.4376	3.986	58
	294	160	189	DFT		0.4337	4.094	59
	314	157	200	DFT		0.4340	4.086	60
BN	837	182	493	DFT	3400	0.3590	8.119	56
	819	195	475	DFT		0.3596	8.078	58
	812	182	464	DFT		0.3591	8.111	59
	853	175	497	DFT		0.3600	8.051	60
GaAs	120.5	55.4	67.4	DFT		0.5508	0.945	61
GaN	285	161	149	DFT	2791 <sup>c</sup>	0.4537	3.299	58
	282	159	142	DFT		0.4460	3.617	56 and 57
	297	126	154	DFT		0.4460	3.617	60
GaP	147	61	79	DFT	1743	0.5340	1.264	54
	157.8	67.9	36.7	DFT		0.5358	1.251	61
GaSb	117.4	63.8	25.7	DFT		0.5939	0.520	61
InN	184	116	177	DFT	2146 <sup>c</sup>	0.4920	1.989	56 and 57
	185	107	80	DFT		0.4970	1.939	60
II-VI								
ZnSe	91.3	56.3	38.3	DFT	1799	0.5645	1.104	62
	107.2	67.5	37.2	DFT		0.5633	1.111	63
	97.8	52.5	47	DFT		0.5619	1.119	64
	95.9	53.6	48.9	DFT		0.5618	1.120	65
ZnTe	85.9	54.7	31.3	DFT	1573	0.6019	0.796	63

<sup>a</sup>From thermal conductivity data.<sup>b</sup>Reference 55.<sup>c</sup>Experimental value of the wurtzite structure.

TABLE III. (a) Single-crystal elastic constants, melting temperature, and lattice parameter data for wurtzite structure III-V and II-VI compound semiconductors. Elastic properties determined by Brillouin scattering (BR), ultrasound (US), surface acoustic wave velocity (SAW) measurement, or resonance (R). Lattice constants and melting temperatures are taken from Landolt-Börnstein series (Refs. 9 and 10). (b) Single-crystal elastic constants and lattice constants determined by theoretical calculation using DFT for wurtzite structure III-V and II-VI compound semiconductors. Melting temperatures are taken from Landolt-Börnstein series (Refs. 9 and 10) unless otherwise referenced.

Compound	$C_{11}$ (GPa)	$C_{12}$ (GPa)	$C_{13}$ (GPa)	$C_{33}$ (GPa)	$C_{44}$ (GPa)	Method	$T_M$ (K)	Lattice constant		$k_B T_M / \Omega$ (GPa)	Ref.
								$a$ (nm)	$c$ (nm)		
(a) IV-IV											
SiC-4H	507	108		547	159	Br	2973	0.3079 <sup>a</sup>	0.5053 <sup>a</sup>	3.959	45
SiC-6H	500	92		564	168	US	2973	0.3079 <sup>a</sup>	0.5053 <sup>a</sup>	3.959	66
III-V											
AlN	345	125	120	395	118	US	3023	0.3112	0.4982	3.996	67
	411	149	99	389	125	Br					68
	410	140	100	390	120	SAW					69
GaN	370	145	110	390	90	SAW	2791	0.3189	0.5186	3.376	69
	377	160	114	209	81.4	US					70
	373	141	80	387	94	Br					71
InN	190	104		182		<sup>b</sup>	2146	0.3533	0.5693	1.926	72
II-VI											
BeO	460.6	127	88	491.6	147.7	US	2840	0.2698	0.4380	5.682	73
	470	168	119	494	153	US					74
CdS	90.7	58.1	51.0	93.8	15.0	R	1678	0.4136	0.6713	0.932	42
	85.8	53.4	46.2	93.7	14.9	US					75
	85.7	53.3	46.1	93.6	14.9	US					76
CdSe	74.1	45.2	39.3	83.6	13.2	R	1537	0.4299	0.7010	0.757	42
	74.9	46.1	39.3	84.5	13.2	US					73
	74.6	46.1		81.7	13	US					77
ZnO	206		118	211	44.3	Br	2242	0.3250	0.5204	2.602	78
	210	121	105	210	45	US					79
	207	118	106	210	44.8	Res					80
ZnS	124.2	60.2	45.5	140	28.6	US	1991	0.3820	0.6260	1.390	73
	123.4	58.5	45.5	139.6	28.9	US					81
	124.2	60.2	45.4	138.1	28.6	R					82
	129.4	68.2	53.4	142.4	27.2	R					83
(b) III-V											
AlN	388	154	84	458	85	DFT	3023	0.3060	0.4910	4.194	56 and 57
	398	142	112	383	127	DFT		0.3112	0.4995	3.986	58
	410	125	79	457	104	DFT		0.3082	0.4947	4.103	59
BN	987	143	70	1020	369	DFT	3400 <sup>c</sup>	0.2540	0.4170	8.061	56
	982	134	70	1077	388	DFT		0.2534	0.4191	8.059	58
	944	149	83	1011	350	DFT		0.2531	0.4194	8.072	59
GaN	346	148	105	389	105	DFT	2791	0.3170	0.5130	3.453	56 and 57
	350	140	104	376	101	DFT		0.3210	0.5237	3.299	58
InN	220	120	91	249	36	DFT	2146	0.3530	0.5540	1.983	56 and 57

TABLE III. (Continued.)

Compound	$C_{11}$ (GPa)	$C_{12}$ (GPa)	$C_{13}$ (GPa)	$C_{33}$ (GPa)	$C_{44}$ (GPa)	Method	$T_M$ (K)	Lattice constant			Ref.
								$a$ (nm)	$c$ (nm)	$k_B T_M / \Omega$ (GPa)	
II-VI											
BeO	439	105	72	463	142	DFT	2840	0.2701	0.4387	5.660	84
	479	113	81	510	153	DFT		0.2634	0.4291	6.085	84
ZnO	218	137	121	229	38	DFT	2242	0.3199	0.5167	2.705	85

<sup>a</sup>SiC-2H data.<sup>b</sup>X-ray diffraction data.<sup>c</sup>Value for cubic structure.

regression lines in Fig. 3(b). The results of the regression for both III-V and II-VI wurtzite structure materials are presented in Table V.

Figure 3(a) shows a clear linear relation between the elastic modulus and the parameter  $k_B T_M / \Omega$  for all five independent elastic constants for the III-V semiconductors with the wurtzite structure. The significance of the correlation coefficients is similar to that found for the sphalerite structure materials save for the data for  $C_{12}$  and  $C_{13}$ . However, this is because they show little change with  $k_B T_M / \Omega$  and thus return a low correlation coefficient (or, in the case of  $C_{13}$ , a negative correlation). Given that the variance of the elastic property data appears to be the same for all elastic moduli, the lower significance for  $C_{12}$  and  $C_{13}$  is perhaps not surprising. In many ways, the excellent correlation observed with  $k_B T_M / \Omega$  for these materials is surprising, given that the melting point data for the nitride semiconductors are extrapolated from high pressure data.

The data from the wurtzite structure II-VI semiconductors are plotted in Fig. 3(b). It displays a similar strong linear correlation with  $k_B T_M / \Omega$ , with lower significance again seen with  $C_{12}$  and  $C_{13}$ , which also shows a smaller variation with  $k_B T_M / \Omega$  than is observed with  $C_{11}$ ,  $C_{33}$ , and  $C_{44}$ .

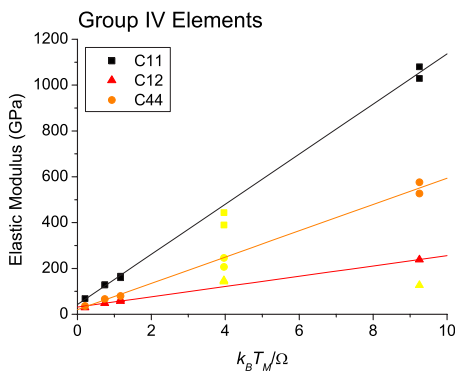


FIG. 1. (Color online) Single-crystal elastic moduli for diamond structure semiconductors (and  $\beta$ -SiC) as a function of  $k_B T_M / \Omega$ . Solid lines show linear relationships as determined by regression analysis. The datum for  $C_{12}$  from diamond is omitted from the regression analysis, as are the data for  $\beta$ -SiC at  $k_B T_M / \Omega = 3.96$ . These data are identified by a yellow color on the plot (light gray in print).

### III. DISCUSSION

The diamond structure semiconductors and sphalerite structure III-V and II-VI semiconductor data are reasonably well described by the correlation, with the III-V compounds showing normalized stiffness values close to those found with the elemental semiconductors. The only IV-IV material for which there are significant data is SiC. On comparing the data presented in Figs. 1 and 2, where SiC is plotted with  $k_B T_M / \Omega = 3.96$ , it can be seen that although the SiC data sit close to the regression line for the elemental semiconductors and the III-V sphalerite structure material, it is significantly different from those for the III-V wurtzite structure material. Thus  $\beta$ -SiC has been tentatively grouped with the elemental semiconductors. The II-VI materials show much lower values for their elastic properties when compared with the elemental IV-IV and III-V semiconductors. This indicates the difference in bonding and greater ionicity of these materials.

Frost and Ashby considered the empirical correlation of  $k_B T_M / \Omega$  with elastic properties of polycrystalline elemental group IV semiconductors. They reported a value of the slope

TABLE IV. Linear regression results from the data for diamond cubic structure semiconductors and sphalerite structure III-V and II-VI compounds.

Elastic modulus	$A_{ij}$ (GPa)	$B_{ij}$	$R$	$P$
Elements				
$C_{11}$	$43.0 \pm 8.5$	$109.3 \pm 1.7$	0.999	$< 10^{-7}$
$C_{12}$	$31.5 \pm 2.3$	$22.4 \pm 0.6$	0.999	$10^{-6}$
$C_{44}$	$20.0 \pm 8.1$	$57.4 \pm 1.6$	0.998	$< 10^{-7}$
III-V				
$C_{11}$	$12.8 \pm 10.1$	$95.8 \pm 2.8$	0.983	$< 10^{-7}$
$C_{12}$	$37.3 \pm 8.4$	$24.7 \pm 2.3$	0.861	$< 10^{-7}$
$C_{44}$	$-4.6 \pm 6.1$	$57.1 \pm 1.7$	0.982	$< 10^{-7}$
II-VI				
$C_{11}$	$31.6 \pm 3.7$	$52.6 \pm 3.8$	0.947	$< 10^{-7}$
$C_{12}$	$23.8 \pm 2.7$	$27.4 \pm 2.8$	0.908	$< 10^{-7}$
$C_{44}$	$8.5 \pm 2.3$	$28.8 \pm 2.3$	0.940	$< 10^{-7}$

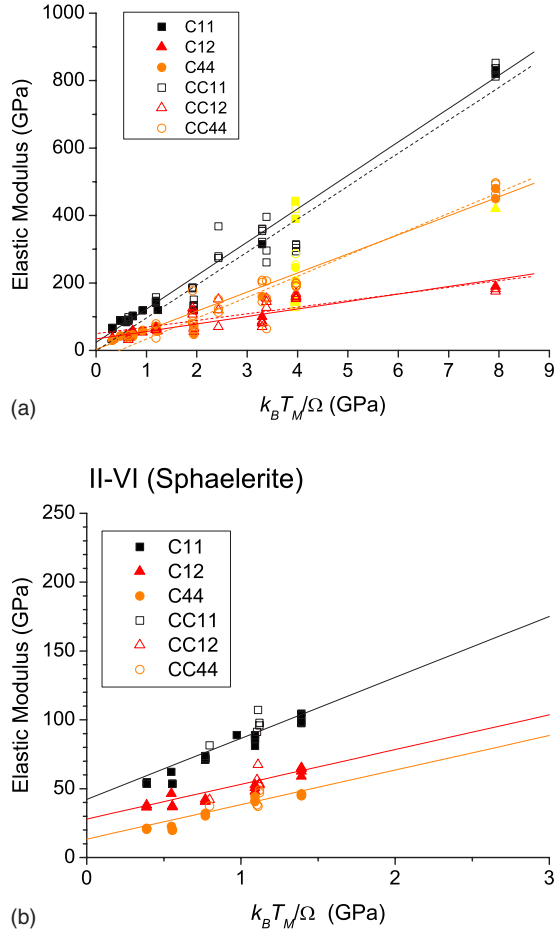


FIG. 2. (Color online) Single-crystal elastic moduli from compound semiconductors with the sphaalerite (zinc blende) crystal structure as a function of  $k_B T_M / \Omega$ . Filled symbols indicate experimental data, open symbols indicate theoretical data from DFT calculations. (a) III-V compounds: The experimental  $C_{12}$  datum from BN is omitted from the regression analysis, as are the experimental data for  $\beta$ -SiC at  $k_B T_M / \Omega = 3.96$ . These data are identified by a yellow color on the plot (light gray in print). The solid lines show the results of linear regression to the experimental data, the broken lines show linear regression to the theoretical data. (b) II-VI compounds: The solid line shows the results of the linear regression applied to the combined experimental, and theoretical data.

of the linear relation  $B = k_B T_M / \Omega = 56 \pm 17$ , where  $\mu$  is the bulk polycrystalline shear modulus.<sup>7</sup> Using the relation  $\mu = \{(1/2)[C_{44}(C_{11} - C_{22})]\}^{1/2}$  and the values of  $B$  [Eq. (3)] in Table IV for the single-crystal elastic properties of group IV semiconductors, we obtain the following value of our linear constant for the polycrystalline shear modulus:  $B = k_B T_M / \Omega = 49 \pm 3$ . Considering that the results obtained by Frost and Ashby used only Si and Ge as their source data and that they appear to have forced the relation through an intercept of zero, these two values are reasonably consistent.

The sphaalerite and wurtzite structures differ only in their second nearest neighbor and higher order coordination. Thus it is reasonable to assume that they should have similar ranges to their elastic properties. Martin made this observation and he derived a geometric transformation for the crystal properties of the sphaalerite structure to an equivalent rhom-

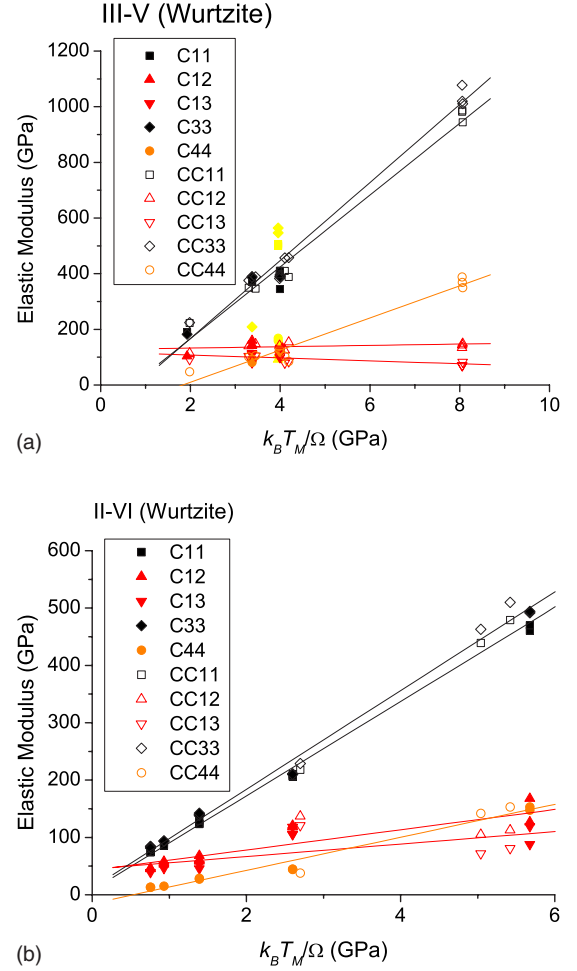


FIG. 3. (Color online) Single-crystal elastic moduli from compound semiconductors with the wurtzite crystal structure as a function of  $k_B T_M / \Omega$ . Filled symbols indicate experimental data, open symbols indicate theoretical data from DFT calculations. Solid lines show linear relationship as determined by regression analysis to the combined experimental, and theoretical data. (a) III-V compounds: The anomalous InN, and GaN data are indicated in yellow (light gray in print), and omitted from the regression analysis, as are the data for  $\alpha$ -SiC at  $k_B T_M / \Omega = 3.96$ . (b) II-VI compounds.

bohedral lattice with crystal axes parallel to those of the wurtzite structure.<sup>86</sup> This transformation for the single-crystal stiffness tensor is given, using Wright's simpler formulation,<sup>87</sup> by

$$C_{11,w} = \frac{1}{6}(3C_{11,s} + 3C_{12,s} + 6C_{44,s}) - \frac{3\Delta^2}{(C_{11,s} - C_{12,s} + C_{44,s})}, \quad (4a)$$

$$C_{12,w} = \frac{1}{6}(C_{11,s} + 5C_{12,s} - 2C_{44,s}) + \frac{3\Delta^2}{(C_{11,s} - C_{12,s} + C_{44,s})}, \quad (4b)$$

$$C_{13,w} = \frac{1}{6}(2C_{11,s} + 4C_{12,s} - 4C_{44,s}), \quad (4c)$$



TABLE V. Linear regression results from the wurtzite structure compound semiconductors plotted in Fig. 3.

Elastic modulus	$A_{ij}$ (GPa)	$B_{ij}$	$R$	$P$
III-V				
$C_{11}$	$-92.2 \pm 28.3$	$129.1 \pm 6.0$	0.985	$< 10^{-7}$
$C_{33}$	$-113.3 \pm 27.3$	$140.2 \pm 5.7$	0.989	$< 10^{-7}$
$C_{12}$	$128.1 \pm 8.9$	$2.4 \pm 1.9$	0.320	0.20
$C_{13}$	$118.3 \pm 9.0$	$-5.2 \pm 1.8$	-0.618	$6.0 \times 10^{-3}$
$C_{44}$	$-105.5 \pm 15.0$	$57.8 \pm 3.1$	0.982	$< 10^{-7}$
II-VI				
$C_{11}$	$8.1 \pm 4.5$	$82.2 \pm 1.5$	0.994	$< 10^{-7}$
$C_{33}$	$11.9 \pm 6.3$	$86.0 \pm 2.1$	0.990	$< 10^{-7}$
$C_{12}$	$42.7 \pm 8.5$	$17.7 \pm 2.9$	0.719	$7.6 \times 10^{-4}$
$C_{13}$	$44.8 \pm 10.4$	$10.9 \pm 3.4$	0.406	$4.7 \times 10^{-4}$
$C_{44}$	$-15.3 \pm 4.2$	$28.9 \pm 1.4$	0.962	$< 10^{-7}$

$$C_{33,w} = \frac{1}{6}(2C_{11,s} + 4C_{12,s} + 8C_{44,s}), \quad (4d)$$

$$C_{44,w} = \frac{1}{6}(2C_{11,s} - 2C_{12,s} + 2C_{44,s}) - \frac{6\Delta^2}{(C_{11,s} - C_{12,s} + 4C_{44,s})}, \quad (4e)$$

$$\text{and } \Delta = \frac{\sqrt{2}}{6}(C_{11,s} - C_{12,s} - 2C_{44,s}), \quad (4f)$$

where the subscripts  $s$  and  $w$  refer to the sphalerite and wurtzite structures, respectively. Note that the inverse transformation from the wurtzite to sphalerite structure is not exact and requires an approximation to obtain average values from the three nonequivalent orthorhombic axial directions.<sup>64</sup> The proposed correlation allows a better test of Martin's hypothesis in that there is a relation between the mechanical properties of the wurtzite and sphalerite structures through comparing the two data sets across a range of values of the parameter  $k_B T_M / \Omega$ .

In Fig. 4, we present all the data for the II-V and II-VI compounds with the sphalerite structure elastic property data resolved onto an equivalent rhombohedral lattice (open symbols) and plotted alongside the data from the wurtzite structure compounds (filled symbols). The transformed and normalized data clearly demonstrate the close mechanical equivalence of all III-V and II-VI compound semiconductors when transformed to a common set of crystal axes and scaled using the parameter  $k_B T_M / \Omega$ . Closer inspection of the data shows that there are differences in the behavior of the wurtzite and transformed sphalerite data sets. The regression gradients for  $C_{11}$  and  $C_{33}$  for the III-V compounds appear significantly different, as do the gradients for  $C_{12}$  and  $C_{13}$  for both III-V and II-VI compounds. In order to formally test the hypothesis that the transformed sphalerite data are equivalent

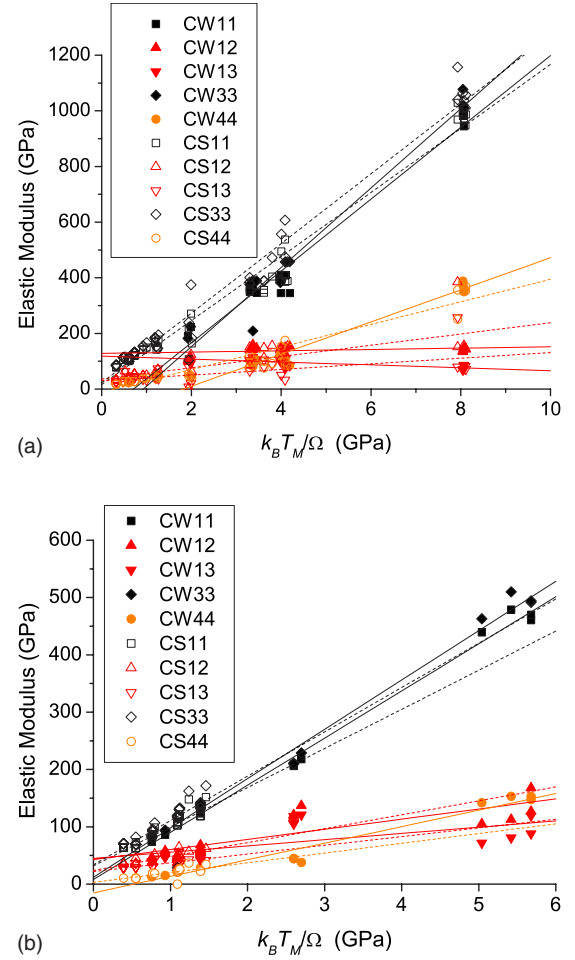


FIG. 4. (Color online) Single-crystal elastic moduli from semiconductors with the wurtzite crystal structure (filled symbols, and continuous regression lines) and data from sphalerite crystal structure materials transformed onto an equivalent rhombohedral lattice (open symbols, and broken regression lines), as a function of  $k_B T_M / \Omega$ . (a) III-V and (b) II-VI compounds.

to the wurtzite data in its relationship with the parameter  $k_B T_M / \Omega$ , an analysis of covariance (ANCOVA) was carried out on the data.

By using ANCOVA, we are assuming that the deviation from the regression displayed by the covariates is approximately normally distributed and that both sets of data have similar variance and regression slopes. The results of the ANCOVA are presented in Table VI in the form of two probability values,  $P_1$  and  $P_2$ .  $P_1$  represents the probability of the null hypothesis that the two regressions (of the wurtzite data and of the transformed sphalerite data) have different slopes, and  $P_2$  tests the null hypothesis that the data sets have the same means (and hence intercepts if the first null hypothesis is satisfied). From the III-V ANCOVA results, we can see that the null hypothesis of common regression slopes can be rejected for all the data using a 5% significance threshold. The II-VI data give different results for  $P_1$ , not allowing the rejection of the null hypothesis with the 5% significance threshold for all save the  $C_{44}$  data. However, in all cases, the  $P_2$  values are such as to reject a common mean and hence coincidence of the data sets.

TABLE VI. ANCOVA results from the data showing the variation of single-crystal elastic constants of semiconductors with  $k_B T_M / \Omega$  for wurtzite structure and sphalerite structure transformed onto an equivalent rhombohedral lattice by Martin's transformation (Ref. 86): (a) III-V semiconductors and (b) II-VI semiconductors.

Elastic modulus	$P_1$	$P_2$
	III-V	
$C_{11}$	$4.5 \times 10^{-2}$	$2.4 \times 10^{-3}$
$C_{12}$	$1.0 \times 10^{-3}$	$1.1 \times 10^{-1}$
$C_{13}$	$1.0 \times 10^{-5}$	$4.4 \times 10^{-2}$
$C_{33}$	$2.5 \times 10^{-2}$	$2.0 \times 10^{-5}$
$C_{44}$	$4.0 \times 10^{-4}$	$5.1 \times 10^{-2}$
	II-VI	
$C_{11}$	0.11	$1.3 \times 10^{-3}$
$C_{12}$	0.34	$3.3 \times 10^{-2}$
$C_{13}$	0.61	$4.9 \times 10^{-3}$
$C_{33}$	0.61	$7.00 \times 10^{-4}$
$C_{44}$	0.02	$1.2 \times 10^{-2}$
	III-V nitrides	
$C_{11}$	0.71	0.42
$C_{12}$	0.28	0.46
$C_{13}$	0.07	0.70
$C_{33}$	0.54	0.02
$C_{44}$	0.56	0.29

However, it should be noted that the III-V data are not truly continuous across the range of  $k_B T_M / \Omega$ . For values of  $k_B T_M / \Omega > 2$ , all the semiconductors are nitrides. The lower part of Table VI displays the ANCOVA results obtained for the wurtzite and sphalerite structures of the nitride semiconductors in isolation. Using the 5% probability significance threshold, this indicates that the elastic constants  $C_{11}$ ,  $C_{12}$ ,  $C_{13}$ , and  $C_{44}$  can be considered as following the same regression line, with the  $C_{33}$  data showing a similar regression slope although with a statistically significant difference in the means. This is reasonably strong evidence that there is some equivalence between the mechanical properties of the sphalerite and wurtzite structure III-V nitride semiconductors. However, this result must be treated with caution because there is little experimental data from both crystal structures and much of the theoretical data are concerned with comparing wurtzite and sphalerite structure properties using similar models and assumptions. Thus there is a possibility that the similarity of the two crystal structures for the III-V nitrides indicated by the ANCOVA results may be an artifact.

Frost and Ashby proposed the concept of the *isomechanical group*,<sup>7</sup> building on the earlier work of Brown and Ashby who investigated correlations for the transport and mechanical properties of materials.<sup>6,88</sup> They hypothesized that within a given isomechanical group, there are a number of simple correlations of material properties which are constant. This earlier work investigated the physical properties of polycrystalline materials. In this work, we have found a similar correlation for the single-crystal elastic properties of semicon-

ductor materials using the grouping of material constants  $k_B T_M / \Omega$ . We can tentatively identify isomechanical groups appropriate for semiconductor elastic properties based on literature data for

- (a) elemental semiconductors and IV-IV compounds,
- (b) III-V sphalerite structure materials,
- (c) III-V wurtzite structure materials (with possible evidence for the III-V nitrides being a distinct subset),
- (d) II-VI sphalerite structure materials, and
- (e) II-VI wurtzite structure materials.

Finally, we consider the physical implications of the proposed correlation for the elastic constants of semiconductors. Frost and Ashby indicate through an analysis of data that the melting temperature is the dominant term in the scaling relation, with the atomic volume acting as a second order effect.<sup>7</sup> The fractional range of values displayed by mean atomic volume in relatively densely packed structures is significantly lower than the range of melting temperature. Thus the greater dependence on melting temperature could simply be a function of the relative range of values spanned by the parameters. This could be tested further by studying the mechanical properties of more open cage structures, e.g., zeolites, but there is little mechanical property or melting data available for these materials.

The parameter product  $C_{ij} \Omega$  is an indication of the stored mechanical energy as a function of bond or unit cell deformation. Similarly,  $k_B T$  represents the thermal energy stored in the structure. The correlation  $k_B T_M / C_{ij} \Omega$  therefore implies some equivalence of the stored thermal energy at the melting temperature and the maximum stored mechanical energy (because for a given crystal structure, the ideal strength of a solid is related to the elastic modulus). Kocks *et al.*, in a monograph on the mechanical properties of materials,<sup>89</sup> considered mechanisms of plasticity in materials. Starting from simple principles such as the intrinsic lattice vibrations of a solid, they concluded that an appropriate temperature normalization for dislocation mechanisms has the form  $k_B / \mu \Omega$ , where  $\mu$  is the shear modulus, and that  $k_B T_M / \mu \Omega$  could be considered a structure insensitive material parameter. It has also been observed for some time that the diffusion constants of crystalline materials converge to very similar values at the melting temperature,<sup>90</sup> the so-called equivalence of melting point diffusivity, indicating that at the melting point certain properties of the crystal lattice converge to common values. Diffusion activation energies are also known to correlate strongly with  $k_B T_M$ .<sup>6</sup> Thus the observed correlation of mechanical properties and melting temperature is consistent with other experimental observations of the equivalence of physical or lattice properties at the melting point of materials.

There is substantial discussion in the literature concerning deviations from Vegard's law and whether the assumed linear dependence of alloy physical properties on lattice parameter is reasonable. An obvious question of considerable practical importance is whether the correlation discussed here can be extended to the mechanical properties of alloys. Frost and Ashby state in their monograph that this could be done by replacing the melting temperature of the compound or element,  $T_M$ , with the solidus temperature of the alloy at a given composition.<sup>7</sup> However, it is not clear that this correlation

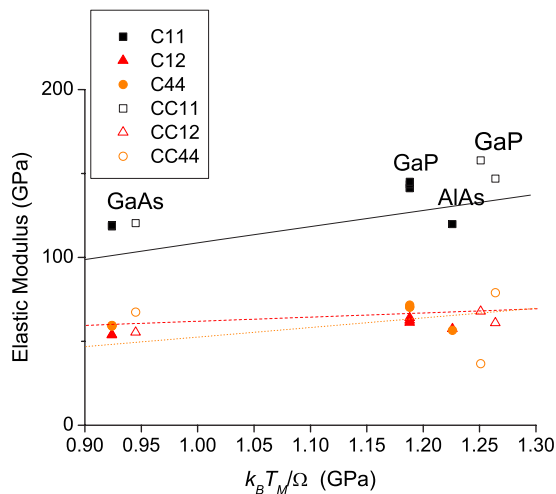


FIG. 5. (Color online) This is an enlargement of the parameter space for the proposed correlation of the elastic properties of III-V sphalerite structure semiconductors, identifying the properties of GaAs and AlAs. Regression lines are as follows:  $C_{11}$ , solid;  $C_{12}$ , dashes; and  $C_{44}$ , dots.

will apply to alloy systems through the simple substitution of the solidus temperature for the unique compound melting temperature. In alloy systems, Gibbs' phase rule states that the solid is in equilibrium with a liquid of different chemical composition and it is not clear whether a scaling with the atomic volume of the solid would be appropriate. In principle, a direct test of this hypothesis could be attempted for semiconductors if there is a robust data set for the variation in physical properties of compound semiconductor alloys. Such data exist for  $\text{Ga}_x\text{Al}_{(1-x)}\text{As}$ ,<sup>91,92</sup> but unfortunately AlAs and GaAs show roughly equal and opposite deviation from the regression lines. This is clearly seen in Fig. 5, which is an enlargement of Fig. 2(a), focusing on the properties of GaAs and AlAs but now showing the regression lines for theoretic

cal and experimental data combined. GaAs shows a positive deviation from the correlation line for both  $C_{11}$  and  $C_{44}$ , and AlAs a similar magnitude negative deviation. Only for  $C_{12}$  do both compounds sit close to the regression value. Thus for the alloy semiconductor system with the most robust data set, there is a large deviation from the correlation with only a small difference in elastic properties for the extremes of the composition of an alloy series. Further work considering the elastic properties of alloy systems is clearly needed to test whether any correlation with  $k_B T^*/\Omega$  has merit, where  $T^*$  is the solidus or some other characteristic temperature.

#### IV. CONCLUSIONS

To conclude, there is compelling evidence for a simple correlation between the single-crystal elastic properties, melting temperature, and mean atomic volume of the compound and elemental semiconductors. The correlation also provides evidence for the mechanical properties of compound semiconductors to be divided into five isomechanical groups consisting of the elemental group IV materials with diamond cubic crystal structure, III-V sphalerite structure materials, III-V wurtzite structure materials (with a possible subgroup of the nitride semiconductors), II-VI sphalerite structure materials, and II-VI wurtzite structure materials, with IV-IV sphalerite structure materials tentatively assigned to the elemental semiconductor group. The correlation identified for the single-crystal elastic properties of elemental semiconductors is found to be consistent with earlier published data for the elastic properties of polycrystalline materials.

This correlation is similar to other correlations observed for lattice dynamic properties such as diffusion and phonon interactions with dislocations. These observations suggest that there is convergence in these properties for a given crystal structure as we approach a material's melting temperature.

- <sup>1</sup>R. W. Keyes, J. Appl. Phys. **33**, 3371 (1962).
- <sup>2</sup>R. M. Martin, Phys. Rev. B **1**, 4005 (1970).
- <sup>3</sup>T. Azuhata, T. Sota, and K. Suzuki, J. Phys.: Condens. Matter **8**, 3111 (1996).
- <sup>4</sup>H. Siethoff, Phys. Status Solidi B **222**, 25 (2000).
- <sup>5</sup>R. R. Reeber and K. Wang, MRS Internet J. Nitride Semicond. Res. **6**, 1 (2001).
- <sup>6</sup>A. M. Brown and M. F. Ashby, Acta Metall. **28**, 1085 (1980).
- <sup>7</sup>H. J. Frost and M. F. Ashby, *Deformation-mechanism Maps* (Pergamon, Oxford, 1982).
- <sup>8</sup>I. Yonenaga and T. Suzuki, Philos. Mag. Lett. **82**, 535 (2002).
- <sup>9</sup>U. Roessler, *II-VI and I-VII Compounds; Semimagnetic Compounds* (Springer, Heidelberg, 1999).
- <sup>10</sup>U. Roessler and D. Strauch, *Group IV Elements, IV-IV and III-V Compounds* (Springer, Heidelberg, 2001).
- <sup>11</sup>A. Tourlog, L. Wei, and J. D. Achenbach, Appl. Phys. Lett. **69**, 3680 (1996).
- <sup>12</sup>R. Vogelgesang, A. K. Ramdas, S. Rodriguez, M. Grimsditch, and T. R. Anthony, Phys. Rev. B **54**, 3989 (1996).
- <sup>13</sup>H. J. McSkimin and P. Andreatch, Jr., J. Appl. Phys. **34**, 651 (1963).
- <sup>14</sup>V. M. Beilin, Y. K. Vekilov, A. E. Kadyshev, and O. M. Krasilni, Sov. Phys. Solid State **10**, 1226 (1968).
- <sup>15</sup>H. J. McSkimin and P. Andreatch, Jr., J. Appl. Phys. **35**, 2161 (1964).
- <sup>16</sup>S. P. Nikanorov, Y. A. Burenkov, and S. A. P., Sov. Phys. Solid State **13**, 2516 (1972).
- <sup>17</sup>D. L. Price, J. M. Rowe, and R. M. Nicklow, Phys. Rev. B **3**, 1268 (1971).
- <sup>18</sup>G. A. Slack, J. Appl. Phys. **35**, 3460 (1964).
- <sup>19</sup>W. R. L. Lambrecht, B. Segall, M. Methfessel, and M. van Schilfgaarde, Phys. Rev. B **44**, 3685 (1991).
- <sup>20</sup>D. W. Feldman, J. H. Parker, W. J. Choyke, and L. Patrick, Phys. Rev. **173**, 787 (1968).
- <sup>21</sup>M. Krieger, H. Sigg, N. Herres, K. Bacher, and K. Köhler, Appl. Phys. Lett. **66**, 682 (1995).
- <sup>22</sup>M. Grimsditch, R. Bhadra, I. K. Schuller, F. Chambers, and G. Devane, Phys. Rev. B **42**, 2923 (1990).

- <sup>23</sup>D. T. Bolef and M. Menes, *J. Appl. Phys.* **31**, 1426 (1960).
- <sup>24</sup>R. Weil, *J. Appl. Phys.* **43**, 4271 (1972).
- <sup>25</sup>M. Grimsditch, E. S. Zouboulis, and A. Polian, *J. Appl. Phys.* **76**, 832 (1994).
- <sup>26</sup>T. D. Sokolovskii, *Inorg. Mater.* **19**, 1311 (1983).
- <sup>27</sup>W. Wettleing and J. Windscheif, *Solid State Commun.* **50**, 33 (1984).
- <sup>28</sup>J. S. Blakemore, *J. Appl. Phys.* **53**, R123 (1982).
- <sup>29</sup>H. J. McSkimin, A. Jayaraman, P. Andreatch, Jr., and T. B. Bateman, *J. Appl. Phys.* **39**, 4127 (1968).
- <sup>30</sup>W. F. Boyle and R. J. Sladek, *Phys. Rev. B* **11**, 2933 (1975).
- <sup>31</sup>R. Weil and W. O. Groves, *J. Appl. Phys.* **39**, 4049 (1968).
- <sup>32</sup>S. Fray, F. A. Johnson, R. Jones, S. Kay, C. J. Oliver, E. R. J. Pike, C. Sennett, J. O'Shaughnessy, and C. Smith, edited by G. B. Wright (Springer, London, 1969), p. 139.
- <sup>33</sup>M. S. Pesin, V. S. Postnikov, S. I. Rembeza, and I. P. Yaroslavtsev, *Fiz. Tverd. Tela (Leningrad)* **18**, 1651 (1976).
- <sup>34</sup>H. J. McSkimin, W. L. Bond, G. L. Pearson, and H. J. Hrostowski, *Bull. Am. Phys. Soc.* **1**, 111 (1956).
- <sup>35</sup>D. Gerlich, *J. Appl. Phys.* **35**, 3062 (1964).
- <sup>36</sup>F. S. Hickernell and W. R. Gayton, *J. Appl. Phys.* **37**, 462 (1966).
- <sup>37</sup>D. N. Nichols, D. S. Rimai, and R. J. Sladek, *Solid State Commun.* **36**, 667 (1980).
- <sup>38</sup>D. Gerlich and M. Wolf, *High Pressure Science, and Technology* (Pergamon, Oxford, 1980).
- <sup>39</sup>L. J. Slutsky and C. W. Garland, *Phys. Rev.* **113**, 167 (1959).
- <sup>40</sup>R. F. Potter, *Phys. Rev.* **103**, 47 (1956).
- <sup>41</sup>V. Wagner, J. Geurts, T. Gerhard, T. Litz, H. J. Lugauer, F. Fisher, A. Waag, G. Landwehr, T. Walter, and D. Gerthsen, *Appl. Surf. Sci.* **123-124**, 580 (1998).
- <sup>42</sup>D. Berlincourt, L. R. Shiozawa, and H. Jaffe, *Phys. Rev.* **129**, 1009 (1963).
- <sup>43</sup>R. D. Greenough, and S. B. Palmer, *J. Phys. D* **6**, 587 (1973).
- <sup>44</sup>H. J. McSkimin, and D. G. Thomas, *J. Appl. Phys.* **33**, 56 (1962).
- <sup>45</sup>W. Martienssen and H. Walimont, *Semiconductors: Springer Handbook of Condensed Matter and Materials Data* (Springer, Berlin, 2004).
- <sup>46</sup>Y. K. Vekilov and A. P. Rusakov, *Fiz. Tverd. Tela (Leningrad)* **13**, 1157 (1971).
- <sup>47</sup>T. Alper and G. A. Saunders, *J. Phys. Chem. Solids* **28**, 1637 (1967).
- <sup>48</sup>R. Cottam and G. A. Saunders, *J. Phys. Chem. Solids* **36**, 187 (1975).
- <sup>49</sup>N. G. Einspruch and R. J. Manning, *J. Acoust. Soc. Am.* **35**, 215 (1963).
- <sup>50</sup>A. Zamebovitch, *J. Phys. (France)* **24**, 1097 (1963).
- <sup>51</sup>B. H. Lee, *J. Appl. Phys.* **41**, 2984 (1970).
- <sup>52</sup>M. Yamada, K. Yamamoto, and K. Abe, *J. Phys. D* **10**, 1309 (1977).
- <sup>53</sup>K. Karch, P. Pavone, W. Windl, D. Strauch, and F. Bechstedt, *Int. J. Quantum Chem.* **56**, 801 (1995).
- <sup>54</sup>P. Rodriguez-Hernandez and A. Munoz, *Semicond. Sci. Technol.* **7**, 1437 (1992).
- <sup>55</sup>K. Osamura and Y. Murakami, *J. Phys. Chem. Solids* **36**, 931 (1975).
- <sup>56</sup>K. Kim, W. R. L. Lambrecht, and B. Segall, *Phys. Rev. B* **53**, 16310 (1996).
- <sup>57</sup>K. Kim, W. R. L. Lambrecht, and B. Segall, *Phys. Rev. B* **56**, 7018 (1997).
- <sup>58</sup>K. Shimada, T. Sota, and K. Suzuki, *J. Appl. Phys.* **84**, 4951 (1998).
- <sup>59</sup>K. Karch and F. Bechstedt, *Phys. Rev. B* **56**, 7404 (1997).
- <sup>60</sup>F. Bechstedt, U. Grossner, and J. Furthmuller, *Phys. Rev. B* **62**, 8003 (2000).
- <sup>61</sup>B. K. Agrawal, P. S. Yadav, S. Kumar, and S. Agrawal, *Phys. Rev. B* **52**, 4896 (1995).
- <sup>62</sup>I. Hamdi, M. Aouissi, A. Qteish, and N. Meskini, *Phys. Rev. B* **73**, 174114 (2006).
- <sup>63</sup>B. K. Agrawal, P. S. Yadav, and S. Agrawal, *Phys. Rev. B* **50**, 14881 (1994).
- <sup>64</sup>J. Sorgel and U. Scherz, *Eur. Phys. J. B* **5**, 45 (1998).
- <sup>65</sup>R. A. Casali and N. E. Christensen, *Solid State Commun.* **108**, 793 (1998).
- <sup>66</sup>G. Arlt and G. R. Schodder, *J. Acoust. Soc. Am.* **37**, 384 (1965).
- <sup>67</sup>K. Tsubouchi, K. Sugai, and N. Mikoshiba, in *Ultrasonics Symposium*, edited by B. R. McAvoy (IEEE, New York, 1981), Vol. 1, p. 375.
- <sup>68</sup>L. E. McNeil, M. Grimsditch, and R. H. French, *J. Am. Ceram. Soc.* **76**, 1132 (1993).
- <sup>69</sup>C. Deger, E. Born, H. Angerer, O. Ambacher, M. Stutzmann, M. Hornsteiner, E. Riha, and G. Fischerauer, *Appl. Phys. Lett.* **72**, 2400 (1998).
- <sup>70</sup>M. Yamaguchi, T. Yagi, T. Azuhata, T. Sota, K. Suzuki, S. Chicibu, and S. Nakamura, *J. Phys.: Condens. Matter* **9**, 241 (1997).
- <sup>71</sup>M. Yamaguchi, T. Yagi, T. Sota, T. Deguchi, K. Shimada, and S. Nakamura, *J. Appl. Phys.* **85**, 8502 (1999).
- <sup>72</sup>A. U. Sheleg and V. A. Savastenko, *Izv. Akad. Nauk SSSR, Neorg. Mater.* **5**, 1598 (1979).
- <sup>73</sup>C. F. Cline, H. L. Dunegan, and G. W. Henderson, *J. Appl. Phys.* **38**, 1944 (1967).
- <sup>74</sup>C. G. Bente, *J. Am. Ceram. Soc.* **49**, 125 (1966).
- <sup>75</sup>H. J. McSkimin, T. B. Bateman, and A. R. Hutchison, *J. Acoust. Soc. Am.* **33**, 856 (1961).
- <sup>76</sup>J. A. Corll, *Phys. Rev.* **157**, 623 (1967).
- <sup>77</sup>B. Bonello and B. Fernandez, *J. Phys. Chem. Solids* **54**, 209 (1993).
- <sup>78</sup>G. Carlotti, D. Fioretto, G. Socino, and E. Verona, *J. Phys.: Condens. Matter* **7**, 9147 (1995).
- <sup>79</sup>T. B. Bateman, *J. Appl. Phys.* **33**, 3309 (1962).
- <sup>80</sup>G. Kurtze, W. Maier, K. Kempf, G. Schmieder, H. Schrey, L. Klingshirn, B. Hönerlage, and U. Rössler, *J. Phys. Soc. Jpn., Suppl.* **49**, 559 (1980).
- <sup>81</sup>E. Chang and G. R. Barsch, *J. Phys. Chem. Solids* **34**, 1543 (1973).
- <sup>82</sup>M. M. Firsova, *Fiz. Tverd. Tela (Leningrad)* **16**, 549 (1974).
- <sup>83</sup>I. A. Dan'kov, I. B. Kobayakov, and S. Y. Davydov, *Fiz. Tverd. Tela (Leningrad)* **24**, 3613 (1982).
- <sup>84</sup>V. Milman and M. C. Warren, *J. Phys.: Condens. Matter* **13**, 241 (2001).
- <sup>85</sup>Z. C. Tu and X. Hu, *Phys. Rev. B* **74**, 035434 (2006).
- <sup>86</sup>R. M. Martin, *Phys. Rev. B* **6**, 4546 (1972).
- <sup>87</sup>A. F. Wright, *J. Appl. Phys.* **82**, 2833 (1997).
- <sup>88</sup>A. M. Brown and M. F. Ashby, *Scr. Metall.* **14**, 1297 (1980).
- <sup>89</sup>U. F. Kocks, A. S. Argon, and M. F. Ashby, *Prog. Mater. Sci.* **19**, 1 (1975).
- <sup>90</sup>J. A. M. v. Liempt, *Z. Phys.* **19**, 534 (1935).
- <sup>91</sup>S. Adachi, *J. Appl. Phys.* **58**, R1 (1985).
- <sup>92</sup>S. Gehrsitz, H. Sigg, N. Herres, K. Bachem, K. Köhler, and F. K. Reinhart, *Phys. Rev. B* **60**, 11601 (1999).