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Impurity pair modes in a diatomic linear chain: nearest neighbour pair

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Abstract. The behaviour of the impurity modes due to a pair of substitutional impurities characterized by both mass as well as force-constant changes and occupying nearest neighbour positions in a diatomic linear chain, is studied. The results are compared with those for the case of impurity pairs occupying next nearest neighbour sites discussed earlier as well as the existing three dimensional calculations of Elliott and Pfeuty. The nearest neighbour impurity pair gap and local modes can be interpreted in terms of two single impurities substituted in the two different sublattices unlike the next nearest neighbour pair modes. The inband resonant modes are totally new features characteristic of the pair. Finally, the predictions of the theory are compared with the available experimental data for Si-impurity-pair-complexes and qualitative agreement is shown.

Keywords. Impurity pairs; impurity modes; defect lattice dynamics.

1 Introduction

In an earlier paper Behera and Patnaik (1975) (hereafter referred as I) have considered the problem of a pair of mass defect impurities occupying next nearest neighbour sites in a diatomic linear chain. This model implied that the two impurities are similar in nature being either cation or anion type and hence go into any one of the two sublattices in an alkali halide crystal. Such a simple model provided a qualitative explanation for the observed gap mode frequencies in some of the alkali-halide-impurity complexes. The model was extended by including the force-constant changes by Patnaik and Behera (1976) (referred as II) in a suitable manner to explain some of the observed inband resonant modes. However, one can have a pair of dissimilar impurities—say, one of the cation type and the other of the anion type—occupying substitutional sites in the crystal. In such a case the impurity pair will go into the two different sublattices and as a result occupy nearest neighbour positions. Some such pairs have been studied experimentally, *e.g.*, Rb^+H^- (Barth and Fritz 1967) and Na^+H^- (Mirlin and Reshina 1966) pairs in KCl. Or else, these can be pairs of similar or dissimilar impurities substituted into the group IV semiconducting crystals such as Si and Ge where again it is expected that the pair will occupy nearest neighbour positions. Extensive experimental studies of Si containing pairs of Boron and its isotope (*see* Angress *et al* 1965, Newman and Smith 1968) phosphorous, BP, BAs

and BSb (Tsvetov *et al* 1968) have been carried out. Similar experimental results are also available on Si (*e.g.*, Feldman *et al* 1966 and Renucci *et al* 1971) containing Ge and vice versa. In all the above mentioned cases, except for Ge pairs in Si, localized modes characteristic of impurity pairs have been observed whereas in the latter case an inband resonant mode is seen in Raman scattering measurements by Renucci *et al* (1971). Three dimensional models for impurity pairs in Si occupying different configurations have been considered earlier by Elliott and Pfeuty (1967) (EP) using the Green's function method. In doing so they have used a model density of states for Si. In this paper we propose a diatomic linear chain model for such nearest neighbour pairs. It is hoped that by comparing the results of this model with those of the three dimensional calculation one can throw some light on the validity of the linear chain calculations. In section 2 we give a brief discussion of the model and present the results of the theory. Section 3 is devoted to a discussion of the results of the calculation and its comparison with those of EP. We conclude by comparing the predictions of the theory with the experimental data in section 4.

2. Theory

The defects characterized by masses M_1' and M_2' are substituted in nearest neighbour positions in the M_1 and M_2 sublattices respectively. Following the same line of argument as discussed in II we shall assume that the force-constant of the spring connecting the impurities gets changed to γ' whereas that connecting the impurities to the neighbouring host atoms remains unchanged and equal to γ. For such a model the equations of motion and hence the Green's function can be determined exactly using the M^*–transformation (*see* Maradudin *et al* 1971). The impurity modes in the various regions of the frequency spectrum are obtained by equating real part of the denominator of the perturbed Green's function to zero. For the inband regions this equation can be solved analytically and the solution becomes (i) $0 < x \leqslant (\omega_a^2/\omega_m^2)$ and $(\omega_0^2/\omega_m^2) \leqslant x < 1$ the inband regions

$$x = \{(\epsilon_1 a + \epsilon_2 b)\,\tau \mp [\tau^2 (\epsilon_1 a + \epsilon_2 b)^2 + 8\epsilon_1\epsilon_2 \times ab\,(1+\tau)]^{\frac{1}{2}}\}/(4\epsilon_1\epsilon_2 ab). \tag{1}$$

For the gap and outside band regions the equations become (ii) $(\omega_a^2/\omega_m^2) < x < (\omega_0^2/\omega_m^2)$, the gap region

$$1 - \{\epsilon_1 a\,(y')^{\frac{1}{2}} - \epsilon_2 b\,(y')^{-\frac{1}{2}}]\,x\,t^{-\frac{1}{2}} - 2\epsilon_1\epsilon_2 ab \times x^2[1-(1-t^{-1})^{\frac{1}{2}}] + \tau\{[1-(1-t^{-1})^{\frac{1}{2}}] \times [1 + 2\,(\epsilon_1 a + \epsilon_2 b)\,x] + \tfrac{1}{2}[(y')^{\frac{1}{2}} - (y')^{-\frac{1}{2}}]\,t^{-\frac{1}{2}}\} = 0 \tag{2}$$

(iii) $x > 1$, the outside band region

$$1 + (\epsilon_1 a y^{\frac{1}{2}} + \epsilon_2 b y^{-\frac{1}{2}})\,x\,(-t)^{-\frac{1}{2}} - 2\epsilon_1\epsilon_2 abx^2 \times [1-(1-t^{-1})^{\frac{1}{2}}] + \tau\{[1-(1-t^{-1})^{\frac{1}{2}} \times [1 + 2\,(\epsilon_1 a + \epsilon_2 b)\,x] - \tfrac{1}{2}(y^{\frac{1}{2}} + y^{-\frac{1}{2}})\,(-t)^{-\frac{1}{2}}\} = 0. \tag{3}$$

where

$$x = (\omega^2/\omega_m^2),\ \epsilon_1 = (M_1' - M_1)/M_1,\ \epsilon_2 = (M_2' - M_2)/M_2 \qquad (4\,a)$$

$$\tau = (\gamma' - \gamma)/\gamma.$$

$$a = 1 + (M_1/M_2), \qquad b = 1 + (M_2/M_1) \qquad (4\,b)$$

$$y = (1 - bx)/(1 - ax), \qquad (y')^{\frac{1}{2}} = \mp\,(-y)^{\frac{1}{2}}, \qquad t = abx\,(1 - x) \qquad (4\,c)$$

and ω_a, ω_0 and ω_m are respectively the zone boundary acoustic, the optic and the maximum optic mode frequencies of the diatomic linear chain. In eq. (4 *c*) the $\mp$ sign carry the same meaning as defined in I. If we put $\tau = 0$ in eqs (1) to (3) we get the results of the simple mass defect theory; and it can be seen from eq. (1) that for this case the resonant mode frequency is given by

$$x = [2\epsilon_1\epsilon_2 ab]^{-\frac{1}{2}}. \qquad (5)$$

From eq. (5) it is clear that a resonant mode can be obtained only if ϵ_1 and ϵ_2 have the same sign, that is, only if both the mass defects are either lighter or heavier than the respective sublattice host masses. This is equivalent to saying that the presence of a second similar impurity in the other sublattice effectively acts to soften the force-constant around the first impurity, or the two impurities repel each other as has been shown by Mazur *et al* (1956). This result is in contrast with that obtained for next nearest neighbour mass defect pair discussed in I. If the two host masses of the diatomic linear chain are identical $M_1 = M_2$ as in the case of Si or Ge then $a = b = 2$ and a pair of extremely light impurities like a pair of vacancies will produce a resonant mode at $\omega_R \simeq 0{\cdot}6\,\omega_m$. As ϵ_1 or ϵ_2 or both increase and approach zero the resonant mode moves towards the top of the band. However, if the impurities happen to be of heavier mass, then, as the mass goes on increasing the resonant mode frequency will go on shifting to the bottom of the band. The three dimensional calculations of Elliott and Pfeuty (1967) also show similar trends as far as the inband modes are concerned. As for example in their case the spectrum remains the same as the host crystal for impurities with mass nearly equal to that of the host mass, but if the impurity mass is drastically lower or higher than the host mass then a strong inband resonant mode appears whose frequency decreases if $\epsilon\ (= \epsilon_1 = \epsilon_2) > 0$ increases, and increases if $\epsilon < 0$ increases.

3. Results and discussion

Equations (1), (2) and (3) are solved numerically to determine the impurity mode frequencies. In order to facilitate the comparison of the results of the present calculation with those obtained in I for the next nearest neighbour impurity pair, the lattice parameters a and b are chosen to be the same as that in I (*i.e.*, those for the KI host). The value of one of the parameters ϵ_1 is taken to be $-0{\cdot}412$, $-0{\cdot}823$ and $2{\cdot}4$ corresponding to Na^+, Li^+ and Cs^+ impurities respectively substituted in the K^+ sublattice and ϵ_2 is varied from -1 to $+4$. At first τ is put equal to zero so that one gets the results for the mass defect case. The variation of the

squared impurity pair mode frequencies as a function of ϵ_2 is shown in figure 1. The resulting impurity pair modes are similar to those obtained in I, in the sense that there are modified single impurity modes as well as pure pair modes. However, unlike the results of I most of the pair modes shown in figure 1 can be understood in terms of two isolated single impurities (*e.g.* Mazur *et al* 1956) substituted in the two sublattices. For example, if $M_1 < M_2$, and ϵ_1 and ϵ_2 both less than zero corresponding to light mass impurities, one would expect a localized mode arising out of ϵ_1 and a localized as well as a gap mode arising out of ϵ_2 and these three modes can be seen clearly for $\epsilon_1 = -0{\cdot}414$ and $-1 < \epsilon_2 < 0$. But for $\epsilon_2 > 0$ one expects no modes and hence only the ϵ_1 local mode should exist as is the case in figure 1. Similarly for $\epsilon_1 > 0$ and $\epsilon_2 < 0$ one expects a gap mode arising out of ϵ_1 and a gap and a local mode arising out of ϵ_2. But as soon as $\epsilon_2 > 0$ no mode is expected out of it so that only a gap mode corresponding to ϵ_1 should exist. Again the plots in figure 1 for $\epsilon_1 = 2{\cdot}4$ and $\epsilon_2 < 0$ agrees with this prediction, but for $\epsilon_2 > 0$, besides the expected single gap mode, an inband resonant mode in the acoustic band or an inband mode in the optic band appears as can be seen from the figure. The existence of these inband resonant modes is a characteristic feature of the pair problem. We have seen in I that for the next nearest neighbour pair the impurity modes cannot be interpreted in a similar way in terms of single impurity results. The variation of the impurity mode frequencies with

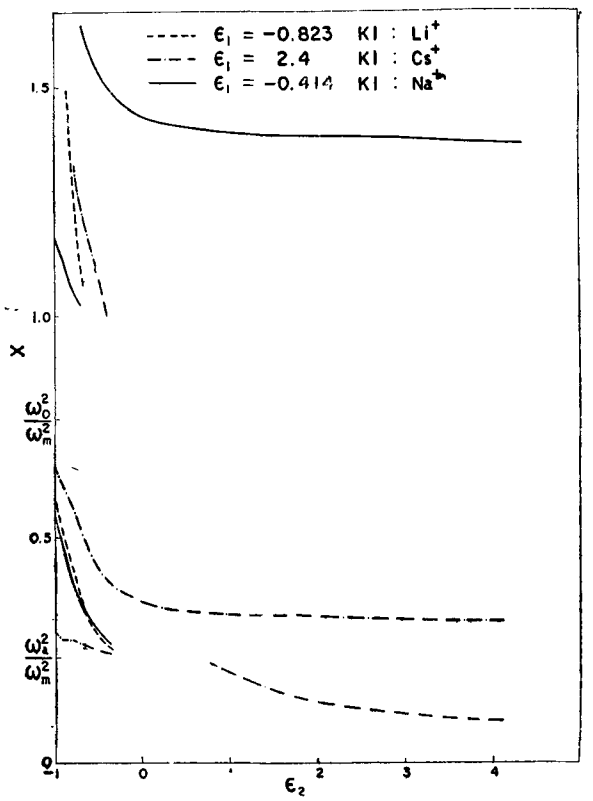

Figure 1. Variation of the impurity pair mode frequencies as a function of ϵ_2 for the mass defect case ($\tau = 0$).

ϵ_2 shown in figure 1 is similar to that of I. Moreover, the three-dimensional calculation of Elliott and Pfeuty (1967) also shows similar behaviour so far as the localized modes are concerned as is evident from their figure 7.

Figure 2 shows the variation of the localized gap and inband pair mode frequencies as a function of the force-constant change parameter τ. For this purpose the mass defect parameters ϵ_1 and ϵ_2 are chosen such that these correspond to pairs of light mass impurities ($\epsilon_1 = -0{\cdot}414$ and $\epsilon_2 = -0{\cdot}721$, $-0{\cdot}370$); a pair consisting of a light mass impurity in the light host sublattice and a heavy mass impurity in the heavy mass sublattice ($\epsilon_1 = -0{\cdot}5$, $\epsilon_2 = 2$); a pair with a heavy mass impurity in the light host sublattice and a light mass impurity in the heavy host sublattice ($\epsilon_1 = 2{\cdot}4$, $\epsilon_2 = -0{\cdot}720$, $-0{\cdot}370$); and a pair of heavy mass impurities ($\epsilon_1 = \epsilon_2 = 2$). In the case of a light mass impurity pair such as the one corresponding to $\epsilon_1 = -0{\cdot}414$ and $\epsilon_2 = -0{\cdot}721$ (one moderately light

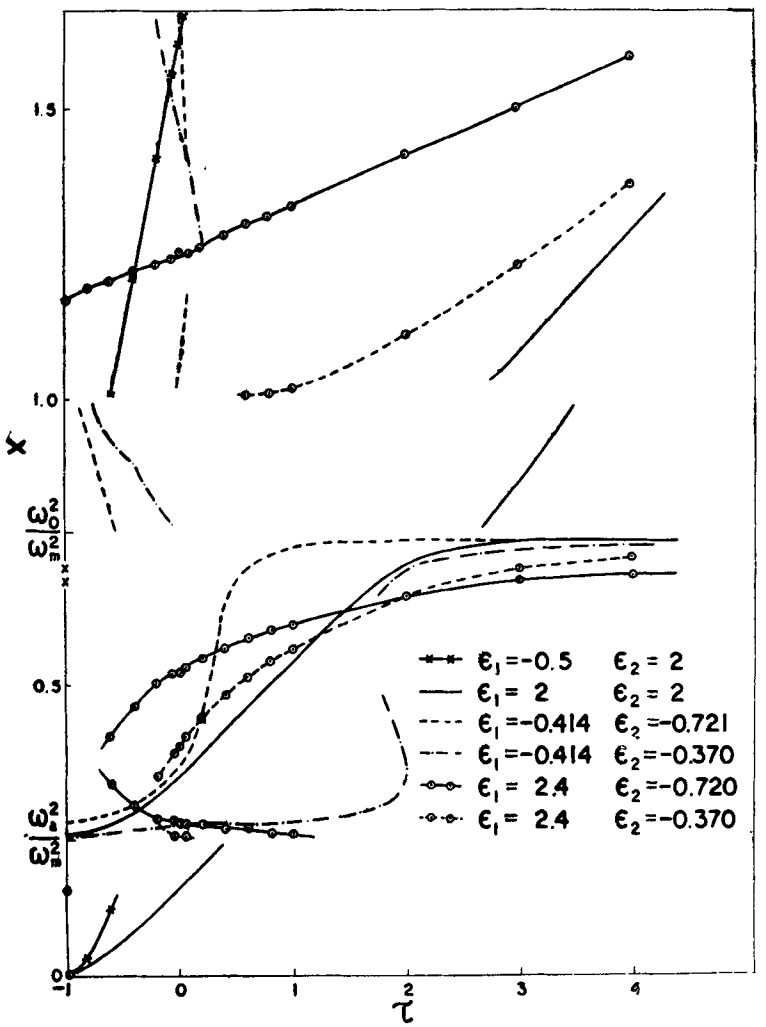

Figure 2. Variation of the impurity pair mode frequencies as a function of the force-constant change parameter τ, for a given pair of mass defect impurities substituted in KI.

and the other extremely light) the mass defect theory predicts two localized modes which are identical to the $\tau = 0$ values in figure 2. As τ is varied from a value of -1, corresponding to no force constant between the two impurities through 0 to a large positive value of 4, it can be seen that the high frequency localized mode decreases rapidly whereas the low frequency localized mode increases and both these modes vanish for $\tau \gtrsim 0{\cdot}1$. For $\epsilon_1 = -0{\cdot}414$ and $\epsilon_2 = -0{\cdot}370$ the mass defect theory predicts only one local mode whose frequency decreases rapidly with increasing τ and vanishes for $\tau \gtrsim 0{\cdot}2$. These results agree partly with the three dimensional calculations of Elliott and Pfeuty (1967), in the sense that with increasing τ the low frequency local mode increases in both the cases. But contrary to the present calculation, Elliott and Pfeuty find that the high frequency local mode also increases with increasing τ. There also exists a gap mode for the light mass impurity pairs as can be seen from figure 1. The variation of these gap mode frequencies with τ is also shown in figure 2. As the force constant softens ($\tau < 0$) the gap mode frequency decreases and aproaches a limiting value as τ tends to -1; and for $\tau > 0$ the gap mode frequency increases and again approaches a limiting value. However, some interesting features develop for a pair of impurities of nearly equal mass for $\tau > 0$ as can be seen for the case of $\epsilon_1 = -0{\cdot}414$ and $\epsilon_2 = -0{\cdot}370$. For $\tau \leqslant 2$ the single gap mode frequency splits into three modes. The pair gap modes were not studied by Elliott and Pfeuty (1967) as they considered impurities in a Si host which has no gap. Besides these local and gap modes, inband resonance modes also appear for $\tau < 0$ in the optic band whose frequency decreases with increasing τ. These inband modes are not present if the pair is characterized only by a change in mass.

In the case of an impurity pair, consisting of an heavy mass substituted into the light mass sublattice and a light mass in the heavy sublattice, the mass defect theory predicts one local mode and two gap modes for $\epsilon_1 = 2{\cdot}4$, $\epsilon_2 = -0{\cdot}720$ and only two gap modes for $\epsilon_1 = 2{\cdot}4$, $\epsilon_2 = -0{\cdot}37$. For the first case the local mode increases uniformly with increasing τ, and a new local mode appears for the second case for $\tau \gtrsim 0{\cdot}6$. whose frequency also increases with increasing τ. Out of the two gap modes the high frequency mode increases and approaches the top of the gap as τ increases and vanishes below a limiting value of $\tau < 0$ (for the first case this limiting value is $-0{\cdot}7$ and for the second pair $-0{\cdot}3$); while the low frequency mode decreases and finally merges with the top of the acoustic band as τ increases. Contrary to the predictions of eq. (5) for the mass defect case, it is possible to have inband resonant modes for a pair of dissimilar impurities provided τ is nearly equal to -1. Such an inband mode also exists for a pair consisting of a light mass impurity in the light host sublattice and a heavy mass impurity in the heavy host sublattice ($\epsilon_1 = -0{\cdot}5$, $\epsilon_2 = 2$). The frequency of this inband mode which lies in the acoustic band increases with decreasing force-constant softening and vanishes rapidly with further increase in τ. For the above case there also appear two gap modes for $\tau = -1$, which are not predicted by the mass defect theory. The frequency of the local mode predicted by the mass defect theory increases with increasing τ. In the case of a pair of heavy mass impurities ($\epsilon_1 = \epsilon_2 = 2$) the mass defect predicted inband and gap mode frequencies increase with increasing τ with a result that the acoustic inband resonant mode vanishes for $\tau > 0{\cdot}4$, and the gap mode frequency stabilizes at the

top of the gap. For large increase in force-constant $\tau > 2{\cdot}5$, there appears two new modes, not predicted by the mass defect theory. The first is an optic inband mode whose frequency increases with increasing τ and vanishes for $\tau \gtrsim 3{\cdot}5$ and the second a localized mode whose frequency goes on increasing with τ.

Figure 3 shows the variation of the impurity modes with τ for the case of substitution in a host like Si ($M_1 = M_2$) which has no gap. The different impurity pairs considered are GeGe, LiP, BAs, BSb in Si host and SiSi in Ge host. It is interesting to note that a pair of light mass Si impurities substituted in Ge can produce an inband resonant mode if τ is finite and this mode decreases with increasing τ. Similarly for sufficiently large force constant changes a pair of heavy mass impurities such as Ge in Si can also give rise to a localized mode.

Finally the variation of the various impurity pair modes when substituted in different hosts with varying gaps is shown in figure 4 (note change of scale below and above $x = 1$). It can be seen that certain local and gap modes persist in all

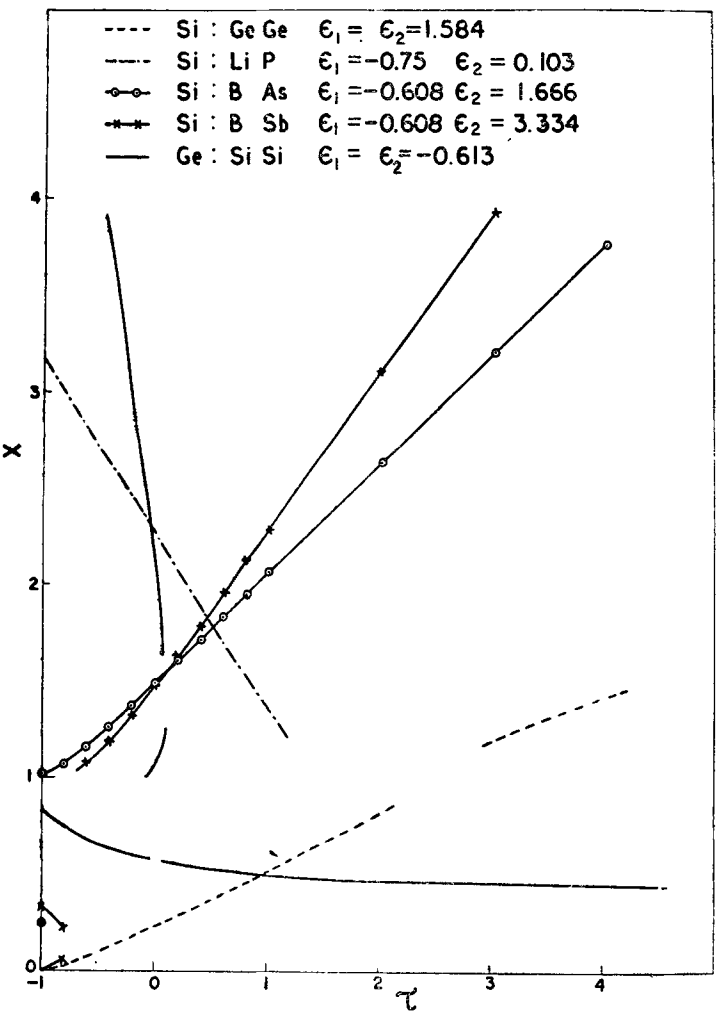

Figure 3. Variation of the impurity pair mode frequencies as a function of τ for impurities substituted in Si and Ge hosts.

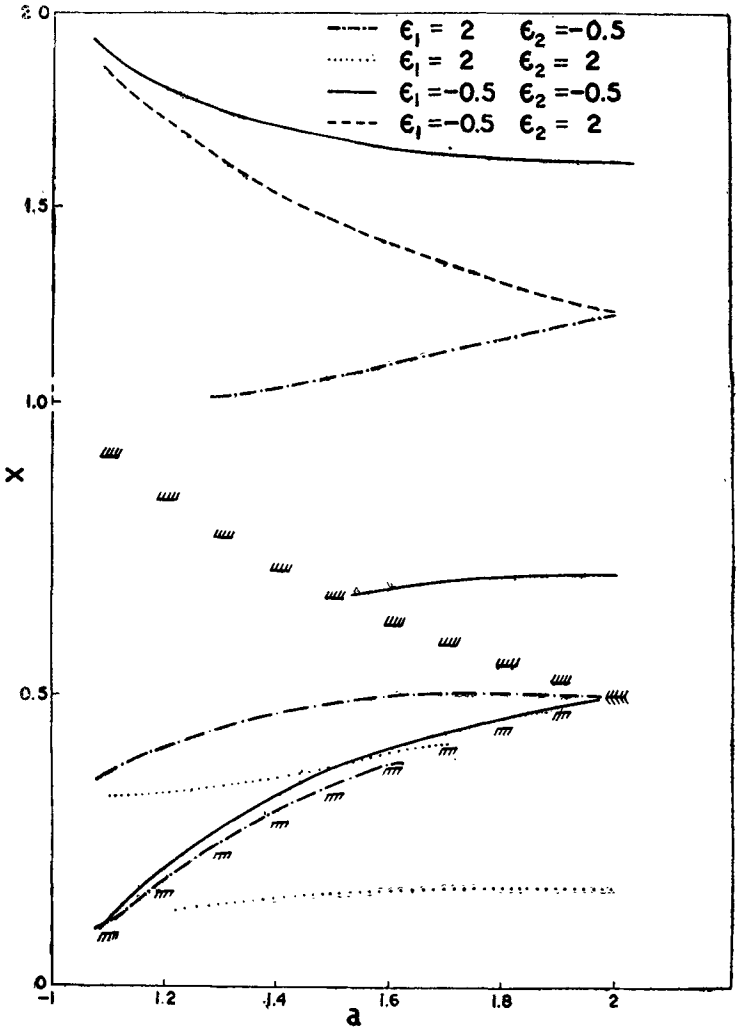

Figure 4. Variation of the impurity pair mode frequencies with the gap in the host crystal is shown. (Note change of scale below and above $x = 1$).

hosts, whereas other local, gap and inband resonant modes disappear as the gap increases or decreases.

4. Conclusion

In concluding we shall compare the predictions of this calculation with the available experimental data. Most of the known experiments were carried out on different impurity pairs substituted in silicon and the impurity modes are studied using infrared (*e.g.*, Angress *et al* 1965, Newman and Smith 1968, Tsvetov *et al* 1968) and Raman spectroscopy (*e.g.*, Feldman *et al* 1966, Renucci *et al* 1971). Silicon when doped with charged impurities can absorb infrared radiation. However, charge compensation demands that pairs of two dissimilar impurities should be substitited in the Si crystal so as to minimize free carrier absorption. As a result impurity pairs such as BP, BAs and BSb occupy nearest neighbour positions in the Si lattice, and the impurity modes become infrared active. On the other

hand pairs of BB or PP if present in Si, their charges have to be compensated by doping Si with Li, the atoms of which usually go to interstitial sites. All these pairs have been studied extensively by infrared absorption (*e.g.* Angress *et al* 1965, Newman *et al* 1968, Tsvetov *et al* 1968). On the other hand for isoelectronic impurities such as Ge substituted in Si or vice versa, the impurity modes as well as the transverse optical modes of the host crystal can be seen by Raman scattering. The experimental data available for such pair modes are tabulated in the 5-th column of table 1, together with the predictions of the present calculation and those of Elliott and Pfeuty (1967) which are given in columns 4 and 6 respectively. It can be seen that in the case of ^{10}B and ^{11}B pairs the high frequency localized modes predicted by our calculations show good agreement with experimental data as well as the results of the Elliott—Pfeuty calculation. But the agreement of the low frequency local mode is rather poor, which is also the case for the Elliott-Pfeuty result. Besides these two local modes the theory also predicts an inband mode at 367·7 cm^{-1} for ^{10}B pair and at 377·7 cm^{-1} for ^{11}B pairs. These are not observed experimentally. In the case of ^{11}B–As and ^{11}B–Sb pairs (Tsvetovs *et al* 1968) the theory predicts local modes at 606.3 cm^{-1} and 601·3 cm^{-1} respectively which are very close to one of the observed modes namely 603·7 cm^{-1} and 611·9 cm^{-1} respectively. However, experimentally one sees three local modes for the former case and two for the latter case. In predicting all these impurity modes the force-constant change parameter τ is taken to be zero. To make sure

Table 1. Observed impurity mode frequencies for different pairs substituted in Si and Ge together with the predictions of the present theory and that of Elliott and Pfeuty.

Sl. No.	System	Defect parameter ϵ_1	ϵ_2	τ	Impurity modes predicted ω_R cm^{-1}	ω_L cm^{-1}	Experimental modes ω_L cm^{-1}	Results of EP calculation ω_L cm^{-1}
1.	Si: ^{10}B ^{10}B	−0·644	−0·644	0	367·7	518·8 745·5	555, 748[a]	590, 751
2.	Si: ^{11}B ^{11}B	−0·608	−0·608	0	377·7	506·9 705·7	547, 720[a]	572, 723[a]
3.	Si: ^{11}B P	−0·608	0·103	0	..	621·2	628, 600·1±0·5[b]	
4.	Si: ^{11}B As	−0·608	1·666	0	..	606·3	636·7±0·4[b] 603·7±0·3 627	
5.	Si: ^{11}B Sb	−0·608	3·334	0	..	601·3	642·7±0·3[b] 611·9±0·3	
6.	Si: GeGe	1·584	1·584	0	232·5	..	~285, 395[c]	
7.	Si: GeGe	1·584	1·584	0·4	285	..	~285, 395[c]	
8.	Ge: Si	−0·613	0	0	..	369	386[c]	
9.	Ge: SiSi	−0·613	−0·613	0	..	300 419	460[c]	
10.	Ge: SiSi	−0·613	−0·613	−0·066	225·7	460	460[c]	

a see Newman and Smith (1968); *b* see Maradudin *et al* (1971); *c* see Mirlin and Reshina (1966)

whether the B impurities occupy nearest neighbour positions or not we have calculated the pair mode frequencies for next nearest neighbour postions using the results presented in I and find that the agreement with the experiment worsens being 656 cm^{-1} and 622 cm^{-1} for ^{11}B pairs and 646·1 cm^{-1} and 596·4 cm^{-1} for ^{11}B pairs.

For Si impurities in Ge the Raman scattering measurements were done by Feldman *et al* (1966) where they observed high frequency modes besides the single impurity Si mode and attributed these to Si pairs. Later Renucci *et al* (1971) confirmed the presence of Si pair modes in Ge and Ge pair modes in Si by performing measurements on mixed crystals of Si and Ge (Ge_{1-c} Si_c). The extrapolated values of these impurity mode frequencies as given by Renucci *et al* (1971) are given in table 1 and compared with the predictions of the present calculation. It can be seen that in order to explain the 285 cm^{-1} pair inband mode due to Ge in Si one has to assume that the Ge–Ge force constant is enhanced by 40% as compared to Si–Si force constant. However for Ge impurities in Si the linear chain model does not explain the second peak observed at 395 cm^{-1}. On the other hand for Si pairs in Ge, the 460 cm^{-1} local mode can be reproduced by assigning a value of −0·066 to τ which amounts to a decrease in Si–Si force-constant by 6·6% as compared to the Ge–Ge force-constant. The other peak at 386 cm^{-1} is the single impurity Si local mode and the present theory predicts it to be at 369 cm^{-1}. As pointed out in II one need not take the force-constant change for single impurities to be the same as for pairs of Si. In evaluating the local and inband mode frequencies in various cases ω_m for Ge is taken to be 293 cm^{-1} and that for Si to be 497 cm^{-1} (see Renucci *et al* 1971). Note that for these cases one need not invoke the criterion of Lucovsky *et al* (1970) for applying the linear chain model to three-dimensional crystals as done in I, because the longitudinal optic and the transverse optic mode frequencies coincide for the hosts.

Thus in concluding we remark that this simple linear diatomic chain model provides qualitative explanation of the existing experimental data and compares well with the existing three-dimensional calculations. The utility of the linear chain model in explaining the experimental optical data has been duly emphasized recently by Barker and Sievers (1975). The success of the linear chain model in explaining the results of the real crystals can be physically understood by noting that, as pointed out in I, for a given impurity configuration, one can always construct a linear chain by taking all the atoms in the direction of the impurity pair. If this direction happens to be one of the symmetry directions of the crystal, then the linear chain provides a good description of the system because all the atoms in each plane perpendicular to the chain direction will vibrate with the same amplitude. Thus the vibrations of the atoms in the crystal will simulate a linear chain.

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