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Vibrational modes of sulphur–copper donor–acceptor pairs in GaP: effects of increasing local force constants by impurity pairing

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Abstract

Sulphur doped GaP crystals compensated by in-diffused Cu show gap modes at 272.5 and 266.2 cm^{-1} from isolated ionized single donors, $^{32}S_P^+$ and $^{34}S_P^+$ respectively, and new gap modes at 311.5 and 304.7 cm^{-1}, attributed to the two isotopes of sulphur present as S_P^+–Cu_{Ga}^{2-} nearest neighbour pairs that are single acceptors. The $^{32}S_P^+$–Cu_{Ga}^{2-} pair also gives rise to a localized vibrational mode (LVM) at 408.1 cm^{-1}. There is evidence that pairing ceases once electrical compensation is achieved when $[S_P^+] = [S_P^+–Cu_{Ga}^{2-}]$. A comparison of the experimental frequencies with simulated values using Green functions methods based on *ab initio* perfect lattice modes shows that the stretch force constant of the S–Ga bond is increased when pairing has occurred. The strong force constant of the S–Cu nearest neighbour pair explains the presence of the LVM. S_{As}^+–Cu_{Ga}^{2-} pairs in GaAs also give rise to an LVM but isolated S_{As}^+ donors do not. The observations link to further LVM data for Si_{Ga}–Cu_{Ga} pairs in GaP and GaAs.

1. Introduction

Calculations using *ab initio* procedures [1] show that, in agreement with neutron scattering measurements [2], there is a gap between the bands of acoustic and optic phonons of GaP from 255 to 326 cm^{-1}. Replacement of a phosphorus atom (^{31}P, 100% abundant) by an impurity with a mass in the range 87 to 37 amu and with no change in the local force constants is expected to give rise to a vibrational gap mode [3]. Infra-red (IR) absorption measurements show that ionized sulphur donors, $^{32}S_P^+$ (95% abundant) and $^{34}S_P^+$ (5%), show gap modes at surprisingly low frequencies of 272.5 and 266.3 cm^{-1}, respectively [4], although their atomic masses are only marginally greater than that of ^{31}P. Very large reductions (around 50%) in the stretch force constant (using a Keating type of description [5]) of nearest neighbour bonds are

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needed to reproduce the measured frequencies. A proposal that the weakening of the force constants is associated with Coulombic repulsion between S_P^+ ions and their positively charged Ga neighbours is discussed briefly in section 4.

Gap modes are not detected for neutral S_P^0 donors, although their frequencies are expected to be little changed from those of S_P^+ since the radius of the Bohr orbit (5.22 Å) is much larger than the nearest neighbour separation (2.36 Å). An explanation for this 'non-observation', involving a large reduction in the dipole moment, has already been proposed [4].

Strong S_P^+ gap modes have only been detected in samples fully compensated by electron traps introduced at room temperature by 2 MeV electron irradiation although weaker lines are detected in samples partially compensated by remote carbon acceptors introduced inadvertently during crystal growth [6]. An alternative way of achieving electrical compensation is to diffuse copper atoms into the crystal. This procedure has been demonstrated for the compensation of silicon-doped *n*-type GaAs [7, 8] and GaP [9, 10]. Diffusing copper atoms are trapped by silicon atoms to form second neighbour Si_{Ga}–Cu_{Ga} pairs, although localized vibrational modes (LVMs) from isolated Si_{Ga} donors are still detected in fully compensated samples. The measurements imply that Cu_{Ga} is a double acceptor in both host crystals. The diffusion of copper into sulphur doped GaP or GaAs should therefore produce S_P^+–Cu_{Ga}^{2-} and S_{As}^+–Cu_{Ga}^{2-} nearest neighbour pairs, respectively, that are expected to be single acceptors. These pairs should then compensate an equal number of isolated S_P or S_{As} donors.

The principal new results of this paper relate to measurements of the vibrational modes associated with (S_P^+–Cu_{Ga}^{2-}) pairs in GaP (section 2) and their analysis in terms of changes in local force constants (section 3): corresponding measurements for GaAs:S–Cu are also reported briefly in section 2.2. These force constant changes are determined using an *ab initio* description of the pure GaP lattice and fitting to the observed frequencies by Green function procedures. It will be shown that the S_P^+–Cu_{Ga}^{2-} bond is stronger than the perfect lattice bonds and the Ga–S_P^+ bond is stronger than the corresponding bond of the isolated S_P^+ impurity.

2. Experimental details

2.1. Sample preparation and measurement techniques

GaP:S and GaP:Si crystals, grown by the liquid encapsulated Czochralski (LEC) method, and GaAs:S and GaAs:Si crystals, grown by the horizontal Bridgman technique, were studied. The sulphur concentrations of four GaP crystals were determined to be 4.2×10^{18}, 3.9×10^{18}, 2.5×10^{18} and 1.5×10^{18} cm^{-3}, using the calibration data discussed in the appendix of [4]: it should be noted that these samples had different thicknesses. The Si concentration in another GaP crystal was 4×10^{18} cm^{-3}. Free carriers in GaP:S and GaP:Si are frozen out at the measurement temperature because of their relatively large ionization energies of 107.3 and 85 meV, respectively: S and Si donors in GaAs are, however, both shallow donors and freeze out does not occur at high doping levels. Some samples from each ingot were fully compensated by 2 MeV electron irradiation at room temperature [4]. Other samples were coated with copper nitrate, sealed in silica ampoules and annealed for approximately 20 hours at 1000 and 930 °C for GaP and GaAs, respectively.

Infrared spectra were obtained using a Bruker IFS 120 HR interferometer operated at a resolution of 0.1 cm^{-1} with the samples at about 10 K. Spectra of undoped crystals were subtracted from these spectra to remove intrinsic two-phonon features. This procedure, used to reveal absorption lines that occur close to the reststrahl, requires careful preparation of sample thicknesses because of the very strong intrinsic absorption in this spectral region: the samples also have to be wedged to prevent interference fringes appearing in recorded spectra.

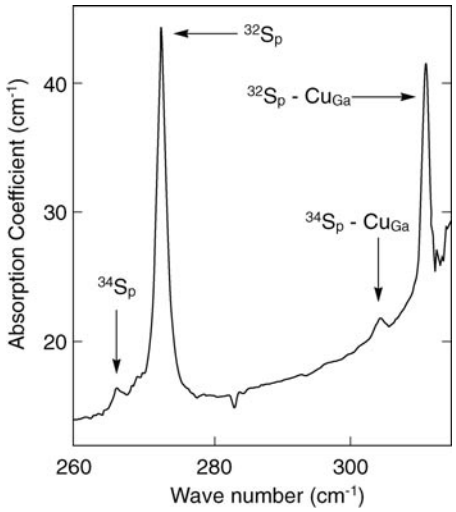

Figure 1. Absorption spectrum of a sulphur doped GaP sample fully compensated by Cu diffusion showing gap modes from the two isolated S isotopes, together with transverse gap modes from the two sulphur isotopes present as S_P–Cu_{Ga} pairs.

2.2. Infrared spectra

The absorption spectrum of a copper-diffused GaP:S sample at frequencies below the reststrahl region (figure 1) shows a gap mode due to $^{32}S_P^+$ at 272.5 and a weak gap mode from $^{34}S_P^+$ (5% abundant) at 266.2 cm^{-1}, giving an isotopic separation of 6.3 cm^{-1}, as reported previously [4]. The sample also shows lines at 311.5 and 304.7 cm^{-1} with a separation of 6.8 cm^{-1} and relative integrated absorption coefficients (IAs) that correspond to the isotopic abundances of ^{32}S and ^{34}S. It is inferred that these lines are due to gap modes of $^{32}S_P$–Cu_{Ga} and $^{34}S_P$–Cu_{Ga} pairs, respectively. No fine splitting of the modes due to the mixed copper isotopes, namely ^{65}Cu (30.9%) and ^{63}Cu (69.1%), was detected.

An LVM at 408.1 cm^{-1}, close to the reststrahl (figure 2) is also assigned to the paired $^{32}S_P$ atoms (C_{3v} symmetry) because, as indicated in figure 3, the ratio IA(LVM)/IA(gap mode at 311.5 cm^{-1}) is, within experimental error, the same for the four samples and is equal to ∼0.3. If (a) the LVM is due to a longitudinal non-degenerate mode and the gap mode is due to doubly degenerate transverse vibrations of the S_P–Cu_{Ga} pairs and (b) the dipole moments associated with the two types of mode were equal, the ratio would be 0.5. Assumption (b) can only be an approximation since displacements of the Cu impurity may be appreciable in the longitudinal LVM eigenvector but not in the transverse gap mode eigenvectors. An LVM with a lower frequency due to $^{34}S_P$–Cu_{Ga} pairs was not detected.

A plot of the sum of the IAs of the modes of S_P–Cu_{Ga} pairs versus the sum of the IAs of the modes of isolated S_P^+ for the four samples is linear with a gradient of 0.56 (figure 4), demonstrating that the ratio of the concentrations $[S_P^+$–$Cu_{Ga}^{2-}]/[S_P^+]$ is the same for all the samples. If $[S_P^+$–$Cu_{Ga}^{2-}]$ were equal to $[S_P^+]$, a gradient of unity might have been expected but only if all the dipole moments were equal (see above). A somewhat smaller ratio of 0.42 was then determined for the sum of the IAs of the modes due to Si_{Ga}–Cu versus the IA of the isolated Si_{Ga} mode present in a Cu diffused GaP:Si sample (figure 5). The lower frequency line (two unresolved modes) at 454.5 cm^{-1} and the higher frequency line at 485.3 cm^{-1} are due to modes of second neighbour Si_{Ga}–Cu pairs: the strongest line at 465.5 cm^{-1} is due to isolated $^{28}Si_{Ga}$

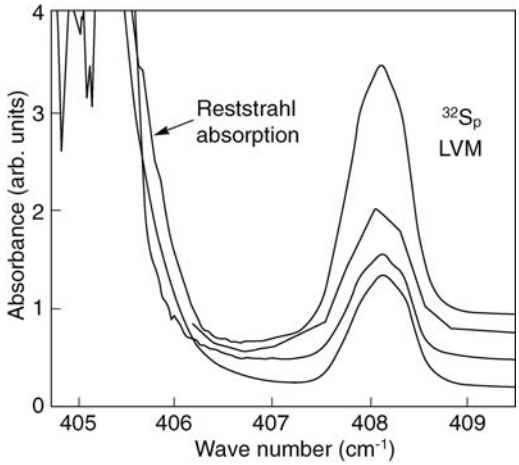

Figure 2. The absorption profiles of the LVM from the $^{32}S_P^+$–Cu_{Ga}^{2-} pair at 408.1 cm^{-1} showing incompletely resolved fine structure for four samples with sulphur concentrations of 4.2×10^{18}, 3.9×10^{18}, 2.5×10^{18} and 1.5×10^{18} cm^{-3}. The very broad absorption for frequencies below 405.7 cm^{-1} is due to the GaP reststrahl band: LVMs centred at or below this frequency would not be detected.

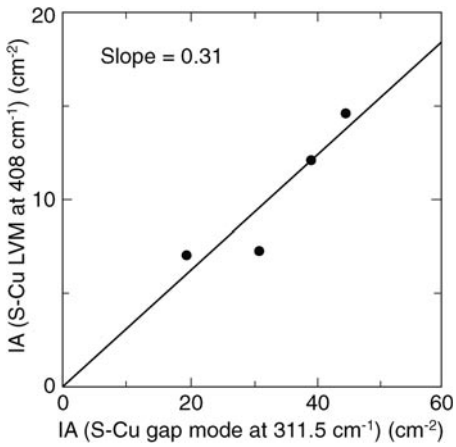

Figure 3. The integrated absorption coefficient, IA, of the LVM at 408.1 cm^{-1} plotted versus the IA of the gap mode at 311.5 cm^{-1} of $^{32}S_P^+$–Cu_{Ga}^{2-} pairs for the same four samples (see figure 2), showing correlation of the strengths of the two IR lines.

donors. We note that the corresponding lowest frequency absorption feature in GaAs is clearly split into two close lines [8]. These results for GaP:Si again imply that the dipole moments for the modes of S_P^+–Cu_{Ga}^{2-} pairs are smaller than those of the isolated S_P^+ donor atoms.

The gap modes due to the $^{32}S_P$–Cu_{Ga} pairs appear as symmetrical absorption lines with full widths at half maximum (Δ) of $\approx$1.0 cm^{-1}, comparable with the widths ($\Delta \approx$ 1.2–1.4 cm^{-1}) of the gap modes of the isolated sulphur atoms (figure 1). This similarity is expected as it was shown previously that the lines from the gap modes are broadened due to the rapid decay of the excitation to modified lattice modes [4] and related lifetime broadening effects are likely for the gap modes from S_P–Cu_{Ga} pairs. The broadening accounts for the absence of fine structure due to the various combinations of ^{69}Ga (60%) and ^{71}Ga (40%) neighbours. Without

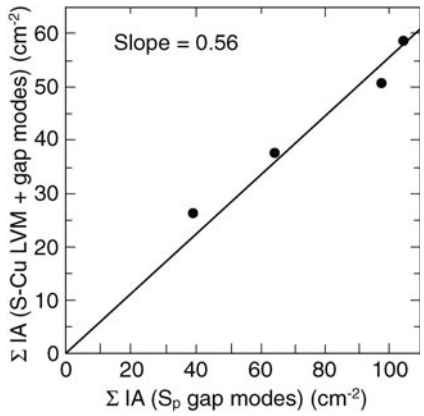

Figure 4. A plot of the total integrated absorption coefficient, $\sum IA$ (gap modes + LVM), of the modes of S_P^+–Cu_{Ga}^{2-} pairs versus the $\sum IA$ of the gap modes of isolated S_P^+ for the same four samples (see figure 2), showing a constant ratio of the IAs for the paired centres and the isolated sulphur donors.

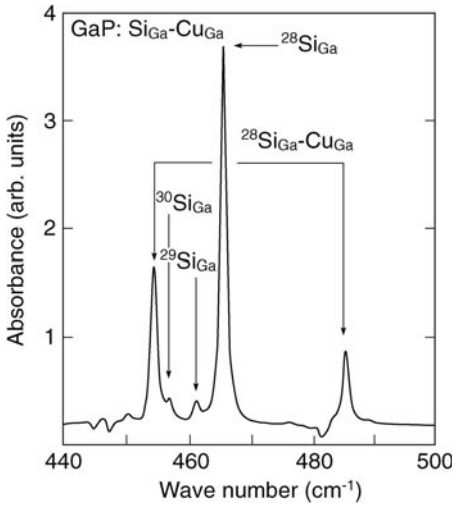

Figure 5. IR absorption from a GaP:Si sample following in-diffusion of Cu, showing the modes due to isolated Si_{Ga} donors (465.6 cm^{-1}) and the modes of Si_{Ga}–Cu_{Ga} pairs (454.5 and 485.3 cm^{-1}) that have C_s symmetry. The lower frequency pair feature is an unresolved superposition of two lines: the corresponding feature for GaAs:Si–Cu is resolved [10].

such broadening, the doubly degenerate transverse mode of the paired S_P donors would show a four-line structure as for other defects with C_{3v} symmetry such as a carbon acceptor paired with an arsenic interstitial atom in irradiated GaAs [11]. Comments concerning weak fine structure observed for the LVM profile (figure 2) are given in section 4.

We also made measurements on sulphur doped GaAs that had been compensated either by 2 MeV electron irradiation at room temperature or by copper diffusion. As found previously, the irradiated GaAs:S crystals did *not* show a $^{32}S_{As}$ LVM [9]. However, Cu diffused samples that incorporated nearest neighbour S_{As}^+–Cu_{Ga}^{2-} pairs showed a featureless LVM, with $\Delta = 1.1\,cm^{-1}$ at 303.5 cm^{-1} on the edge of the reststrahl band (figure 6).

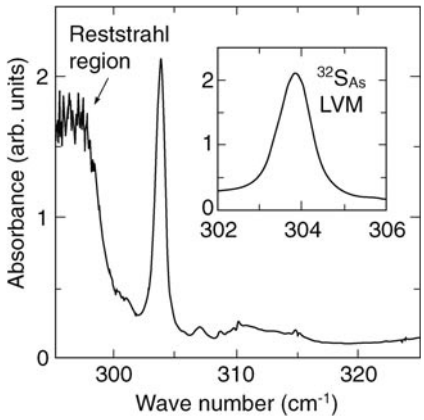

Figure 6. The LVM at 303.5 cm^{-1} attributed to the longitudinal mode of the $^{32}S^{+}_{As}$–Cu^{2-}_{Ga} pair in GaAs. This line is located about 4 cm^{-1} above the edge of intense absorption from the GaAs reststrahl band that fortuitously appears small because of the differencing with an undoped GaAs reference sample with a closely matched thickness (see section 2.1).

3. Theoretical analysis of gap mode frequencies

In this section, results obtained from modelling of the sulphur–copper pairs in GaP are obtained and compared with measurements reported in the previous section. The initial stage is to construct Green functions for the pure host crystal from normal mode eigenvectors and frequencies calculated [1] for GaP by an *ab initio* local density functional response technique [3, 12] using pseudopotentials to represent core electrons. The corresponding Green functions for the defective lattice containing the impurity atoms are formed by the standard Lifshitz procedure [13] and require values for the changes in force constants around the impurity. We specify these force constants using a Keating type of description [5]: stretch and bend force constants are designated by α and β, respectively. The gap mode frequencies are identified by poles in the Green functions of the defective lattice.

The nearest neighbour stretch force constant (α) for pure GaP using the Keating model is close to 38 N m^{-1}. The principal change when an isolated S_P impurity is present is a large reduction, $\delta\alpha$, for the bond between the S_P atom and its nearest neighbour Ga atoms [4]. The gap mode frequencies obtained with $\delta\alpha = -19.3$ N m^{-1} (and no other change in force constants) are 266.14 cm^{-1} for the $^{34}S^{+}_{P}$ impurity and 272.4 cm^{-1} for the $^{32}S^{+}_{P}$ impurity, reproducing the measured values.

We next determine the changes in the local force constants that would reproduce the observed impurity-related vibrational frequencies of S_P–Cu_{Ga} pairs. In our simplest model, we allow only changes of two force constants, namely for the stretch in the bonds between the S_P atom and its three nearest neighbour Ga atoms ($\delta\alpha$) and for the stretch in the bond between the S_P atom and its Cu_{Ga} neighbour ($\delta\alpha'$). The changes are adjusted to give a fit to the two measured frequencies for the modes of the $^{32}S_P$–Cu_{Ga} pair, i.e. the doublet gap mode at 311.5 cm^{-1} and the singlet LVM at 408.1 cm^{-1}. The gap mode frequency is essentially independent of the choice made for $\delta\alpha'$ and the experimental value (311.5 cm^{-1}) is reproduced by taking $\delta\alpha = -10.1$ N m^{-1}. This reduction in the force constant for the S–Ga bonds is only about 50% of the reduction (-19.3 N m^{-1}) required to reproduce the experimental frequency (272.5 cm^{-1}) of the isolated sulphur impurity. The derived frequency of 304.5 cm^{-1} of the $^{34}S_P$–Cu_{Ga} pair then agrees with the measured value. To obtain the LVM frequency for

Table 1. Calculated fine structure of the $^{32}S_P^+$–Cu^{2-} LVM at 408 cm^{-1}, taking account of the presence of ^{63}Cu and ^{65}Cu as well as ^{69}Ga and ^{71}Ga.

Cluster composition	Weighting factor	Calculated LVM frequency (cm^{-1})
$^{69}Ga_3\ ^{32}S_P\ ^{63}Cu_{Ga}$	0.149	408.114
$^{69}Ga_2\ ^{71}Ga\ ^{32}S_P\ ^{63}Cu_{Ga}$	0.299	408.102
$^{69}Ga\ ^{71}Ga_2\ ^{32}S_P\ ^{63}Cu_{Ga}$	0.199	408.091
$^{71}Ga_3\ ^{32}S_P\ ^{63}Cu_{Ga}$	0.044	408.080
$^{69}Ga_3\ ^{32}S_P\ ^{65}Cu_{Ga}$	0.067	406.919
$^{69}Ga_2\ ^{71}Ga\ ^{32}S_P\ ^{65}Cu_{Ga}$	0.133	406.907
$^{69}Ga\ ^{71}Ga_2\ ^{32}S_P\ ^{65}Cu_{Ga}$	0.089	406.896
$^{71}Ga_3\ ^{32}S_P\ ^{65}Cu_{Ga}$	0.020	406.884

the $^{32}S_P$–Cu_{Ga} pair, $\delta\alpha'$ is set equal to +14.5 N m^{-1}. The derived frequency of the LVM of $^{34}S_P$–Cu_{Ga} pairs is calculated to be at 402.1 cm^{-1}, down-shifted by 6.0 cm^{-1} from that for the $^{32}S_P$–Cu_{Ga} pair: this shift cannot be verified experimentally as the line would be obscured by the intense reststrahl absorption up to 405.7 cm^{-1} (figure 2).

A more detailed set of calculations for the ^{32}S–Cu_{Ga} pair, with the same two changes in force constant but taking account of the isotopes of both copper and gallium, was then made to investigate fine structure effects. The results for the LVMs are given in table 1: the upper block is for pairs incorporating ^{63}Cu and the lower block for ^{65}Cu. The weighting factors given for the different isotopic arrangements are obtained from the natural isotopic abundances. The LVMs included in the upper block have frequencies greater than those in the lower block by roughly 1.2 cm^{-1}, while the overall spread in each block, due to the mixed ^{69}Ga and ^{71}Ga isotopes, is only 0.035 cm^{-1}. The model therefore implies that the LVM from the paired $^{32}S_P$ atom should show a two-line fine structure due to the mixed copper isotopes but this simple structure is not observed (figure 2). It should be noted that the frequencies, especially for modes involving the ^{65}Cu isotope, are not much above the reststrahl band. It is possible that with a more extended set of force constant changes the predicted motion of the Cu atom in the LVM could be increased with a consequent downshift of the ^{65}Cu components into the reststrahl band. Softening of the force constants between the Cu atom and its three P neighbours would have this effect. This would mean that the observed simple structure was due solely to the $^{32}S_P$–$^{63}Cu_{Ga}$ combination. For the gap modes, the atomic displacements are essentially perpendicular to the S–Cu bond and the calculated frequencies for the ^{63}Cu and ^{65}Cu blocks of modes differ by only 0.013 cm^{-1}. Ga isotope effects are more important for these modes and lead to a spread within each block of 0.515 cm^{-1}. As discussed earlier, there may be broadening of the gap modes due to anharmonicity that would veil this structure.

The effect of making some additional changes to force constants was examined, including an increase in the Ga–S–Ga bond angle force constant ($\delta\beta$) by 16.6 N m^{-1} and changes to $\delta\alpha$ (-13.0 N m^{-1}) and $\delta\alpha'$ ($= +12.1$ N m^{-1}). These further modifications to the calculations did not lead to any significant increase in the fine structure due to the mixed Ga isotopes.

4. Summary and discussion

IR measurements show that the pairing of sulphur donors with nearest neighbour substitutional copper double acceptors leads to the presence of associated gap modes and a local mode situated

just above the reststrahl region of the GaP lattice. Gap modes of the trigonal complexes incorporating $^{32}S_P$ and $^{34}S_P$ are separated by 6.8 cm^{-1} and are assigned to the doubly degenerate transverse modes. These modes have higher frequencies (+39 cm^{-1}) than the corresponding pair of modes from isolated sulphur donors that are separated by 6.2 cm^{-1}. The LVM is assigned to the non-degenerate longitudinal mode of $^{32}S_P$–Cu pairs.

The frequencies of all the modes are reproduced by our theoretical analysis and this also shows that the LVM from $^{34}S_P$–Cu pairs would be resonant with the reststrahl region of the GaP lattice so that it could not be detected. Theoretical modelling of the $^{32}S_P$–Cu pairs required the stretch force constant for the $^{32}S_P$–Ga bond (α) to be greater than that for isolated $^{32}S_P$ atoms by around 10 N m^{-1}, to explain the higher frequency of 311.5 cm^{-1} of the gap mode of the pair centre. An increase in the stretch constant of the $^{32}S_P$–Cu_{Ga} bond by 14.5 N m^{-1} compared with the constant for $^{32}S_P$–Ga is required to account for the emergence of the observed LVM.

The observations imply the cessation of pairing at the stage when there are essentially equal concentrations of isolated and paired S_P^+ donors. However, it is certain that excess Cu would have been introduced by the diffusion at the high temperature. It is speculated that the excess copper atoms are located at sites remote from the sulphur donors in the form of small precipitates. Recent positron annihilation measurements have indicated that diffusion of copper into GaAs:Te_{As} leads to the formation of high concentrations of Ga vacancies that are then decorated with copper atoms [14]. Similar processes are expected in GaP:S samples. It has also been established from IR measurements of both GaAs:Si [7, 9, 15] and GaP:Si [8] that grown-in Si_{Ga}–V_{Ga} second neighbour pairs are absent after copper diffusion due to their conversion to Si_{Ga}–Cu_{Ga} pairs [9]. The IR measurements of GaP:S described in section 2.2 are clearly in accord with those for other III–V compounds.

It is evident from the observed LO–TO splitting at the Γ-point [2] that the perfect crystal is partially ionic with ionicity around 0.7 e. An isolated S^+ impurity atom, replacing a P atom, would repel its four neighbouring positively charged Ga atoms, leading to longer and weaker bonds. On the other hand, a Cu_{Ga}^{2-} impurity would strongly attract its neighbouring S_P^+ donor, so that this bond would be shortened and strengthened. The three remaining S_P^+–$Ga^{(+)}$ bonds would still be 'weak' due to the mutual repulsion of the atoms: however, the Cu^{2-} atom would be more strongly repelled towards the sulphur atom by its three negatively charged P neighbours. Our arguments assume that ion size effects (such as those due to the large size of the Cu ion) are unimportant compared with coulombic effects. A further possible deficiency of our modelling is that no force constant changes were made to the Cu_{Ga}–P bonds. Relative changes in these bond lengths cannot be determined by the type of argument above.

The data in table 1 imply that the LVM due to the $^{32}S_{Ga}$–Cu pairs should have a double peaked structure with the strengths of the high and low frequency components in the ratio of the natural abundance of ^{63}Cu to that for ^{65}Cu, i.e. approximately 7:3. The separation of the peaks is estimated to be about 1.0 cm^{-1} and broadening from Ga isotope effects should be very small. However, the observed structure, common to four samples (see figure 2), shows a single broadened peak ($\Delta \approx 0.7$ cm^{-1}) with some indication of shoulders of equal strength that are separated by around 0.4 cm^{-1}. We have suggested the possibility that only the ^{32}S–^{63}Cu components are observed with the other components (^{32}S–^{65}Cu, ^{34}S–^{63}Cu and ^{34}S–^{65}Cu) being downshifted into the reststrahl band.

The observations for GaP:S–Cu and GaAs:S–Cu are of general interest because, to the best of our knowledge, they provide the only examples of LVMs that are pulled out from the continuum of lattice modes by the formation of a complex with increased force constants.

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