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LETTER TO THE EDITOR

A photoluminescence investigation of local mode vibrations of the beryllium pair centre in silicon

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Abstract. A detailed examination of the spectrum of the isoelectronic bound exciton (IBE) recombination attributed to Be pair centres in Si reveals the presence in the sidebands of a previously unreported sharp local mode phonon of energy 104.7 ± 0.5 meV (844 ± 4 cm^{-1}). The energy of this local vibrational mode is in excellent agreement with a recent prediction of 860 cm^{-1} for the vibrational energy of a pair of Be atoms aligned along a ⟨111⟩ crystal direction where one of the atoms occupies a substitutional site and the other an adjacent tetrahedral interstitial site. This result provides the most convincing evidence to date for assigning the IBE spectrum to Be pair centres with this configuration.

The intense photoluminescence (PL) observed for silicon doped with beryllium has been the subject of several investigations (Henry *et al* 1981, Killoran *et al* 1982, Thewalt *et al* 1982). From the outset, the spectrum was immediately identifiable, by the characteristic zero-phonon line structure and relative line intensities, as the recombination radiation of electron–hole pairs at an isoelectronic centre. The isoelectronic centre was assumed to be a substitutional–interstitial pair of Be atoms that would provide the electrically neutral defect required for the creation of an isoelectronic bound exciton (IBE). Uniaxial stress and Zeeman measurements confirmed the axial nature of the defect, indicating a ⟨111⟩ symmetry axis (Davies, 1984). However, the data did not discriminate between a substitutional–interstitial pair aligned along ⟨111⟩ and a split interstitial (or interstitialcy), where neither of the two atoms occupy the substitutional site.

The formation of complex defects by beryllium in silicon was recently addressed by Tarnow *et al* (1990). These authors calculated the energies of several Be complexes, including the substitutional–interstitial pair and the split interstitial (SIP and SI, respectively). The calculations predicted the SIP to be the most favourable configuration for the Be pair, with a ⟨111⟩ symmetry axis. Furthermore, the modes of vibration of the pair of Be atoms were calculated, and values of 310 cm^{-1} and 860 cm^{-1} predicted for the energies of the symmetric and anti-symmetric modes, respectively. These predictions can be tested by several experimental methods including photoluminescence. In this letter we report the results of a detailed examination of the phonon sidebands of the Be pair IBE recombination spectrum. Sharp well-resolved lines not previously reported are observed

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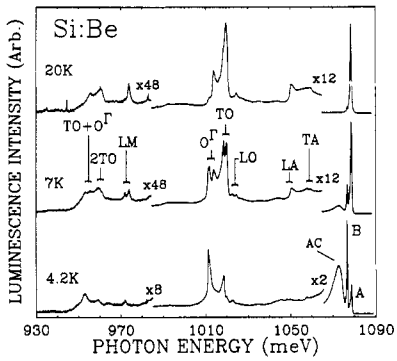

Figure 1. Photoluminescence spectra of Si:Be recorded at 4.2 K, 7 K and 20 K, The spectra have not been corrected for the spectral response of the apparatus. Gain changes for different regions of the spectrum are given in the figure. The labelling of the lines is explained in the text.

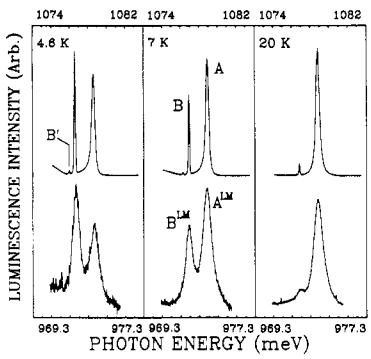

Figure 2. A comparison of the zero-phonon lines and sharp features observed in the sidebands of the Si:Be photoluminescence. The energy axes are shifted to align the A and A^{LM} lines in the diagram.

in the sidebands and found to be in excellent agreement with some of the theoretical predictions for the SIP configuration.

In figure 1 we show PL spectra of Si:Be for several temperatures between 4 K and 20 K. Details of the experimental techniques are described by Henry *et al* (1981, 1987). The strong sharp curves in the region of 1078 meV are the zero-phonon lines, labelled A and B in the figure. Lines A and B originate in the $J = 1$ and $J = 2$ states, respectively, of the IBE. The A transitions ($J = 1$ to $J = 0$) are electric dipole allowed whereas the B transitions ($J = 0$ to $J = 0$) are forbidden. The axial strain at the defect mixes the $J = 1$ and $J = 2$ states, relaxing the latter selection rule somewhat. The strain also causes a small splitting of the $J = 2$ manifold of states producing three levels, two of which are involved in radiative transitions in the absence of external perturbations (Killoran *et al* 1982). The subject of IBE recombination is described thoroughly in a review by Dean and Herbert (1979). Below 4 K, the B lines and their sidebands dominate the spectrum, but for 20 K, the spectrum is composed almost entirely of line A and its sidebands. This change in the spectrum with increasing temperature enables the principal features in the sidebands to be readily identified with particular zero-phonon lines. These identifications have previously been reported but are included here for completeness. Table 1 lists the energies and identifications of the peaks in the spectum; these are also labelled fully in figure 1.

We are concerned principally with the details of the sideband structure in the regions of 970 meV and 1042 meV where the local mode phonon replicas of the zero-phonon lines are expected to occur. In figure 2 we present a comparison of the zero-phonon lines and sharp line structure observed in the 970 meV region. The spectra are displaced in energy to align the positions of line A and the line at 974.2 ± 0.5 meV labelled A^{LM}. There is a direct correspondence between the two regions of the spectrum. The thermal activation energies of the pairs of lines are equal within experimental error. We conclude that these are phonon sidebands of lines A and B involving the creation of local mode vibrations of the pair of Be atoms, as predicted by Tarnow *et al* (1990) for the Be SIP. Our experimental measurements of 104.7 ± 0.5 meV is in excellent agreement with their calculated value of ~107 meV (860 cm^{-1}).

Table 1. Line energies, identifications and energy shifts of phonon sidebands from corresponding zero-phonon lines (ZPL).

	Line energy (meV)	Identity	Energy shift from ZPL (±0.4 meV)
	1078.68	A	—
ZPL	1076.71	B	—
(±0.05 meV)	1076.05	B′	—
Phonon	1071.7	B′(AC)	4.2
sidebands	1059.4	A (TA)	19.3
(±0.3 meV)	1057.6	B (TA)	19.1
	1050.6	A (LA)	28.1
	1048.7	B (LA)	28.1
	1024.6	A (LO)	54.0
	1022.8	B (LO)	53.9
	1019.9	A (TO)	58.8
	1018.6	B (TO)	58.1
	1014.0	A (O^{Γ})	64.7
	1012.4	B (O^{Γ})	64.6
	1011.8	B′(O^{Γ})	64.2
	974.0	A (LM)	104.7
	972.2	B (LM)	104.6
	960.1	A (2TO)	118.6
	958.0	B (2TO)	118.7
	955.7	A (TO + O^{Γ})	122.9
	953.3	B (TO + O^{Γ})	123.4

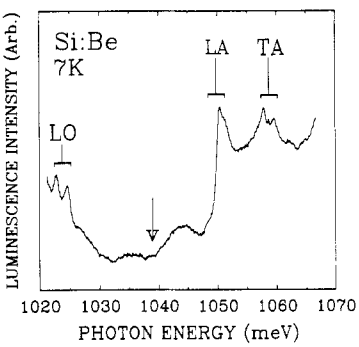

Figure 3. Details of the Si : Be photoluminescence spectrum in the region of 1042 meV for a temperature of 7 K. The arrow indicates the position at which the local mode sideband would be expected.

A local mode vibration of energy 310 cm^{-1} was also predicted by Tarnow *et al* (1990). In figure 3 we show the region of the spectrum in which the corresponding local mode phonon replicas of the IBE zero-phonon lines should occur, indicated by the arrow in the figure. It should be noted that a substantial uncertainty is expected for this calculation. Weak broad peaks are observed in the region of interest. The intensity of the broad peak centred at about 1044 meV diminishes with increasing temperature, indicating a connection with the B lines. The separation of the peak from the B′-line energy agrees with the sum of the AC and LA energies, so we rule out this peak as a local mode replica.

Although the feature at 1035 meV is a possible candidate, the evidence is clearly far too weak for a positive identification.

We have presented a detailed analysis of the phonon sidebands of the Be pair IBE recombination spectrum in Si. A sharp local mode phonon replica of the zero-phonon lines is observed, in addition to a range of one- and two-phonon sidebands involving lattice phonons. The energy of the local mode is in excellent agreement with a predicted anti-symmetric mode of vibration for a Be_s–Be_i substitutional–interstitial pair of Be atoms aligned along a ⟨111⟩ direction. This result is also consistent with previously published Zeeman and uniaxial stress data for the zero-phonon lines and it provides the most conclusive evidence to date for the atomic configuration of the Be pair defect in Si. The excellent agreement between the measured and calculated energies provides strong support for the model used by Tarnow *et al* (1990) for the calculation of defect energies and structures.

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