## Effects of point defects on lattice parameters of semiconductors

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A model for analyzing the correlation between lattice parameters and point defects in semiconductors has been established. The results of this model for analyzing the substitutes in semiconductors are in accordance with those from Vegard's law and experiments. Based on this model, the lattice strains caused by the antisites, the tetrahedral and octahedral single interstitials, and the interstitial couples are analyzed. The superdilation in lattice parameters of GaAs grown at low temperatures by molecular-beam epitaxy can be interpreted by this model, which is in accordance with the experimental results. This model provides a way of analyzing the stoichiometry in bulk and epitaxial compound semiconductors nondestructively. [S0163-1829(96)05336-2]

### I. INTRODUCTION

The lattice parameters of semiconductors have a close correlation with the characteristics of semiconductor devices<sup>1</sup> and the stoichiometry of compound single crystals.<sup>2,3</sup> Point defects such as substitutes, antisites, and interstitials play an important role in deviations in the lattice parameters of semiconductors.<sup>4,5</sup> Both the superdilation of undoped As-rich GaAs grown at low temperatures of 200-250 °C (LT GaAs) by molecular-beam epitaxy (MBE),<sup>6-8</sup> and the lattice contraction of heavy carbon-doped GaAs grown by MBE,<sup>9-12</sup> are significant in the x-ray doublecrystal diffractometry (XDCD) measurements. Although vacancies and dislocations may also affect lattice parameters of single crystals, their effects can be neglected compared with those of substitutes, antisites, and interstitials.<sup>13</sup> A precise measurement of lattice parameters of single crystals can be generally accomplished by Bond<sup>14</sup> and improved methods<sup>15,16</sup> utilizing an x-ray double-crystal diffractometer. Because it is a nondestructive measurement, XDCD is preferred in a measurement of the stoichiometry of compound semiconductors,<sup>1,2</sup> even though there is not a theoretical model for the analyses. For analyzing the causes of the deviation in lattice parameters, the original form of Vegard's law was used,<sup>13</sup> based upon the chemical covalent radii given by Pauling.<sup>17</sup> However, the elasticity of crystals was not a concern there. In addition, the commonly used Vegard's law (which will be discussed in Sec. II) is invalid for some dopants in semiconductors, such as carbon in GaAs. Although some other efforts have also been adopted,18-20 the mechanism of the deviation in lattice parameters still remains ambiguous.

A model for analyzing the deviations in lattice parameters caused by point defects will be established in this paper. The effects of the substitutes and the antisites are analyzed in Sec. II, the effects of single interstitials and interstitial couples are discussed in Sec. III, a discussion is given in Sec. IV, and final conclusions are given in Sec. V.

#### **II. EFFECTS OF THE SUBSTITUTES AND ANTISITES**

The unit cells of diamond and blend crystals are similar. Both of them are composed of two interlaced face-centered cubes, as shown in Fig. 1. (Atoms A and B are the same for the diamond structure.) Although the atmospheres of the nonequivalent atoms of the two cubes are not completely the same, they both have a common feature, i.e., each has four nearest neighbors sitting at four apexes of a regular tetrahedron, as shown by the smaller cube in Fig. 1. The distance between the two nearest atoms is

$$d_0 = AB = r_a + r_b, \qquad (1)$$

where  $r_a$  and  $r_b$  are the chemical covalent radii of atoms A and B, respectively. If there are substitutional or antisite defects in a single crystal, the distance becomes

$$d_0 = r_s + r_b$$
 or  $r_s + r_a$  (substitute of A or B),  
(2a)

 $d_0 = 2r_a$  or  $2r_b$  (antisite  $A_B$  or  $B_A$ ), (2b)

with the chemical covalent radius  $r_s$  of the substitutional atom.



FIG. 1. The unit cell of blend or diamond (atoms A=B) structure. Each atom has four nearest neighbors (smaller cube).

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In order to calculate the lattice strain caused by a point defect, we take account of a small cube as shown in Fig. 1. When the distance between the two nearest atoms changes from  $d_0$  to d, an elastic strain along  $\langle 111 \rangle$  direction occurs:

$$\varepsilon = \frac{\Delta d}{d_0} = \frac{d - d_0}{d_0}.$$
(3)

The components of  $\varepsilon$  projecting on the three axes  $\langle 100 \rangle$ ,  $\langle 010 \rangle$ , and  $\langle 001 \rangle$  are the same:

$$\boldsymbol{\varepsilon}_{x} = \boldsymbol{\varepsilon}_{y} = \boldsymbol{\varepsilon}_{z} = \boldsymbol{\varepsilon}. \tag{4}$$

According to Hook's law, a stress along (001) caused by the strain will be

$$\sigma_z = c_{11}\varepsilon_z + c_{12}(\varepsilon_x + \varepsilon_y) = (c_{11} + 2c_{12})\varepsilon, \qquad (5)$$

where  $c_{11}$  and  $c_{12}$  are the stiffness coefficients of the crystals. Then the equivalent principal strain along  $\langle 001 \rangle$  is

$$E_z = \frac{\sigma_z}{c_{11}} = \frac{c_{11} + 2c_{12}}{c_{11}} \varepsilon = \mu \varepsilon, \qquad (6)$$

where  $\mu = (c_{11} + 2c_{12})/c_{11}$ . If the strains among atoms other than the nearest neighbors can be neglected, the lattice strains caused by the substitutes and the antisites will be

$$\frac{\Delta a}{a_0} = \frac{\mu}{d_0 N_0} \sum_p \Delta d_p N_p, \qquad (7)$$

where  $N_p$  and  $N_0$  are the densities of the point defects and the matrix atoms of the crystal, respectively, and the sum is for all the possible point defects described by Eq. (2).  $\Delta a = a - a_0$  is the difference between measured and standard lattice parameters.

As an example, we take account of GaAs. In such case,  $r_{As}$  and  $r_{Ga}$  are 1.18 and 1.26 Å, respectively, and  $c_{11}=11.88$ ,  $c_{12}=5.38(\times 10^{11} \text{ dyn/cm}^2)$ ,<sup>21</sup> and  $\mu=1.9057$ . Then the lattice strain caused by the indium substitute In<sub>Ga</sub> ( $r_{In}=1.44$  Å) in In<sub>x</sub>Ga<sub>1-x</sub>As is

$$\frac{\Delta a}{a_0} = \mu \; \frac{r_{\rm In} - r_{\rm Ga}}{r_{\rm Ga} + r_{\rm As}} \frac{[{\rm In}_{\rm Ga}]}{N_0} = \mu \; \frac{r_{\rm In} - r_{\rm Ga}}{r_{\rm Ga} + r_{\rm As}} \frac{x}{2} = 7.0922 \times 10^{-2} x, \tag{8}$$

where  $[In_{Ga}]$  is the concentration of In on the site of Ga, and  $[In_{Ga}]/N_0 = x/2$ . Figure 2 shows a comparison of these results with those obtained from Vegard's law (dashed line):

$$a_{A_xB_{1-x}C} = xa_{AC} + (1-x)a_{BC}.$$
(9)

An In-doped  $\langle 100 \rangle$  GaAs wafer grown by the liquidencapsulated Czochralski (LEC) technique was measured by XDCD and, subsequently, photoluminescence (PL) methods. The peak of the PL spectrum is  $\lambda$ =8780 Å, as shown in Fig. 3. The component *x* of indium can be calculated from the equation<sup>22</sup>

$$E_{g} = 1.425 - 1.337x + 0.27x^{2}. \tag{10}$$

The lattice parameter of the sample is a=5.6577 Å, obtained from XDCD measurement with the Bond method. The values of x are 0.011, 0.010, and 0.011, obtained, respectively, by this model, PL measurement, and Vegard's law. It is un-



FIG. 2. Lattice strains  $\Delta a/a_0$  in  $\ln_x \text{Ga}_{1-x}$ As obtained by this model and Vegard's law (dashed line), respectively.

ambiguous that the result of this model is consistent with the results of PL measurement and Vegard's law.

Figure 4 shows the lattice strains caused, respectively, by  $As_{Ga}$ ,  $C_{As}$ ,  $Si_{Ga}$ ,  $Si_{As}$ , and  $Te_{As}$ , with  $N_0=4.42\times10^{22}$  cm<sup>-3</sup>,  $r_c=0.77$  Å, and  $r_{Te}=1.32$  Å. The substitutional impurity caused deviations in lattice parameters that are quite in accordance with the experimental results.<sup>9-13,21</sup>

# III. EFFECTS OF SINGLE INTERSTITIALS AND INTERSTITIAL COUPLES

Except for some substitutes with large chemical covalent radii, most of the point defects cause the lattice parameter of GaAs to contract. From Fig. 4 we know that the arsenic antisite defects  $As_{Ga}$  do not have obvious effects on the lattice parameters of GaAs. In this section we will deal with the effects of interstitials on the lattice parameters of semiconductors.

For a unit cell of blend crystals consisting of atoms A and B (A = B for diamond crystals), the four atoms sitting on the four diagonals of the unit cell form a hollow tetrahedron, as shown by the smaller cube in Fig. 5. There are four similar



FIG. 3. PL spectrum of  $In_xGa_{1-x}As$ .



FIG. 4. Lattice strains  $\Delta a/a_0$  of GaAs caused, respectively, by (from the bottom) C<sub>Ga</sub>, Si<sub>Ga</sub>, As<sub>Ga</sub>, Si<sub>As</sub>, and Te<sub>As</sub>, with the densities of  $N_p$  in logarithms.

hollow tetrahedrons in the four corners of the cell without diagonal atoms. The atoms in the center of such hollow tetrahedrons, if there are any, are called single tetrahedral interstitials. There are four hollow octahedrons between each hollow tetrahedron in the corner and the central one, as shown in Fig. 6. Similarly, the atoms in the center of such hollow octahedrons are called single octahedral interstitials. If two atoms share one matrix site in a metastable state, the two atoms are called an interstitial couple, as shown in Fig. 7. All kinds of interstitials will be discussed, respectively, as follows.

### A. Single tetrahedral interstitials

The distance between a tetrahedral interstitial and its nearest neighbors is



FIG. 5. Unit cell of blend crystals. The four diagonal atoms form a hollow tetrahedron (in smaller dashed cube).

![](_page_2_Figure_9.jpeg)

FIG. 6. Hollow octahedron in blend crystals.

$$d_a = r_i + r_a$$
 or  $d_b = r_i + r_b$   
(interstitial in tetrahedron A or B) (11)

where  $r_i$ ,  $r_a$ , and  $r_b$  are the chemical covalent radii of the interstitial, atom A, and atom B, respectively. If the distances  $d_a$  and  $d_b$  are less than the distance between the center and the apex of the hollow tetrahedron, i.e.,  $d_0 = r_a + r_b$ , the effects of the interstitials on the lattice parameters can be neglected. Otherwise, the interstitials will cause the lattice parameters to dilate. For convenience in the following calculation, we suppose that  $r_a \leq r_b$ . When  $r_a < r_i \leq r_b$ , only the interstitials in the hollow tetrahedrons formed by atom B (tetrahedron B) account for the dilation in lattice parameters. According to the results derived in Sec. II, the lattice strain caused by the interstitials is

$$\frac{\Delta a}{a_0} = \mu \varepsilon_b \, \frac{N_{bi}}{N_0},\tag{12}$$

where

$$\varepsilon_b = \frac{\Delta d_b}{d_0} = \frac{d_b - d_0}{d_0}.$$
(13)

In Eq. (12),  $N_{\rm bi}$  is the density of the interstitials in the tetrahedron *B*.

![](_page_2_Figure_17.jpeg)

FIG. 7. An interstitial couple in a tetrahedron.

If  $r_i > r_b$ , the interstitials will affect the lattice parameters whether they are in tetrahedron A or B. The total lattice strain caused by such interstitials is

$$\frac{\Delta a}{a_0} = \frac{\Delta a_a}{a_0} + \frac{\Delta a_b}{a_0} = \frac{\mu}{N_0} \left( \varepsilon_a N_{ai} + \varepsilon_b N_{bi} \right), \tag{14}$$

where

$$\varepsilon_a = \frac{\Delta d_a}{d_0} = \frac{d_a - d_0}{d_0}.$$
 (15)

 $N_{ai}$  is the density of the interstitials in tetrahedron A.

The influence of the single tetrahedral arsenic interstitials in GaAs on the lattice parameters can be neglected, because  $r_{As}=r_a=r_i < r_b=r_{Ga}$ .

#### **B.** Single octahedral interstitials

The hollow octahedron in a unit cell of blend crystals is shown in Fig. 6. It can be derived that the distance between two diagonal atoms of the octahedron is

$$q_0 = \overline{25} = \frac{\sqrt{11}}{4} a_0 = \frac{\sqrt{11}}{4} \frac{4}{\sqrt{3}} (r_a + r_b) = \sqrt{\frac{11}{3}} d_0. \quad (16)$$

When an interstitial is pushed into the octahedron, the distance becomes

$$q = \overline{25} = 2r_i + r_a + r_b = 2r_i + d_0.$$
(17)

If  $q < q_0$ , i.e.,  $r_i < (\sqrt{11/3} - 1)d_0/2$ , the effects of such octahedral interstitials on the lattice parameters can be neglected. Otherwise, there are lattice strains within the crystal:

$$\frac{\Delta a}{a_0} = \mu \varepsilon \, \frac{N_{qi}}{N_0} \tag{18}$$

with

$$\varepsilon = \frac{\Delta q}{q_0} = \frac{q - q_0}{q_0}.$$
 (19)

 $N_{qi}$  in Eq. (18) is the density of octahedral interstitials. For example, the octahedral arsenic interstitial As<sub>qi</sub> in GaAs will cause a relative increase in lattice parameters:  $\Delta a/a_0 = 0.05456N_{qi}/N_0$ .

Figure 8 shows a double-crystal x-ray rocking curve measured from the (004) undoped GaAs grown at low temperature (LT GaAs, at 250 °C for this sample) by molecularbeam epitaxy technique on a semi-insulating (SI) GaAs substrate. It can be seen from the angular difference between the two peaks that the lattice strain in the epilayer is about 0.03%, which needs  $5.33 \times 10^{20}$  cm<sup>-3</sup> of single octahedral arsenic interstitials. Because the formation energy of octahedral interstitials is much higher than that of tetrahedral interstitials and arsenic antisites,<sup>23</sup> there would be more tetrahedral interstitials and arsenic antisites in GaAs crystals if there were high density of octahedral interstitials there; i.e. there would be several tenths of an excess arsenic atoms in the epilayer. Obviously, this is quite unreasonable for a single crystal.

![](_page_3_Figure_20.jpeg)

FIG. 8. Double-crystal x-ray rocking curve from the (004) undoped MBE LT GaAs grown on a SI GaAs substrate.

### C. Interstitial couples

In order to analyze the dilation in lattice parameters caused by the interstitial couples, we consider the case that an interstitial couple occupies a matrix site of atom A. Figure 9 shows the projection of the cube, including the tetrahedron B shown in Fig. 7 on the (110) plane. The dashed rectangle in Fig. 9 shows the projection of the cube without the interstitial couple. Suppose, at the beginning, that one atom of the couple moves from point O upwards to point A satisfying  $\overrightarrow{OA} = r_i$  and  $\overrightarrow{AK} = r_i + r_b$ .

From the two similar triangles of  $\triangle OBC$  and  $\triangle OKG$ , it can be derived that the distance between points *O* and *K* is

$$d = \overline{OK} = \sqrt{3} \ \overline{OG} = \frac{\sqrt{3}}{3} \ \overline{OA} + \sqrt{\overline{AK^2} - \frac{2}{3}\overline{OA^2}}.$$
 (20)

For the interstitial couples in tetrahedron B, the distance becomes

$$d_b = \frac{\sqrt{3}}{3} r_i + \sqrt{(r_i + r_b)^2 - \frac{2}{3}r_i^2},$$
 (21)

![](_page_3_Figure_28.jpeg)

FIG. 9. The projection of a cube including a tetrahedron with an interstitial couple on a  $(\overline{1}10)$  plane.

and the lattice strain caused by them is

$$\frac{\Delta a_b}{a_0} = \mu \varepsilon_b \, \frac{N_{bc}}{2N_0},\tag{22}$$

where  $\varepsilon_b$  is as the same form as Eq. (13), and  $N_{bc}$  is the density of single interstitial atoms in tetrahedron *B*. Similarly, the lattice strain caused by the interstitial couples in tetrahedron *A* is

$$\frac{\Delta a_a}{a_0} = \mu \varepsilon_a \, \frac{N_{ac}}{2N_0},\tag{23}$$

where  $\varepsilon_a$  is as the same form as Eq. (15),  $N_{ac}$  is the density of single interstitial atoms in tetrahedron A, and

$$d_a = \frac{\sqrt{3}}{3} r_i + \sqrt{(r_i + r_a)^2 - \frac{2}{3}r_i^2}.$$
 (24)

When (1)  $d_a \leq d_b \leq d_0$ , the effects of interstitial couples on the lattice parameters can be neglected; for instance  $O_2$  $(r_0=0.66 \text{ Å})$  in GaAs,  $d_b=2.2249 < d_0=2.44 \text{ Å}$ ; (2)  $d_a < d_0 \leq d_b$ , only the interstitial couples in tetrahedron *B* cause the lattice parameters to dilate; and (3)  $d_b \geq d_a > d_0$ , the interstitial couples affect the lattice parameters wherever they are. The lattice strain caused by such interstitial couples is

$$\frac{\Delta a}{a_0} = \frac{\Delta a_a}{a_0} + \frac{\Delta a_b}{a_0} = \frac{\mu}{2N_0} \left(\varepsilon_a N_{ac} + \varepsilon_b N_{bc}\right).$$
(25)

As an example, we consider the arsenic interstitial couples occupying the matrix site of arsenic in GaAs. In this case, only one atom of an interstitial couple is the excess atom. If the density of such excess arsenic atoms is  $N_c$ , the lattice strain caused by the arsenic interstitial couples, according to Eq. (22), is

$$\frac{\Delta a_b}{a_0} = \mu \varepsilon_b \frac{N_c}{N_0}.$$
(26)

For the LT-GaAs discussed above, the relative increase in lattice parameters  $\Delta a/a_0 = 0.03\%$  needs  $3.40 \times 10^{19}$  cm<sup>-3</sup> of excess arsenic atoms.

# **IV. DISCUSSION**

Look, Grant, and Sizelove<sup>24</sup> and Liliental-Weber et al.<sup>25</sup> supposed the existence of dimeric interstitials in GaAs before. Although the formation energy of tetrahedral interstitials is high, dense arsenic tetrahedral interstitials may appear near the melting temperature in melt-grown GaAs. When an interstitial arsenic is ionized, it becomes positively charged  $As_i^{3+}$  or  $As_i^{+}$ <sup>24</sup> It will be attracted to one of the nearest matrix arsenic atoms when the positively charged  $As_i^{3+}$  or  $As_i^+$  deviates from the center of the tetrahedron due to thermal vibration. Then the two mutually attracted particles will share the same matrix site and form a metastable interstitial couple, as shown in Fig. 7. The arsenic interstitial couples may appear in LT GaAs, as well. The GaAs grown by MBE requires the interaction of gallium and arsenic species impinging on a heated substrate surface. Either As<sub>4</sub> molecules and Ga atoms, or As<sub>2</sub> molecules and Ga atoms, are used as constituent molecular-beam species. If the temperature of the substrate surface is not high enough, the arsenic and gallium species impinging on it will not completely interact, and some dimeric arsenic will remain as interstitial couples in MBE LT GaAs. The fact that the arsenic interstitial couples decrease with the increasing of growing temperature can be interpreted by this model very well. The better interaction of As<sub>2</sub> and Ga than that of As<sub>4</sub> and Ga can also explain the decrease in point defects of LT GaAs grown with As<sub>2</sub> and Ga species.<sup>26</sup>

The lattice location of the excess arsenic has been detected with ion channeling experiments.<sup>27</sup> Because the existence of the arsenic interstitial couples in LT-GaAs is metastable, rocking curve measurements on annealed samples show that lattice parameters of the epilayers gradually decrease as the samples are annealed at temperatures higher than 300 °C, and finally resume the value of the substrate when the annealing temperature reaches 450 °C.

The main effects of dislocations on XDCD measurements are the broadening of the x-ray-diffraction profile, which can be neglected when the density of the dislocations is lower than  $10^5$  cm<sup>-2</sup>. Note that the rocking curve of the XDCD measurement cannot tell the difference between a LEC GaAs substrate with a vacancy concentration of  $10^{18}$  cm<sup>-3</sup>, and epitaxial GaAs with vacancy concentration of 10<sup>15</sup> cm<sup>-3</sup>.<sup>13</sup> The effects of vacancies on the lattice parameters can also be neglected. With this model the lattice parameter of GaAs will be contracted by As<sub>Ga</sub>. This is reasonable. Except for the shorter covalent radius of As,  $As_{Ga}$  is generally positively charged in GaAs, i.e., As<sub>Ga</sub><sup>2+</sup>. The covalent tetrahedron composed of the five As atoms will be tightened due to the stronger Coulomb attraction. Even if the five As atoms are all positively charged like  $As_{Ga}^+$ , the Coulomb repelling energy is too small to make the lattice dilated, for the covalent radius only becomes about 0.01 Å longer. That is why the  $As_{Ga}$ defects are stable up to 1000 °C.<sup>28</sup>

#### V. CONCLUSIONS

In summary, we have established a model for analyzing the correlation between lattice parameters and point defects in semiconductors. The results of this model are in accordance with those from Vegard's law and experiments. We conclude that the dilation in the lattice parameters of GaAs is not caused by the  $As_{Ga}$  defects. The effects of various interstitials on the lattice parameters have been discussed systematically based on a theoretical model. The superdilation in the lattice parameter of LT GaAs can be interpreted in this model as due to the As interstitial couples. This model has provided a way of analyzing the stoichiometry in bulk and epitaxial compound semiconductors by nondestructive x-ray double-crystal diffractometry measurements.

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- <sup>1</sup>Y. Fujisaki, J. Cryst. Growth **126**, 77 (1993).
- <sup>2</sup>Y. Takano, T. Ishiba, N. Matsunaga, and N. Hashimoto, Jpn. J. Appl. Phys. **24**, L239 (1985).
- <sup>3</sup>A. N. Morozov and V. T. Bublik, J. Cryst. Growth **97**, 475 (1989).
- <sup>4</sup>D. Korytar, J. Cryst. Growth **126**, 30 (1993).
- <sup>5</sup> R. E. Pritchard, S. A. McQuaid, L. Hart, R. C. Newman, J. MaKinen, H. J. von Bardeleben, and M. Missous, J. Appl. Phys. **78**, 2411 (1995).
- <sup>6</sup>D. C. Look, D. C. Walters, M. O. Manasreh, J. R. Sizelove, C. E. Stutz, and K. R. Evans, Phys. Rev. B **42**, 3578 (1990).
- <sup>7</sup>F. W. Smith, A. R. Calawa, C. L. Chen, M. J. Mantra, and L. J. Mahoney, IEEE Electron. Device Lett. EDL-9, 77 (1988).
- <sup>8</sup>A. C. Warren, J. M. Woodall, J. L. Freeouf, D. Grischkowsky, D. T. McInturff, M. R. Melloch, and N. Otsuta, Appl. Phys. Lett. **57**, 1331 (1990).
- <sup>9</sup>C. Abernathy, S. Pearton, R. Caruso, F. Ren, and J. Jovalchik, Appl. Phys. Lett. 55, 1750 (1989).
- <sup>10</sup>R. J. Malik, R. N. Nottemberg, E. F. Schubert, J. F. Worlker, and R. W. Ryan, Appl. Phys. Lett. **53**, 2661 (1988).
- <sup>11</sup>M. C. Hanna, Z. H. Lu, and A. Majerfeld, Appl. Phys. Lett. 58, 164 (1991).
- <sup>12</sup>C. R. Abernathy, S. J. Pearton, M. O. Manasreh, D. W. Fischer, and D. N. Talwar, Appl. Phys. Lett. **57**, 294 (1990).
- <sup>13</sup>C. M. H. Driscoll, A. F. W. Willoughby, J. B. Mullin, and B. W. Straughan, Inst. Phys. Conf. Ser. 24, 275 (1975).
- <sup>14</sup>W. L. Bond, Acta Crystallogr. **13**, 814 (1960).

<sup>15</sup>W. J. Bartels, J. Vacuum Sci. Technol. B 1, 338 (1983).

- <sup>16</sup>M. Fatemi, J. Cryst. Growth **96**, 316 (1989).
- <sup>17</sup>L. Pauling, *The nature of the chemical bond and the structure of molecules and crystals*, 3rd ed. (Cornell University Press, Ithaca, NY, 1960), Chap. 7.
- <sup>18</sup>J. B. Mullin and B. W. Straughan, J. Appl. Phys. 47, 2584 (1976).
- <sup>19</sup>H. Kuwamoto and D. E. Holmes, J. Appl. Phys. 59, 656 (1986).
- <sup>20</sup>J. Hornstra and W. J. Bartels, J Cryst. Growth 44, 513 (1978).
- <sup>21</sup>J. C. Brice, *Properties of Gallium Arsenide*, 2nd Ed., EMIS Data Review Series No. 6 (INSPEC, City 1991), Chap. 1.
- <sup>22</sup>R. E. Nahory, M. A. Pollack, and J. C. DeWinter, J. Appl. Phys. 46, (1975) 775.
- <sup>23</sup>S. B. Zhang and J. E. Northrup, Phys. Rev. Lett. 67, 2339 (1991).
- <sup>24</sup>D. C. Look, J. T. Grant, and J. R. Sizelove, Appl. Phys. Lett. **61**, 1329 (1992).
- <sup>25</sup>Z. Liliental-Weber, A. Ishikawa, M. Tarianchi, and M. Tanaka, in *Advances in Surface and Thin Film Diffraction*, edited by T. C. Huang, P. L. Cohen, and D. J. Eagleshaw, MRS Symposium Proceedings, No. 208 (Materials Research Society, Pittsburgh, 1991) p. 183.
- <sup>26</sup>P. W. Yu, D. C. Reynolds, and C. E. Stutz, Appl. Phys. Lett. **61**, 1432 (1992).
- <sup>27</sup>K. M. Yu, M. Kaminska, and Z. Liliental-Weber, J. Appl. Phys. 72, 2850 (1992).
- <sup>28</sup>Z. Liliental-Weber, X. W. Lin, and J. Washburn, Appl. Phys. Lett. **66**, 2086 (1995).