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A photoluminescence study of defects in non-stoichiometric gallium arsenide using concurrent electrical and structural characterization

C. M. H. DRISCOLL, A. F. W. WILLOUGHBY
Engineering Materials Laboratories, The University, Southampton, UK

E. W. WILLIAMS
Royal Radar Establishment, Malvern, Worcestershire, UK

Photoluminescence has been used to identify centres associated with point defects and impurities in single crystal gallium arsenide, and this has been correlated with electrical and structural characterization of the same samples. Five different types of defect centre have been identified by this technique in material grown under different conditions of stoichiometry. These studies show systematic differences between the photoluminescence data obtained from stoichiometric and non-stoichiometric gallium arsenide. Precision lattice parameter and density measurements on the same gallium arsenide specimens indicate a deviation from stoichiometry on the arsenic-rich side of the gallium arsenide phase and it is suggested that defects primarily responsible for this stoichiometric deviation are arsenic interstitials in concentrations up to 3×10^{18} cm^{-3}. Photoluminescence measurements associate these defects in arsenic-rich gallium arsenide with an energy level of 0.036 eV.

1. Introduction

Luminescence studies on control specimens, or combined with information obtained from other techniques, have been shown to provide useful information concerning the nature, energy levels and in certain circumstances, the concentration of impurities and point defects in gallium arsenide [1, 2]. A review of simple and associated defect levels identified in gallium arsenide by photoluminescence has been made by Williams [3]. Of particular interest to the present study of non-stoichiometry in gallium arsenide is the identification of photoluminescence centres found only under non-stoichiometric conditions [2, 4-6].

In the present investigation, front surface photoluminescence, employing the technique described previously [7], has been used to analyse defect centres in gallium arsenide single crystals, grown under different conditions of stoichiometry. Information obtained from photoluminescence measurements has been combined and compared with that obtained from electrical and mass spectometric studies on the same specimens to aid in the interpretation of the observed photoluminescence centres. Precision lattice parameter measurements, using the APEX technique described previously [7, 8], and hydrostatic density measurements, using the differential method of Ratcliffe [9], have also been made to aid in the material characterization of the gallium arsenide specimens.

The results from the photoluminescence study are presented and interpreted in Section 3, and are discussed in Section 4 in comparison with previous work, additional information from the supplementary studies and the expected nature of non-stoichiometric defects in gallium arsenide.

2. Experimental

Undoped gallium arsenide crystals grown by several different techniques have been examined in this investigation. Samples grown by Czochralski liquid encapsulation under stoichiometric and gallium excess conditions have been supplied by the Royal Radar Establishment, Malvern. Horizontal Bridgman n-type gallium arsenide, grown under different conditions of excess arsenic (with arsenic reservoir temperatures ranging from 609 to 637°C), have been supplied by the Allen Clark Research Centre (Plessey Co) and Mullard Laboratories (Redhill). In addition, heavily n-doped gallium arsenide (100) layers grown by liquid epitaxy have been supplied by SERL (Baldock).

Melt-grown samples, sectioned and ground parallel to a (100) plane for lattice parameter measurement at a Bragg angle of 80° [8], were polished in a 10% bromine-methanol solution to give a mirror surface for front surface photoluminescence at 20 and 77 K in the wavelength range 8000 to 10 000 Å. The electrical properties of the gallium arsenide specimens were assessed using the Hall effect and electrical conductivity measurements. A study of the variation of the electrical properties of these samples with temperature over the range 77 to 300 K was conducted with the object of ascertaining the electrical characteristics of possible non-stoichiometric defects and the prominent scattering mechanisms limiting the mobility of the electrical carriers in gallium arsenide.

Van der Pauw specimens [10], used for electrical measurements, were lightly ground on silicon carbide paste and chemically polished in a bromine-methanol solution. Low resistance non-rectifying contacts were made by heating each sample, with small spheres of indium solder positioned on the circumference of each leaf segment, in an inert atmosphere at 400°C.

The differential density method [9] is comparative, in which the weights of specimens in air and in liquid (distilled water) are compared alternately with those of a standard specimen as a function of time. Interpolation of the weights of all specimens to a common time was used to relate all weighings to the same environmental conditions.

Arsenic concentrations in the melt were obtained from the known arsenic reservoir temperatures, using the T–x diagrams of Boomgaard and Schol [11] and Koster and Thoma [12].

3. Results

3.1. Photoluminescence data as a function of the arsenic concentration in the melt

Photoluminescence measurements at 20 K have identified five different types of defect level in the horizontal Bridgman n-type gallium arsenide, as shown in Fig. 1 and summarized in Table I. The peak, indexed A, was observed in all samples in the melt concentration range 50 to 57 at. % arsenic. The peaks, indexed E and F, were observed only in samples grown close to stoichiometric conditions, while the peak, indexed B, was observed only in samples grown in the concentration range 50 to 55 at. % arsenic. Only samples grown under extreme conditions of excess arsenic (56 to 57 at. % arsenic in the melt) showed the luminescence peaks C and D.

Photoluminescence measurements on the same samples at 77 K showed only A, E and F peaks in some specimens, possibly related to the increased probability of non-radiative recombination and thermal quenching of the luminescent emission at higher temperatures. These results are summarized in Table II.

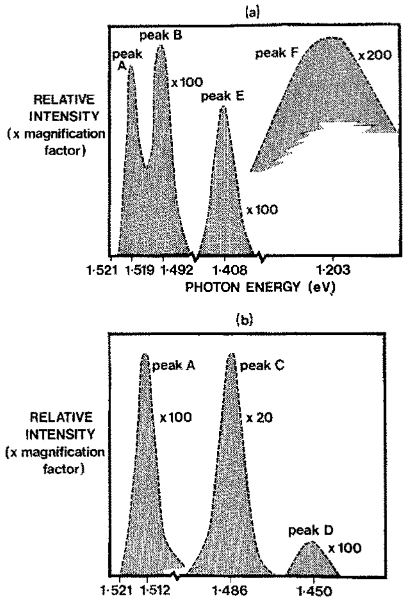

Figure 1 Photoluminescence spectra at 20 K for gallium arsenide grown under different conditions of stoichiometry: (a) with 50 at. % As in the melt; (b) with 57 at. % As in the melt.

3.2. Interpretation of photoluminescence peaks

3.2.1. Peak indexed A

The shallow defect levels, indexed A, were observed in all n-type Bridgman samples, grown under different conditions of stoichiometry. The

TABLE I Photoluminescence data at 20 K on horizontal Bridgman n-type GaAs as a function of at. % As in the melt

	Conditions of growth: at. % As in melt				
Level type and index	50	52	55	56	57
A. Hydrogenic donor impurity	*$E = 0.002$ $L = 0.016$ $I = 115$	$E = 0.006$ $L = 0.014$ $I = 25$	$E = 0.008$ $L = 0.009$ $I = 110$	$E = 0.011$ $L = 0.008$ $I = 45$	$E = 0.009$ $L = 0.006$ $I = 130$
B. Hydrogenic acceptor impurity	$E = 0.029$ $L = 0.020$ $I = 140$	$E = 0.015$ $L = 0.015$ $I = 55$	$E = 0.029$ $L = 0.011$ $I = 100$		
C. Native defect				$E = 0.037$ $L = 0.009$ $I = 1650$	$E = 0.035$ $L = 0.007$ $I = 650$
D. Phonon replica of native defect peak				$E = 0.073$ $L = 0.009$ $I = 60$	$E = 0.071$ $L = 0.009$ $I = 25$
E. Acceptor impurity-arsenic vacancy complex	$E = 0.113$ $L = 0.023$ $I = 95$	$E = 0.063$ $L = 0.025$ $I = 5$			
F. Donor impurity-gallium vacancy complex	$E = 0.318$ $L = 0.071$ $I = 75$	$E = 0.281$ $L = 0.081$ $I = 70$			

*E = optical activation energy (eV) of photoluminescence level, equal to the peak energy subtracted from the band gap energy of 1.521 eV at 20 K.
L = line width (eV) at half maximum height of photoluminescence peak.
I = relative peak intensity.

TABLE II Photoluminescence data at 77 K on horizontal Bridgman n-type GaAs as a function of at. % in the melt

	Conditions of growth: at. % As in melt			
Level type and index	50	51.5	52	55
A. Hydrogenic donor impurity		*$E = 0.003$ $L = 0.024$ $I = 800$	$E = 0.005$ $L = 0.024$ $I = 30$	$E = 0.006$ $L = 0.020$ $I = 17$
E. Acceptor impurity-arsenic vacancy complex	*$E = 0.095$ $I = 10$	$E = 0.087$ $I = 250$		
F. Donor impurity-gallium vacancy complex			$E = 0.271$ $I = 40$	

*E = optical activation energy (eV) of photoluminescence level, equal to the peak energy subtracted from the band gap energy of 1.513 eV at 77 K.
L = line width (eV) at half maximum height of photoluminescence peak.
I = relative peak intensity.

activation energies and line shapes of these peaks generally conform to the predicted values for donors treated in the hydrogenic approximation [13, 14]. That these levels were observed at temperatures of 20 K and above would tend to rule out a general interpretation in terms of excitons since strong quenching of exciton associated luminescence begins to occur at 10 K [3].

A systematic decrease in the half-width of this level with increasing arsenic content in the melt has been observed, and is shown in Fig. 2 for measurements both at 20 and 77 K. Pankove [1] has shown that the half-width of a luminescence profile of a hydrogenic defect is a sensitive function of the concentration of centres responsible for the peak, since it reflects the broadening of the impurity level into a band as the impurity concentration increases. Similar effects have been reported for indium phosphide at 80 K [15]. Using Pankove's results [1], an

TABLE III Electrical and mass spectrometric data on horizontal Bridgman n-type GaAs as a function of at. % As in the melt

	Conditions of growth: at. % As in melt			
Measurement parameter	close to 50	52	55	> 56
μ* (293 K)	4000	3600	4000	1400
n (293 K)	3×10^{17}	2×10^{17}	7×10^{16}	3×10^{16}
n (77 K)	2×10^{17}	1.5×10^{17}	5×10^{16}	1×10^{16}
m	2×10^{17}	2×10^{17}		1×10^{17}
Major impurities from mass spectrometry at concentrations above 2×10^{16} cm^{-3}	Si C O_2	O_2 C		C S O_2

*μ = the Hall mobility of the carriers (cm^2 volt-sec^{-1}).
n = the electron carrier concentration (cm^{-3})
m = the total impurity concentration, assessed by mass spectrometry (cm^{-3}).
Errors in electrical parameters: < 10%.

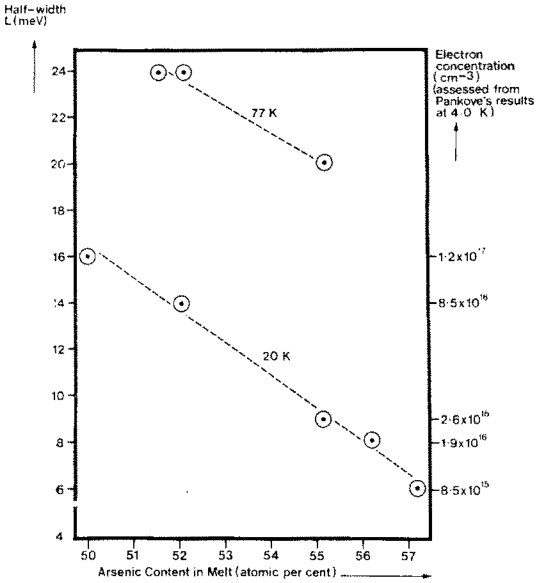

Figure 2 Observed dependence of the half-width of the luminescence peak, indexed A, at 20 and 77 K on the arsenic content in the melt for horizontal Bridgman gallium arsenide (compared through the half-width with the electron concentration given by Pankove's results [1]).

interpretation of the observed behaviour of the half-width of this shallow level suggests that the concentration of these centres is decreased from about 10^{17} cm^{-3} at 50 at. % arsenic to about 10^{16} cm^{-3} at 57 at. % arsenic in the melt. This is generally confirmed by the electrical analysis at 77 K of the electron carrier concentration in the samples as a function of arsenic content in the melt, as shown in Table III.

The linear dependence of the half-width on the concentration of arsenic in the melt might suggest that this behaviour is due to the effect of arsenic pressure on the solubility of an impurity or impurities on an arsenic site. If it were due to impurities substituting on a gallium site, one would expect the impurity concentration to be enhanced by increasing the arsenic pressure.

Mass spectrometric analysis on these samples, as shown in Table III, indicates that donor impurities in sufficient concentrations are either group IV or VI. The group IV impurities are generally amphoteric, with group IV donors replacing gallium atoms in the gallium arsenide lattice, so this means that group VI donors must be responsible.

A possible choice from the group VI donors (substituting on arsenic sites) would be oxygen, since it readily diffuses into gallium arsenide under most growth conditions and has been analyzed at significant concentrations in the Bridgman samples by mass spectrometry. However, the reported activation energies of oxygen associated levels are much greater than those observed [16]. Of the other group VI impurities, Te_{As}, Se_{As} and S_{As} have been reported with shallow donor levels [5, 17, 18] and, of these, sulphur is more likely to occur as a contaminant.

3.2.2. Peak indexed B

The shallow luminescence B peaks generally observed at 30 ± 1 meV from the band edge in gallium arsenide specimens grown close to stoichiometry (Table I) are identified as simple hydrogenic acceptor levels, in agreement with the activation energies observed for such centres [3, 19].

As was observed for the hydrogenic donor levels, one might expect that the half-width of the luminescence profile of a hydrogenic acceptor level to be a sensitive function of the concentration of centres responsible for this peak. There is a trend of decreasing half-width with increasing excess arsenic conditions during growth, which might suggest an interpretation of the acceptors responsible for this peak in terms of those substituting on arsenic sites. From mass spectrometric analysis (Table III) and activation energies of shallow acceptor impurities previously reported [3, 17], the most likely acceptor impurities to explain the B luminescence peaks are Si_{As} at 0.029 eV [20, 21] and C_{As} at 0.015 eV [17].

3.2.3. Peaks indexed C and D

The luminescence emission profile, indexed C, was observed only at 20 K with an optical activation energy of about 36 meV. Two possible interpretations of this line have to be considered. Firstly, the C peak could be similar in nature to the hydrogenic acceptor impurity levels (e.g. Si_{As}) associated with the B peaks, shifted to lower photon energies due to increased acceptor doping or compensation [3, 22]. Photoluminescence measurements at 5 K on epitaxial gallium arsenide have recently associated the silicon acceptor with a binding energy of 35.2 meV [23].

Secondly, the C peak has a number of features (such as activation energy and line shape) in common with the so-called native defect emission profile, observed independently by Williams [2, 5] and Hwang [4] in both melt-grown and epitaxial gallium arsenide, prepared under non-stoichiometric conditions.

The C peaks were only observed in the present experiments in samples grown under non-stoichiometric conditions (i.e. under extreme conditions of arsenic excess). The relative intensities of these peaks were significantly greater than those observed for the associated hydrogenic impurity B peaks (Table I), which would indicate that the number of radiative centres for the C emission was greater.

If the C peak were associated with an acceptor impurity substituting on an arsenic site (e.g. Si_{As}), one would expect that the number of radiative centres would decrease under arsenic excess conditions, rather than the observed increase. Although acceptor impurities substituting on gallium sites (e.g. Cd_{Ga}) have been reported [3, 23] with activation energies close to that of the C emission line, there is no evidence from mass spectrometry (Table III) for high concentrations of these acceptors in the present samples. Thus, it is considered that the C emission is of different nature to the B acceptor impurity emission, and may be due to a native defect, the nature of which is discussed in Section 4.

The luminescence profile, indexed D, at an energy of 36 meV below the photon energy of the C peak is identified as a longitudinal optical phonon replica, as reported by Williams [2, 5]. Further evidence for associating the C peak with the native defect level is the observation that the intensity of the D peak relative to the C peak remains constant from sample to sample [5]. Also, from high temperature annealing experiments, previously reported [7], the shape and photon energy of the C peak were changed by annealing under potentially different conditions of gallium excess, which indicated that the concentration of this level was changed by the heat-treatments.

A possible reason for the lower intensity of the C peak at 57 at. % arsenic with respect to that at 56 at. % arsenic in the melt (Table I) may be the greater probability of non-radiative transitions, at the extreme arsenic excess condition, due to increased inhomogeneous distribution of defects responsible for the emission, as discussed in Section 4.

3.2.4. Peaks indexed E and F

Bridgman gallium arsenide grown under conditions close to stoichiometry show a photoluminescence peak, indexed E, in the energy range 63 to 113 meV from the band edge emission. The activation energy of this type of emission line is consistent with those reported for complex centres associated with an arsenic vacancy and acceptor impurity [6, 24, 25], as shown in Fig. 3. Considering the limited experimental evidence available, there appears to be a basic difference in the temperature dependence of photon energy between those arsenic vacancy complexes which have acceptor impurities which replace gallium atoms (e.g. V_{As}–Cd_{Ga} and V_{As}–Zn_{Ga} [24]) and those which replace arsenic atoms (e.g. V_{As}–Ge_{As} [6]) in the gallium arsenide lattice, as shown in Fig. 3. If it is assumed that the E peaks observed at 20 and 77 K in the sample grown at the stoichiometric composition (S50) are associated with the same centre, then an interpretation of this centre in terms of a complex involving an arsenic vacancy and an impurity substituting for gallium in the gallium arsenide lattice might be consistent with the observed similarity in the temperature dependence of photon energy. The E peaks observed in samples grown with approximately 52 at. % arsenic in the melt (S52) show reasonable consistency at the two temperatures of measurement with a complex centre involving an arsenic vacancy and an impurity substituting for arsenic in the gallium arsenide lattice (e.g. V_{As}–Ge_{As} [6] or V_{As}–Si_{As} [6, 26]).

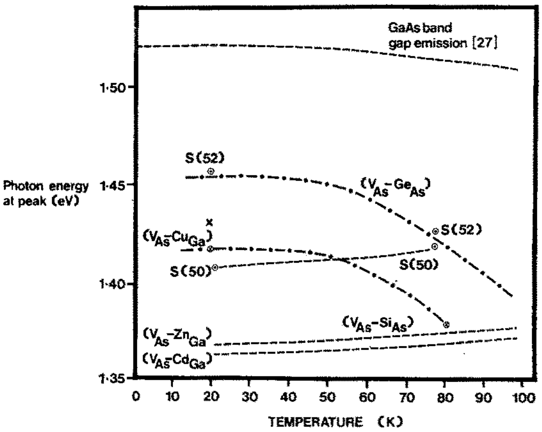

Figure 3 Comparison of the emission peak energy as a function of temperature of the photoluminescence profile, indexed E, for samples grown with 50 at. % (indicated as S(50)) and approximately 52 at. % (indicated as S(52)) arsenic in the melt with those previously published for the arsenic vacancy-acceptor impurity complexes in gallium arsenide: (V_{As}–Zn_{Ga}) and (V_{As}–Cd_{Ga}[24]; (V_{As}–Cu_{Ga}) isolated measurement [25]; (V_{As}–Ge_{As}) and (V_{As}–Si_{As}) [6] (a possible variation of the peak energy of (V_{As}–Si_{As}) complex has been inferred [26] through the two isolated measurements [6], following that given for the (V_{As}–Ge_{As}) complex). (A possible variation through two isolated measurements is also indicated for S(50).)

The optical activation energies in the range 0.271 to 0.318 eV for the luminescence emission, indexed F, observed at 20 and 77 K in samples grown close to stoichiometry are consistent with those in the range 0.289 to 0.340 eV at 77 K for the gallium vacancy-donor impurity complexes, reported by Williams [18]. However, as in the interpretation of the E peaks, there is insufficient reported information, in this case at low enough temperatures, to make a more definite identification of these peaks in terms of the specific donor or donors that are involved in the complex.

3.3. Photoluminescence measurements on other gallium arsenide material

Photoluminescence measurements on Czochralski melt-grown gallium arsenide, grown under gallium excess or stoichiometric conditions, revealed peaks similar in nature to peaks B and E, although there was also evidence of copper or copper associated peaks [2, 3]. This material was either p-type or semi-insulating. There was no evidence in material grown under gallium excess conditions for peaks similar in nature to peaks C and D, observed in the Bridgman samples.

Photoluminescence measurements on heavily tellurium doped epitaxial gallium arsenide showed only an emission line with an optical activation energy of 53 meV, which might be associated with tellurium.

4. Discussion

As a function of growth stoichiometry, the photoluminescence data on the n-type Bridgman gallium arsenide indicated that material grown close to the stoichiometric composition had a significant concentration of both gallium and arsenic vacancies associated with substitutional impurities or complexed with nearest or next nearest neighbour impurity atoms [18]. As the growth conditions became more non-stoichiometric on the arsenic-rich side of the phase, the concentration of these centres decreased, until at growth conditions corresponding to 56 at. % arsenic in the melt, only shallow substitutional donors, responsible probably for the n-type conduction, were observable optically. However, at these high non-stoichiometric melt concentrations, a new centre, possibly associated with a native defect, was observed in the photoluminescence spectra.

Lattice parameter and density measurements were performed on the gallium arsenide specimens in order to ascertain the nature of the defects responsible for the native defect level. These results, summarized in Table IV (the lattice parameter measurements have been reported previously [8]), show that both the lattice parameter and density increase with increasing arsenic content in the melt, becoming significant above arsenic melt concentration of 56 at. %. Thus, the gallium arsenide samples grown under extreme arsenic excess conditions, which show the native defect level, are also the only samples to show significant changes in lattice parameter and density.

TABLE IV Lattice parameter and density data on horizontal Bridgman GaAs as a function of at. % As in the melt

	Conditions of growth: at. % As in melt		
Measurement parameter	50	56	57
$a^* \pm \Delta a$	5.653 241 ± 0.000 003	5.653 263 ± 0.000 009	5.653 278 ± 0.000 027
ρ	5.317 2	5.317 5	5.317 9

$^*a$ = the lattice parameter (Å), corrected for refraction, at 300 K (the error in a is less than ± 0.000 003 Å)
Δa = the variation in lattice parameter, given as a standard deviation on a, across a sample.
ρ = the density (g cm^{-3}) at 300 K (the error in ρ is ± 0.0002 g cm^{-3}).

From this evidence and an analysis of the number of atoms per unit cell in stoichiometric and arsenic-rich gallium arsenide, as shown in the Appendix, it is possible that the defects primarily responsible for deviations from stoichiometry in arsenic-excess material are arsenic interstitials, in concentrations up to 3 × 10^{18} cm^{-3}, and that these defects may be associated with an energy level of 0.036 eV, as observed by photoluminescence. Antistructure disorder, which may also account for the observed changes in lattice parameter and density, generally requires charge and size similarity between the atoms involved in the replacement [28], and may not be likely in the partially ionic sphalerite structure of gallium arsenide. Since this structure is fairly open, it may favour an interstitial disorder occurring in potentially arsenic-rich material. Other possible causes for the experimental observations, in terms of gross inhomogeneities, variations in impurity concentration or dislocation density, have been analysed and appear unlikely [8].

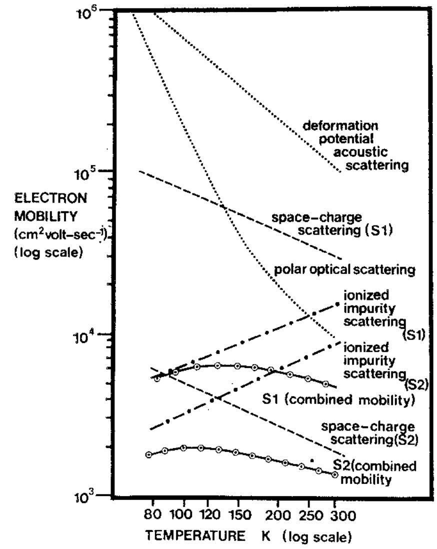

Figure 4 Analysis of the temperature dependence of electron mobility for gallium arsenide grown close to the stoichiometric composition (S1) and grown under extreme conditions of excess arsenic (S2) (the combined mobilities, calculated from the theoretical mobility curves, are shown through the experimental points).

The general inhomogeneity of gallium arsenide samples, grown under excess arsenic conditions, as monitored by the non-uniformity in the lattice parameter, appears to increase with increasing arsenic content in the melt [8] (Table IV). An independent assessment of homogeneity has been made electrically on the Bridgman specimens by an analysis of the electrical carrier mobility as a function of temperature in terms of ionized impurity scattering [29] and space charge scattering from inhomogeneous regions [30], allowing for other scattering mechanisms [31], as shown in Fig. 4. (A full account of this technique has been given by Wolfe *et al.* [31]). For a sample, grown with less than 56 at. % arsenic in the melt, ionized impurity scattering is found to be the most important scattering mechanism limiting the carrier mobility over the measured temperature range, combining with polar optical scattering at the higher temperatures. For such a sample, space charge scattering is only of secondary importance. For a sample grown with more than 56 at. % arsenic in the melt, space charge scattering is important over the entire temperature range, combining with ionized impurity scattering below about 200 K. These results suggest that non-stoichiometric point defects, associated with arsenic excess, are inhomogeneously distributed within crystals grown under extreme conditions of excess arsenic, and thus tend to confirm the observations regarding inhomogeneity obtained from lattice parameter measurement.

No change in lattice parameter or density was observed for the gallium arsenide grown under gallium excess conditions compared with that for the stoichiometric material, confirming photoluminescence observations. The effect of heavy doping on the lattice parameter of gallium arsenide has already been discussed in a previous paper [8].

5. Conclusions

1. Systematic differences between the photoluminescence data obtained from gallium arsenide single crystals grown under conditions close to stoichiometry and those grown under extreme arsenic excess conditions have been observed.

2. The linear dependence of the half-width of a photoluminescence profile associated with a shallow donor (and acceptor) impurity centre, observed in gallium arsenide grown under both stoichiometric and non-stoichiometric conditions, on the concentration of arsenic in the melt suggests that this behaviour is due to the effect of arsenic pressure on the solubility of a donor impurity or impurities on an arsenic site.

3. Gallium arsenide grown close to the stoichiometric composition appears from the photoluminescence measurements to have a significant concentration of both gallium and arsenic vacancies, associated with substitutional impurities or complexed with nearest or next nearest neighbour impurity atoms. As the growth conditions become more non-stoichiometric on the arsenic-rich side of the phase, the concentration of these centres is decreased.

4. Under growth conditions of extreme excess arsenic, gallium arsenide shows the presence of a photoluminescence centre associated with a native defect with an activation energy of about 36 meV. Materials which show this native defect level have lattice parameters and densities significantly higher than materials which do not show such a photoluminescence centre.

5. It is suggested that defects present in arsenic-rich gallium arsenide are arsenic interstitials in concentrations up to 3×10^{18} cm^{-3}.

6. Electrical and lattice parameter measurements indicate that the non-stoichiometric defects associated with arsenic excess are inhomogeneously distributed within crystals grown under extreme conditions of excess arsenic.

6. No detectable extent to the gallium-rich side of the gallium arsenide phase was observed from lattice parameter, density and photoluminescence measurements.

6. Appendix

Analysis of the mode of non-stoichiometric incorporation from measurements of lattice parameter and density

A compound A_xB_y, containing on average x A atoms and y B atoms, is assumed to be stoichiometrically correct when it contains one A atom and one B atom per unit cell. The respective masses of one A atom and one B atom are Z_A/N_0 and Z_B/N_0, where N_0 is Avogadro's number, and Z_A and Z_B are the respective constituent's atomic weights. Thus, the average mass of one unit cell of A_xB_y is equal to $(xZ_A + yZ_B)/N_0$.

The density, ρ, of homogeneous compound A_xB_y is equal to the average density of one unit cell, i.e.

$$\rho = (xZ_A + yZ_B)/N_0 v \qquad (1)$$

where v, the volume of one unit cell for a cubic crystal, equals a^3, where a is the lattice parameter.

For a stoichiometric crystal,

$$\rho_0 = (Z_A + Z_B)/N_0 v_0 \, . \qquad (2)$$

For vacancy disorder on the A sublattice, $x < 1$, $y = 1$, and, therefore, $(Z_A + Z_B) > (xZ_A + Z_B)$, so, from Equations 1 and 2,

$$(\rho v)_{A_xB} < (\rho_0 v_0)_{AB} \, .$$

Similarly, for vacancy disorder on the B sublattice,

$$(\rho v)_{AB_y} < (\rho_0 v_0)_{AB} \, . \qquad (3)$$

For interstitial disorder on the A sublattice, $x > 1$, $y = 1$, and, therefore, $(Z_A + Z_B) < (xZ_A + Z_B)$, so, from Equations 1 and 2,

$$(\rho v)_{A_xB} > (\rho_0 v_0)_{AB} \, .$$

Similarly for interstitial disorder on the B sublattice,

$$(\rho v)_{AB_y} > (\rho_0 v_0)_{AB} \, . \qquad (4)$$

Antistructure disorder can be treated in a similar way. If an average fraction, g, of one atom type is involved in substitution on the sites of the other atom type, such that $x = 1 - g$, $y = 1 + g$, then, from Equations 1 and 2, $g = (v\rho N_0 - (Z_A + Z_B))/(Z_B - Z_A)$ and

$$(\rho v)_{A_xB_y}/(\rho_0 v_0)_{AB} = 1 + [g(Z_B - Z_A)/(Z_B + Z_A)] \, . \qquad (5)$$

These relations hold for simple defects, assuming no interaction.

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