Experimental doping dependence of the lattice parameter in *n*-type Ge: Identifying the correct theoretical framework by comparison with Si

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The lattice parameter of Ge films doped with phosphorus, arsenic, and antimony was measured as a function of the dopant concentration. When the observed trends are compared with similar measurements in doped Si, a clear pattern emerges in support of the Cargill-Keyes theory that computes the doping dependence of the lattice parameter as the sum of a purely electronic contribution, proportional to the absolute deformation potential for the states occupied by the dopant carriers, plus a size mismatch contribution that depends on the universal topological rigidity parameter for Si-Ge systems. It is shown that when considered from the same global perspective, *ab initio* calculations of the structural effects of doping are in remarkable agreement with the Cargill-Keyes theory.

The lattice parameter of doped semiconductors changes as a function on the dopant concentration, a fact that has been known for more than half a century [1]. The dependence is linear below the dopant solubility limit, which is typically two orders of magnitude less than the host atomic concentration. Accordingly, it is customary to define a coefficient β such that $\Delta a/a = \beta N_I$, where $\Delta a/a = (a_{\text{doped}} - a_{\text{undoped}})/a_{\text{undoped}}$, and N_I is the dopant concentration. The most obvious theory of β is based on the difference in atomic radii r_I and r_H between the dopant (I) and the host (H). This leads to [2]

$$\beta = \beta_{\text{size}} = \frac{(r_I/r_H - 1)}{N_H} = \frac{2}{N_H}\frac{\Delta R}{R}, \tag{1}$$

where N_H ($= 8/a^3$ in diamond-structure materials) is the host atomic density $\Delta R = r_I - r_H$ and $R = 2r_H$. This result is often referred to as "Vegard's law" for the lattice parameter dependence on doping. As noted by Keyes and others [3,4], however, there is an additional contribution to Δa that is purely electronic in character. Consider for example a semiconductor with a density N_I of shallow substitutional donors. A hydrostatic deformation beyond the distortion caused by the dopant-host size mismatch would change the total energy per unit volume by the amount $\Delta E = 3a_c N_I \varepsilon + \frac{9}{2}B\varepsilon^2$ [3], where ε is the strain, a_c is the so-called absolute deformation potential (ADP) associated with the conduction-band states from which the donor states are derived, and B is the bulk modulus. This expression has a minimum for a nonzero $\varepsilon = -a_c N_I/(3B)$. Thus an electronic-induced deformation must be added to the size mismatch effect, and the full doping dependence of the lattice parameter becomes [5]

$$\frac{\Delta a}{a} = \beta N_I = (\beta_{\text{size}} + \beta_{\text{e}})N_I, \tag{2}$$

where β_{size} accounts for the size mismatch effect and $\beta_{\text{e}} = -a_c/(3B)$. A similar reasoning for the case of shallow acceptors leads to an analogous equation with $\beta_{\text{h}} = a_v/(3B)$, a_v being the valence-band ADP.

Equation (2) has been proposed by Cargill *et al.* [5] and Kavanagh and Cargill [6] as an elegant way to determine the

elusive ADPs, which play a fundamental role in the theory of carrier mobilities [7,8] and in the strain dependence of band offsets [9]. Its major success has been the explanation of the counterintuitive experimental finding that the Si lattice *contracts* upon As doping, despite the prediction $\beta > 0$ from Eq. (1). However, the usefulness and even the correctness of the Cargill-Keyes (CK) theory have been challenged on multiple grounds. An important drawback is the lack of independent evidence concerning the magnitude of the size contribution β_{size}. One possibility is to use Eq. (1). Alternatively, Cargill *et al.* proposed starting from experimental values of the impurity-host bond length $R + \Delta R$ as obtained from extended x-ray absorption fine-structure spectroscopy (EXAFS). However, it is well known that the bond length of a substitutional isoelectronic impurity, such as Ge in Si or In in GaAs, is *not* related to the change in lattice parameter as in Eq. (1) because bond lengths in $Si_{1-x}Ge_x$ or $Ga_{1-x}In_xAs$ alloys do not follow Vegard's law between the end-point compounds [10,11]. In fact, if one assumes that the size contribution from a dopant atom has the same functional dependence as the size contribution from an isoelectronic impurity, it is easy to show that instead of Eq. (1) one should use [6]

$$\beta_{\text{size}} = \frac{2}{a^{**}N_H}\frac{\Delta R}{R}, \tag{3}$$

where a^{**} is the so-called topological rigidity parameter (also relaxation parameter [10]), which is $a^{**} = 0.7$ in the Si-Ge system [11,12]. However, the superior accuracy of Eq. (3) relative to Eq. (1) has never been independently confirmed.

The problem of separating the size and electronic contributions also affects *ab initio* calculations in which the change in lattice constant is obtained from optimizing the structure of large supercells containing a dopant atom [13,14]. Moreover, *ab initio* theoretical attempts to compute separately the electronic contribution [14–16] to the lattice constant change have led some to conclude that this effect is not well represented by the CK theory [14,15]. Experimentally, the application of the hole version of Eq. (2) to Ga-doped Si seems to yield a deformation potential a_v with the wrong sign [6], indirectly supporting the theoretically based claims [14,15] that the theory behind Eq. (2) may be inadequate. Even the apparent success with the Si:As system has been questioned on the basis

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that the experimental data were obtained from epitaxial films in which there is a significant shear strain component. This shear strain splits the six-degenerate valleys at the bottom of the Si conduction band, which changes the energy expression used above to compute the ADP contribution [17]. Ignoring such effects has been claimed to lead to large errors in the ADPs derived from Eq. (2). Finally, the experimental challenges in obtaining accurate measurements of β and ΔR should not be underestimated. The changes in lattice parameter are small, requiring highly doped samples with very uniform doping profiles of substitutional impurities. These are very hard to fabricate, which probably explains the disagreement between published reports. Even in the case of Si:As—perhaps the best example to date in support of the CK theory—published values for β that range from 2.5 times higher (Ref. [18]) to 5 times smaller (Ref. [19]) than reported in Ref. [5]. If we add to this the experimental uncertainties associated with EXAFS measurements of the dopant-host bond lengths, we are led to the conclusion that an experimentally validated theory of the doping dependence of the lattice parameter in elemental semiconductors is still lacking.

In this Rapid Communication, we report a study of the lattice parameter of Ge doped with P, As, and Sb. We show that a comparison of lattice constant *trends* for the same series of isoelectronic dopants—such as P, As, and Sb—in Si and Ge offers the key insights from which the correct theoretical framework to describe the effect of doping can be determined. This is because for the same concentration of any of these dopants, the electron-induced deformation should remain the same, whereas the size contribution should vary dramatically, making it possible to separate the two contributions. Moreover, since the relevant ADPs in Si and Ge correspond to different valleys and have opposite signs [9], the presence of a substantial electronic contribution should manifest itself as a systematic difference in the effect of the same dopant on Si and Ge. The conclusion from our analysis is that the experimental evidence offers strong support for the CK theory represented by Eqs. (2) and (3). Furthermore, we show that when existing *ab initio* calculations are considered from the same global perspective, a remarkable agreement emerges with the CK theory.

Our experimental study of doped Ge was greatly facilitated by the recent development of $P(GeH_3)_3$ and $As(GeH_3)_3$ precursors for *in situ* doping of Ge-on-Si epitaxial films [20–22]. These precursors promote the substitutional incorporation of the dopant at very low temperatures, leading to very high doping levels with extremely flat profiles, as required for measurements of the doping dependence of the lattice constant. We also introduce here deuterated stibine (SbD_3) as a Sb source that allows us to complete the sequence of n-type dopants in Ge. It is important to mention that electrons in n-type Ge reside in conduction-band valleys along the (111) direction of the Brillouin zone. These valleys are not split by epitaxial shear strain in (001)-oriented thin films so that—unlike the case of doped Si—no shear strain contribution to the total energy needs to be considered or corrected for in our Ge films [17].

Our samples were grown on Si(001) substrates using $Ge_{0.95}Si_{0.05}$ intermediate buffer layers to reduce the lattice mismatch with the doped film. This approach leads to higher crystal quality as compared to growth directly on Si, while

allowing for an easy determination of the lattice parameter in the doped film. Pure Ge buffers were also used at the highest Sb doping concentrations for which the x-ray diffraction (XRD) peaks for the doped film and buffer are well separated. The buffer layers were grown by gas source molecular epitaxy on 4-in. high-resistivity Si(001) wafers at temperatures near $370\,^\circ\text{C}$, using the Ge_4H_{10} and Si_4H_{10} precursors. They were subjected to a 3-min annealing step at $650\,^\circ\text{C}$ to reduce dislocations and then loaded into a separate ultrahigh vacuum chemical vapor deposition reactor. The doped films were grown at temperatures close to $330\,^\circ\text{C}$ using reactions of Ge_3H_8 and the appropriate dopant precursors $P(GeH_3)_3$, $As(GeH_3)_3$, and SbD_3. Growth details for $P(GeH_3)_3$ and $As(GeH_3)_3$ are the same as in Refs. [21,22], respectively. Details for the novel SbD_3 precursor will be published elsewhere. The average doped film thickness was 200 nm. The doping levels were determined from Hall effect and infrared spectroscopic ellipsometry (IRSE) measurements. In the case of Sb doping, the amount of Sb incorporated into the film could also be determined directly from Rutherford backscattering (RBS) experiments. Assuming a Hall factor $\gamma_H = 1$, as usually performed in semiconductor studies, we find nearly perfect agreement between RBS and Hall measurements, suggesting 100% substitutionality. On the other hand, the best estimate for the Hall factor in heavily doped Ge is $\gamma_H = 0.83$ [23,24]. Accordingly, we have used this value, which reduces the carrier concentrations by 17% relative to those obtained assuming $\gamma_H = 1$. The carrier concentrations obtained from the IRSE data are about 20% lower than the Hall values if we assume an effective mass $m^* = 0.12 m_e$, where m_e is the free-electron mass [20]. This discrepancy is reduced if one uses a higher value of the effective mass to account for nonparabolicity effects [25], although band-gap renormalization could partially compensate the nonparabolicity increase. For the purposes of this Rapid Communication we use the Hall values of the carrier concentration and estimate the concentration error as the difference between IRSE and Hall measurements.

The relaxed lattice parameter of the films was determined from XRD measurements. The in-plane $a_\parallel$ and out-of-plane $a_\perp$ lattice constants were obtained from $\theta-2\theta$ scans for the (004) reflection and reciprocal space maps (RSMs) for the (224) reflection. No epilayer tilt was detected in (004) RSMs. Figure 1 shows examples of the x-ray results for Ge:Sb, demonstrating a significant lattice expansion as a function of the doping concentration. The relaxed cubic lattice parameter was obtained from the measured $a_\parallel$ and $a_\perp$ using standard elasticity theory. We used elastic constants for bulk Ge without any correction for doping. This is a good approximation because the C_{12}/C_{11} elastic constant ratio is a very weak function of doping [26]. The results are plotted in Fig. 2. The figure includes measurements from 19 additional pure Ge films grown by a similar method on Si substrates. The standard deviation of a for the pure Ge films was taken as the error of the relaxed lattice parameter for the doped films. For Ge:As, we also include earlier measurements by Isherwood and Wallace [27]. The parameter β was extracted from a linear fit using an orthogonal distance regression method to account for errors both in the lattice parameter and in the doping concentrations.
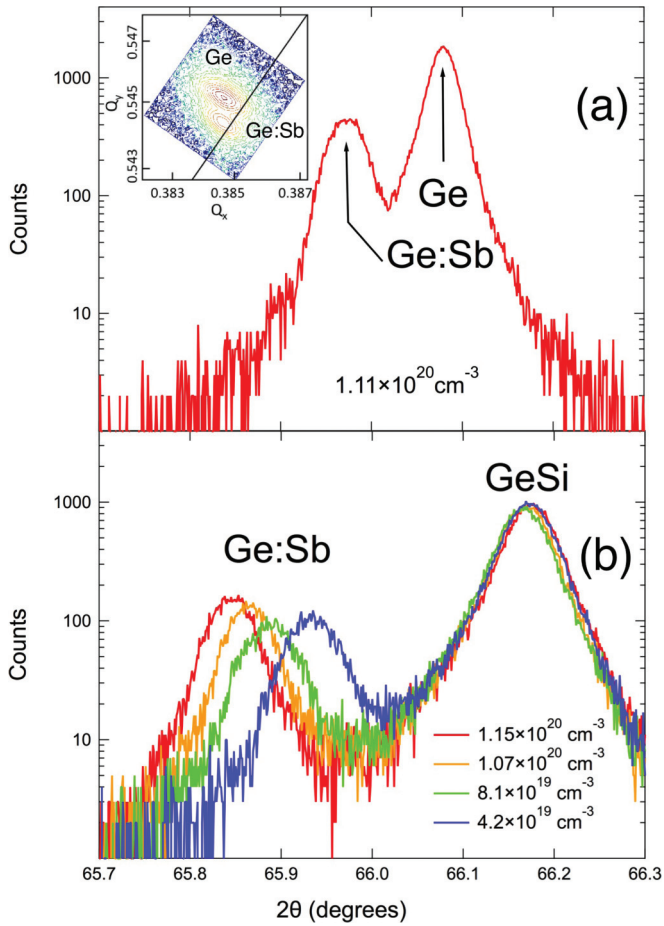
FIG. 1. θ-2θ scans for the 004 reflection in several Sb-doped Ge films. (a) Film grown on Ge-buffered Si. The inset shows a reciprocal space intensity map around the 224 reflection; (b) films grown on $Ge_{0.95}Si_{0.05}$. The peaks at high angles in both panels correspond to the buffer layers.
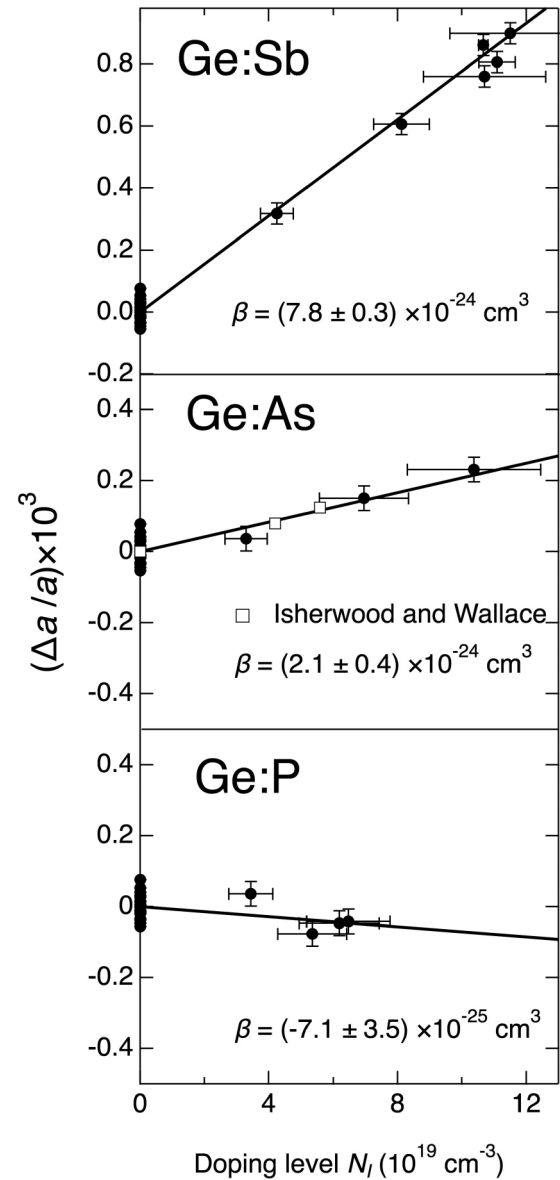

FIG. 2. Relative change in the lattice parameter as a function of carrier concentration in Ge doped with P, As, and Sb. The linear fit coefficients are shown in the corresponding panels. The white squares show Ge:As results from Ref. [25].

For a comparison of our results for doped Ge with earlier work on doped Si, Eqs. (1) and (3) suggest that we define the dimensionless parameter $\beta^* = \beta N_H$. The experimental values of β^* are compared in Fig. 3(a) with the predictions from Vegard's theory in Eq. (1) using Phillips covalent radii [28]. The data for Si:P were taken from Refs. [29–31]. For Si:As, we used results from Refs. [5,19,32], and for Si:Sb the data were taken from Refs. [33,34]. We see that the quantitative agreement is marginal. More importantly, a systematic trend is readily apparent: Whereas all germanium values lie above the Eq. (1) line, the corresponding Si values are below the line. This is a clear indication of electronic effects since, as indicated above, these effects have opposite signs in Si and Ge. A comparison of Ge:As and Si:As offers a dramatic example of the inadequacy of the Vegard theory: The covalent radii of Ge and As are the same, whereas that of Si is much smaller, yet the doping dependence of the lattice parameter is much stronger in the Ge:As system than in Si:As. Even the good agreement for Si:Sb appears to arise from a fortuitous combination of two errors: the overestimation of the experimental values for smaller $\Delta R/R$ (Si:P and Si:As), combined with the fact that

the slope of 2 in the theoretical line [Eq. (1)] is clearly smaller than suggested by the experimental data.

In Fig. 3(b) we first compare the experimental β^*'s with *ab initio* calculations for Ge [13] and Si [35]. All values are plotted against *ab initio* values of $\Delta R/R$ from Refs. [13,36]. This is performed for later comparison with the CK theory, but we first concentrate on the accuracy of the predicted values of β^*, ignoring the $\Delta R/R$ information. We note that the agreement is substantially improved relative to the Vegard theory represented by Eq. (1). In fact, the remaining discrepancies are within the range that might be expected on account of possible systematic errors in the doping concentrations and the difficulty in ruling out the presence of a residual fraction of nonsubstitutional donors. Even the wrong sign of β^* for Ge:P, the only remaining qualitative discrepancy between *ab initio* theory and experiment, does not appear too serious if
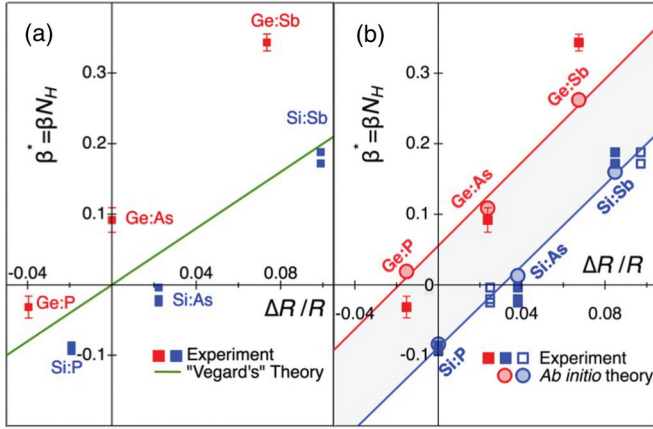
FIG. 3. (a) Normalized β^* coefficients for doped Ge (our Rapid Communication) and doped Si from Refs. [5,19,29–34] compared with Vegard's theory from Eq. (1) with $\Delta R = r_I - r_H$ and $R = 2r_H$. The atomic radii r_H and r_I are from Ref. [28]. (b) The same normalized β^* coefficients for doped Ge and doped Si are plotted against *ab initio* theoretical values of $\Delta R/R$ from Refs. [13,36] (solid squares) and EXAFS values of $\Delta R/R$ (empty squares). The light red and blue circles correspond to *ab initio* values of β^* from Refs [13,35] for Ge and Si, respectively. The solid red (blue) line is a linear fit of the *ab initio* results for Ge (Si). The slopes of both lines turn out to be nearly identical to the value $2/a^{**}$ predicted from Eq. (3). The intercept at the origin represents the electronic contribution, and it has the opposite sign in both materials due to the opposite sign of the corresponding deformation potentials.

one observes that the magnitude of β^* in this case is small. As can be seen in Fig. 2, the change in lattice constant in Ge:P is not much larger than the fluctuation of the measured lattice parameter in pure Ge.

From the foregoing analysis we conclude that *ab initio* calculations of the doping dependence of the lattice parameter are in very satisfactory agreement with experiment. This, however, has no obvious implication for the validity of the CK theory since, as indicated above, the problem of separating the size and electronic contributions affect both the experimental data and the *ab initio* calculations. On the other hand, if we perform linear fits of the *ab initio* values of β^* versus $\Delta R/R$, we obtain the red and blue lines in Fig. 3(b). The slope of these lines is 2.96 (Ge) and 2.89 (Si). This is in excellent agreement with the slope $2/a^{**} = 2/0.7 = 2.86$ predicted from Eq. (3). Moreover, the ordinates at the origin have opposite signs, and when equated to $-3a_c N_H/B$, the value predicted by Eq. (2), we obtain $a_c = -1.86$ eV (Ge) and $a_c = 3.30$ eV (Si). Combined with predicted $a_v = 2.23$ eV (Ge) and $a_v = 2.38$ eV (Si) in Ref. [37], these values imply band-gap deformation potentials $a = -4.1$ eV (Ge) and $a = 0.9$ eV (Si), in good agreement with the experimental values $a = -3.6$ eV (Ge, Ref. [38]) and $a = 1.5$ eV (Si, Ref. [39]). Other direct calculations of ADPs are also in good agreement with the values determined with our procedure. For example, Van de Walle finds $a_c = -1.5$ eV (Ge) and $a_c = 4.18$ eV (Si) [9]. We thus conclude that, far from disagreeing with the CK theory in Eqs. (2) and (3), as previously claimed, *ab initio* calculations provide strong support for it and, in particular, demonstrate fairly conclusively that Eq. (3) is the correct way to account for size effects.

The analysis so far demonstrates that *ab initio* results are in good agreement with experiment and with the Cargill-Keyes theory. However, the definitive validation of the CK theory requires a study of the experimental β^*'s as a function of *experimental* $\Delta R/R$ values. We have done so in Fig. 3(b) for the cases in which EXAFS data for $\Delta R/R$ are available [5,40] (empty squares), and we see that the difference with the $\Delta R/R$ from *ab initio* calculations is small and, if anything, the agreement with the theoretical β^*'s is improved. In fact, for Si:As even closer agreement with the *ab initio* $\Delta R/R$ value is reported by Koteski *et al.* [41] The similarity between *ab initio* and EXAFS values of $\Delta R/R$ can be expected based on the observation that *ab initio* calculations of Raman spectra in alloy semiconductors with significant bond length mismatch are in excellent agreement with experiment [42]. Errors in the compositional dependence of optical phonon frequencies are no larger than 4%, which, given the fact that Grüneisen parameters are on the order of unity, imply comparable errors in $\Delta R/R$ (Ref. [43]). We thus conclude that the CK theory is fully consistent with the experimental evidence. Still, the objection could be raised that the $\Delta R/R$ values from both EXAFS measurements and *ab initio* calculations are themselves affected by the electronic contribution so that we might be counting this contribution twice. However, as demonstrated by Chizmeshya [13], the size effect is strongly localized around the dopant atom, whereas the electronic contribution is uniformly spread over the lattice. Thus the error incurred is on the order of N_I/N_H, which is negligible under normal conditions.

So far we have limited ourselves to n-type systems, but the CK theory applies to p-type systems as well. Unfortunately, there are no available data to create the equivalent of Fig. 3(b) for p materials. Moreover, the valence-band ADPs for Ge and Si have the same signs and similar magnitudes so that the separation between size and electronic effect would not be equally obvious. An individual case that has been studied in detail is Si:B. *Ab initio* calculations predict $\Delta R/R = -0.107$ [44]. Thus the size contribution from Eqs. (2) and (3) is predicted to be $\beta^*_{size} = -0.31$. In addition, using $a_v = 2.38$ eV [37], we obtain $\beta^*_h = 0.06$. The total $\beta^* = -0.25$ is in reasonable agreement with experimental values in the -0.31 to -0.26 range [45–47]. On the other hand, in the above-mentioned Si:Ga case [6] a_v is determined to be negative. We notice, however, that Si:Ga is somewhat anomalous because there is no consensus on the value of $\Delta R/R$. EXAFS gives $\Delta R/R = 0.025$ but could not completely rule out $\Delta R/R \sim 0$ [6], whereas *ab initio* calculations range from $\Delta R/R = 0.013$ (Ref. [48]) to 0.017 (Ref. [49]). These particular results underscore the fact that extracting deformation potentials from measurements on one single host-dopant system may lead to incorrect conclusions. Only when the results are considered globally, as in Fig. 3(b), does the validity of the CK approach become apparent.

To summarize, we have presented measurements of the doping dependence of the cubic lattice parameter for a complete series of shallow donors in Ge. When the experimental results and *ab initio* theoretical calculations are combined with similar measurements and calculations on doped Si, a clear pattern emerges that supports the Cargill-Keyes theory for the doping dependence of lattice parameters in semiconductors.

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