Impurity pair modes in a diatomic linear chain

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The modes of vibration of pair of mass-defect impurities occupying next-nearest-neighbor positions in a diatomic linear chain are examined using the Green's-function method. The existence of new localized, gap, and inband resonant modes corresponding to pairs of light, heavy, and a combination of light and heavy impurities, respectively, is predicted. The calculations are carried out for two different cases; first, for a pair of impurities in the heavy host sublattice and secondly, for the case when the impurity pair is substituted in the light host sublattice. The Lucovsky-Brodsky-Burstein criterion is used for applying the theory to three-dimensional crystals. The localized and gap pair mode frequencies thus estimated for different impurities in KI, KCl, and NaCl hosts show qualitative agreement with the corresponding experimental values.

I. INTRODUCTION

Recently much attention has been given to the experimental study of lattice impurity pair modes[1-7] using far-infrared spectroscopy. These pair modes are identified from the characteristic concentration dependence of the strength of absorption, which goes as a quadratic in impurity concentration. The observations are confined mostly to the alkali-halide–impurity systems with relatively high impurity concentrations. The first[1] pair mode to be observed happened to be the local mode due to H^-H^-, H^-D^-, and D^-D^- pairs substituted in KCl. Since then, impurity-pair resonant, gap, and localized modes have been observed for different impurities substituted in KCl, KI, and NaCl hosts. Ward and Clayman[4] have reported the infrared-active gap modes at 73.8 cm^{-1} due to pairs of Br^- and at 72.02, 80.26, and 82.84 cm^{-1} due to pairs of Cl^- impurities in KI. Similar measurements have also revealed the existence of resonant pair modes for F^- pairs[3] in NaCl at 32.7, 40.02, 44.3, and 48.4 cm^{-1} and for Cl^- pairs[5] in KI at 36 cm^{-1} (see Table I). In all the above-mentioned measurements the impurities are always substituted in the heavy-mass sublattice of the host crystal. However, measurements have also been carried out in systems where the impurities are substituted in the light-mass sublattice of the host. The observation of local modes[6] due to H^-, H^--D^-, and D^- pairs in KCl at 463.5, 535, 512.5 cm^{-1}; 351, 508, 511 cm^{-1}; and 331.5, 375.5, 368 cm^{-1}, respectively, essentially belongs to this second category. Besides, there also exists evidence for pair modes due to[7] Rb^+ and[4] Na^+ in KI whose frequencies are given in Table I. The experimental investigation of these pair modes has also indicated that certain impurity modes (e.g., the 73.8-cm^{-1} gap mode[8] due to Br^- in KI) which were earlier thought to be single-impurity modes are actually due to pairs.[4]

Attempts to provide a theoretical understanding of these pair modes have so far been confined to either extremely simple models or to very approximate calculations. To understand the local pair modes due to H^- and D^- a simple model of two coupled localized oscillators was proposed by DeSouza and Luty.[6] A molecular model, where only the impurities and their nearest neighbors are allowed to vibrate keeping the rest of the lattice rigid, was first proposed by Jaswal[9] to explain the Na^+-pair resonant mode in KCl. Subsequently it was extended by Ward and Clayman[10] to take into account two different impurity configurations and hence two different molecular complexes. However, both these models give only qualitative results in their prediction of pair-mode frequencies cies, because of the neglect of the dynamics of the host lattice. But from these molecular models[10] it becomes obvious that the pair of impurities (cation or anion) either occupy next-nearest-neighbor sites with an anion or cation between them in the [100] direction, or they occupy nearest-neighbor positions in the [110] direction. Green's-function calculations[11] are confined to extremely restricted defect spaces, again resulting in qualitative results.

Recently the potentiality of a diatomic-linear-chain model to explain the optical-absorption data of mixed crystals has been ably demonstrated by Sen and Hartmann.[12] They developed a theory based on the calculation of a single defect[13] in a diatomic linear chain, in order to explain the one-mode, two-mode, and mixed-mode behavior of mixed crystals. However, it is well known that a single mass defect in a diatomic linear chain can never produce an in-band resonant mode. In view of the success of their theory, we investigate the problem of a pair of mass-defect impurities in a diatomic linear chain with a view to explain the above-mentioned experimental data on pair modes. In what follows we shall demonstrate the existence of in-band resonant modes, gap modes, and localized modes characteristic of pairs of impurities be-

TABLE I. Impurity-pair-mode frequencies for ionic crystal-impurity pair complexes, obtained from the experimental data and the calculations of the present theory.

			Host-lattice frequencies (cm^{-1})				Impurity-mode frequencies and nature calculated		Experimental frequencies (cm^{-1})		
	System	ϵ_2, ϵ_2'	ω_{TO}[f]	ω_{LO}[f]	$(\omega_A)_{max}$[g]	$(\omega_O)_{min}$[g]	ω_G (cm^{-1})	ω_L (cm^{-1})	ω_R	ω_G	ω_L
1.	KI : Br^-Br^-	−0.378	101	139	69	98	91.62 gap mode	118.21 no local mode	...	73.8[a]	...
2.	KI : Cl^-Cl^-	−0.721	101	139	69	98	96.39 gap mode	126.06 no local mode 139.8 marginal local mode	36[d]	72.02[a] 80.26 82.84	
3.	KCl : Na^+Na^+	−0.414	142	214	no gap		111.5 no gap mode	170.98, 185.92 no local mode	44[c]	...	...
4.	NaCl : F^-F^-	−0.463	164	264	no gap		142.08 no gap mode	209.18, 221.02 no local mode	32.7[b] 40.2 44.7 48.4	...	...
5.	KI : Na^+Na^+	−0.414	101	139	69	98	81.16 gap mode	132.99, 138.67 no local mode	...	76.18[a] 84.2	...
6.	KI : Rb^+Rb^+	1.183	101	139	69	98	63.2 no gap mode	...	49[e]	86.17[e]	...

[a]See Ref. 4.
[b]See Ref. 3.
[c]See Ref. 2.
[d]See Ref. 5.
[e]See Ref. 7.
[f]See Ref. 20.
[g]See Ref. 21.

sides the existence of modified characteristic single-impurity modes. The statement of the problem with its exact solution is given in Sec. II. The results of the pair-mode calculations are presented and discussed in Sec. III. In Sec. IV we incorporate the criterion proposed by Lucovsky, Brodsky, and Burstein (LBB)[14] for applying the diatomic-linear-chain model to real crystals and conclude by comparing the predictions of the present theory with the existing experimental data.

II. THEORY

Consider an ionic diatomic linear lattice with masses M_1 and M_2 situated at even and odd sites, respectively. The defects being either cation or anion type when substituted in the crystal will go into only one of the two sublattices, and we shall henceforth assume that the defect sublattice is the one with masses M_2. The pair of defect atoms with masses M_2' and M_2'' will therefore occupy next-nearest-neighbor positions with a host atom of mass M_1 situated between the two. For convenience we choose their positions to be 1 and -1, and γ is the nearest-neighbor force constant. The diatomic lattice is treated by the Green's-function method using the M^* transformation developed by Maradudin *et al.*[15,16] This method has the advantage of reducing the equation of motion of the Green's function for the diatomic lattice to that of a monatomic lattice which has a frequency-dependent mass M^*.

The perturbed Green's functions for this problem can be solved exactly. The impurity modes are given by the zeros of the real part of the denominator of the perturbed Green's function. In the three different regions corresponding to the in-band, gap, and localized modes these equations can be written as given below.

(i) In-band regions $0 < x \leq \omega_a^2/\omega_m^2$ and $\omega_o^2/\omega_m^2 \leq x < 1$:

$$1 + 8\epsilon_2\epsilon_2' b^2 x^2 y^{-1}(1-t) = 0 \,. \tag{1}$$

(ii) Gap region $\omega_a^2/\omega_m^2 < x < \omega_o^2/\omega_m^2$:

$$1 \mp (\epsilon_2 + \epsilon_2')bx(y')^{-1/2}(t)^{-1/2} - 4\epsilon_2\epsilon_2' b^2 x^2 (y')^{-1} \times\{2(t-1) + 2[t(t-1)]^{1/2} - (1-t^{-1})^{1/2}\} = 0 \,. \tag{2}$$

(iii) Outside-band region $x > 1$:

$$1 + (\epsilon_2 + \epsilon_2')bx\, y^{-1/2}(-t)^{-1/2} + 4\epsilon_2\epsilon_2' b^2 x^2 y^{-1} \times\{2(t-1) + 2[t(t-1)]^{1/2} + (1-t^{-1})^{1/2}\} = 0 \,. \tag{3}$$

In Eqs. (1)–(3),

$$x=\omega^2/\omega_m^2,\quad \epsilon_2=(M_2'-M_2)/M_2,\quad \epsilon_2'=(M_2''-M_2)/M_2, \tag{4a}$$

$$b=1+M_2/M_1,\qquad a=1+M_1/M_2, \tag{4b}$$

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

and ω_a, ω_o, and ω_m are, respectively, the zone-boundary acoustic, optic, and maximum optic mode frequencies. Solutions of Eqs. (1)–(3) give, respectively, the in-band resonant, gap, and localized impurity-pair modes. The values of b and a defined by Eq. (4b) get interchanged if M_2 changes from the heavy-mass to the light-mass sublattice, and as a result the sign of $(y')^{1/2}$ will change depending on whether the impurity is substituted into the heavy-mass sublattice or the light-mass sublattice. Thus the upper minus sign in Eq. (2) corresponds to the light-mass sublattice case and the plus sign to the heavy-mass sublattice case. If we put $\epsilon_2'=0$ in Eqs. (1)–(3) these reduce to the results of the single-impurity case.

III. RESULTS AND DISCUSSION

Equations (1)–(3) are solved numerically and the zeros are determined. In order to study the variation of the in-band resonant, gap, and localized mode frequencies as a function of the mass-defeat parameters ϵ_2 and ϵ_2', it is necessary to choose the parameters a and b so as to correspond to a host lattice with a large gap. Keeping this in mind the parameters a and b are chosen to be 1.307 and 4.256, respectively, corresponding to the case of KI, when the defect sublattice M_2 happens to be the heavy-mass sublattice. On the other hand if the defect is substituted in the light-mass sublattice of mass M_2 then the values of a and b will be interchanged. It is well known from neutron-diffraction studies[17] that KI has a gap between 69 and 98 cm^{-1}. When the defects are substituted in the heavy-mass sublattice, i.e., the iodine-ion sublattice, the values of one of the mass-defect parameters, ϵ_2, are -0.721, -0.378, and 2, corresponding to a Cl^-, Br^-, and a heavy impurity with a mass three times that of the iodine mass, respectively. Similarly when the defects are substituted in the light-mass or K^+ sublattice the values of ϵ_2 are -0.823, -0.414, 1.183, and 2.4, corresponding to Li^+, Na^+, Rb^+, and Cs^+ mass defects, respectively. In both cases, the other parameter ϵ_2' of the second impurity is varied from -1, corresponding to the limiting case of a vacancy, to 4, which is an impurity of mass five times heavier than that of the host mass. The variations of the pair-mode frequencies as a function of ϵ_2' for both heavy- and light-mass sublattices are plotted in Figs. 1 and 2, respectively. In what follows we shall discuss these results one at a time. Each of the above-mentioned cases reproduce the single-impurity result when ϵ_2' goes to zero.

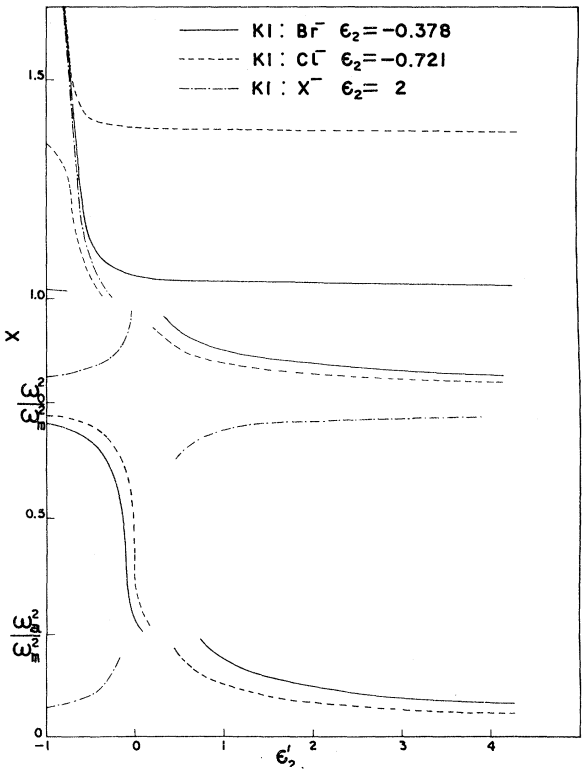

FIG. 1. Variation of the localized, gap, and in-band resonant mode frequencies as a function of ϵ_2'. The solid lines correspond to Br^- with $\epsilon_2=-0.378$, the dashed lines to Cl^- with $\epsilon_1=-0.721$, and the chain lines to some heavy impurity X^- with $\epsilon_2=2$ in KI. The impurities are substituted in the heavy-mass sublattice.

It is well known that when a single light-mass impurity[13] is substituted in the heavy-mass sublattice a gap mode and a local mode appear and if the impurity mass happens to be heavier than the heavy-sublattice-host mass then no impurity modes are produced. In Fig. 1, $\epsilon_2'=0$ corresponds to the former situation and hence the gap and the localized modes appearing at this point are characteristics of the single impurity with mass-defect parameter ϵ_2. It is clear from Fig. 1 that introduction of the second impurity modifies the single-impurity modes and as a result their frequencies shift. If the second impurity happens to be of lighter mass the gap and localized mode frequencies (for $\epsilon_2<0$) belonging to the single impurity increases rapidly with decreasing mass of the second impurity and stabilizes when ϵ_2' approaches -1. On the other hand if $\epsilon_2'>0$ the gap-mode frequency decreases rapidly towards the acoustic band edge and disappears with a subsequent appearance of an in-band resonant mode within the acoustic band when ϵ_2' increases. With the further increase of ϵ_2' the frequency of this in-band mode also decreases attain-

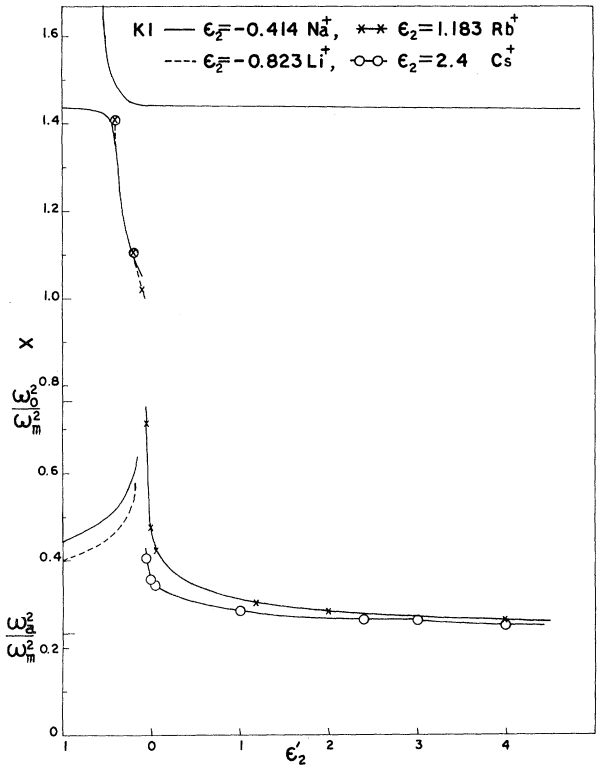

FIG. 2. Variation of the localized and gap mode frequencies as a function of ϵ_2', for the case of the impurity substitution into the light-mass sublattice. The solid lines correspond to Na^+, $\epsilon_2 = -0.414$, the dashed lines to Li^+, $\epsilon_2 = -0.823$, the solid line with crosses to Rb^+, $\epsilon_2 = 1.183$, and the solid line with circles to Cs^+, $\epsilon_2 = 2.4$.

ing a stabilized value for very heavy defects. At the same time the characteristic single-impurity localized-mode frequency decreases with increasing value of ϵ_2' and attains a constant value for heavier impurity masses.

A careful examination of Fig. 1 reveals that aside from the appearance of these gap, localized, and acoustic-band resonant modes that are identified as modified single-impurity modes, there also exist localized, gap, and in-band (both acoustic and optic) resonant modes that are purely characteristic pair modes. Such a pair localized mode appears when both the impurities have lighter masses, and its frequency increases with decreasing value of ϵ_2', which again attains a stabilized value when ϵ_2' approaches -1. This mode does not exist when $\epsilon_2' \cong 0$. For positive and somewhat large values of ϵ_2' there appears a resonant mode in the optical band whose frequency decreases with increasing ϵ_2'. If ϵ_2 increases and approaches zero, the frequency of this in-band resonant mode increases and approaches the top of the optic band. Similarly new modes that are characteristic of pairs of impurities, also appear for $\epsilon_2 > 0$. For this case if ϵ_2' has a value near about -1, two resonant modes appear, one in the acoustic and the other in the optic band, whose frequencies increase with increasing ϵ_2' and disappear around $\epsilon_2' = 0$. Aside from these two resonant modes, a localized mode also appears whose frequency rapidly increases as ϵ_2' tends to -1. For $\epsilon_2' > 0$ a gap mode appears whose frequency increases with increasing ϵ_2'. Such modes can never be expected in the case of the single impurity because it is well known that a heavy impurity substituted into the heavy sublattice does not produce any new mode. From Fig. 1 one can also conclude that a resonant mode will appear only if ϵ_2 and ϵ_2' have opposite signs or only if one of the impurities is of lighter mass and the other of heavier mass. Addition of a second heavy impurity in the presence of a single light impurity seems to be equivalent to a softening of the force constant around the light impurity, thus giving rise to an in-band resonant mode, when the impurities are substituted in the heavy-mass sublattice.

Similarly Fig. 2 shows the variation of the impurity-pair-mode frequencies as a function of ϵ_2' when the impurity is substituted into the light-mass sublattice. Again we see that when $\epsilon_2' = 0$ the single-impurity results are reproduced; that is, there appears a localized mode when a lighter-mass impurity is substituted, and a gap mode when a heavier-mass impurity is substituted into the light-mass sublattice.[13] Besides, one can also find the modified single-impurity local and gap modes as well as other local and gap modes which are characteristic of pure pairs. However, one distinguishing feature of Fig. 2 as compared to Fig. 1 is that the impurity-pair in-band resonant modes are almost absent in Fig. 2 except for one mode in the optical band corresponding to $\epsilon_2 = -0.414$ and $\epsilon_2' = 0.05$. Hence it can be concluded that in-band resonant pair modes are not produced easily when the impurities are substituted into the light-mass sublattices. Thus the introduction of a second impurity produces more dramatic effects in the case of the heavy-mass sublattice than the light-mass sublattice.

Figure 3 shows the variation of the impurity-pair-mode frequencies with the properties of the host lattice, that is, with the decrease in the gap of the host lattice. Three different impurity pairs are chosen for this purpose: one pair of lighter masses $\epsilon_2 = \epsilon_2' = -0.5$; the second pair consists of one lighter- and the other heavier-mass impurities with $\epsilon_2 = -0.5$ and $\epsilon_2' = 2$, respectively; and the third is a pair of heavy-mass impurities with $\epsilon_2 = \epsilon_2' = 2$. The impurity modes are calculated for the case of the substitution into the heavy-mass sublattice. The gap of the host is varied by varying M_2 ($M_2 > M_1$) from zero (corresponding to $M_2 = M_1$)

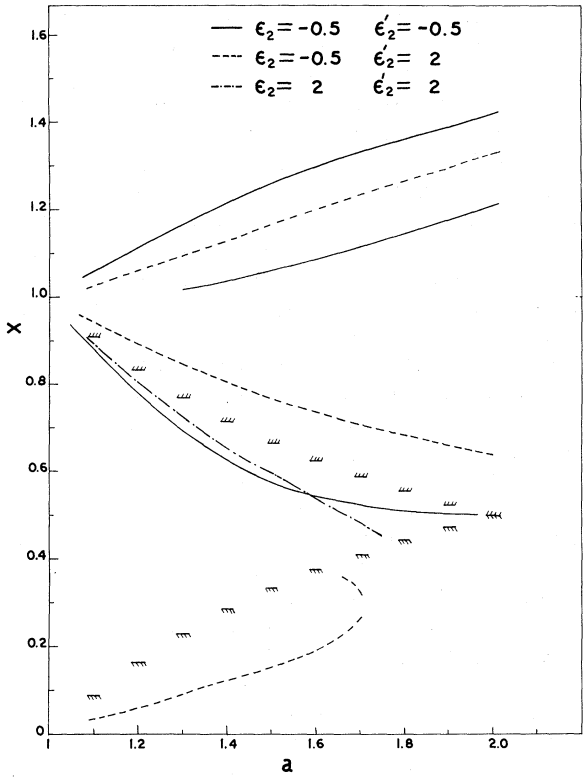

FIG. 3. Variation of the local, gap, and in-band resonant modes as a function of the gap of the host lattice. The solid lines correspond to a pair of light-mass impurities $\epsilon_2 = \epsilon_2' = -0.5$, the dashed lines to the case of a light- and a heavy-mass impurity pair with $\epsilon_2 = -0.5$ and $\epsilon_2' = 2$, and the chain line to a pair of heavy-mass impurities with $\epsilon_2 = \epsilon_2' = 2$, where all the pairs are substituted into the heavy-mass sublattice.

to 0.819 (corresponding to $M_2 = 10\,M_1$). It is interesting to note that some of the local, gap, and in-band modes exist for all the hosts, whereas some other local, gap, and in-band modes disappear either when the gap increases or decreases beyond a certain critical value. For example, in the case of a pair of light-mass impurities, out of the two local and one gap modes the high-frequency local mode and the gap mode persist for all hosts, whereas the low-frequency local mode disappears when the gap or the mass ratio M_2/M_1 increases beyond a certain value. Similarly for the second impurity pair the local mode and the in-band resonant mode in the optic band persist for all hosts, whereas the in-band mode in the acoustic band disappears when the gap decreases beyond a certain value. An interesting feature worth noting is that for values of the gap slightly larger than the critical value at which the acoustic-band resonant mode disappears, there appears a second resonant mode, which also vanishes with the first. In Fig. 3 this second acoustic in-band mode can be seen for values of the gap between 0.198 and 0.177. The acoustic-band pair-resonant-mode frequency increases with decreasing gap. This behavior is similar to that of the single-impurity resonant-mode frequency as a function of lattice constant.[18] Finally, for the heavy impurity pair the gap mode does not occur for hosts with small gap (i.e., masses nearly equal to each other).

IV. CONCLUSION

In this section we shall compare the predictions of the present theory with the available experimental data. In order to compare the predictions of the simple theory with the existing experimental data, the linear-chain model should be modified so as to make it applicable to three-dimensional crystals. The prescription for the modification of the linear-chain model to the calculation of local-mode frequencies due to single substitutional impurities was given by LBB,[14] and is achieved by introducing the longitudinal-optical-mode frequency ω_{LO} through the sum rule

$$3\omega_m = 2\omega_{TO} + \omega_{LO}\,, \tag{5}$$

which in turn is used to calculate the maximum frequency of the diatomic linear chain. Then the local mode will exist if

$$\omega_L > \omega_{LO}\,. \tag{6}$$

We shall apply Eqs. (5) and (6) to the calculation of the local-mode frequencies due to pairs of impurities and a generalization[19] of the LBB result to the existence of impurity-pair gap modes as given by

$$(\omega_A)_{max} < \omega_G < (\omega_O)_{min}\,, \tag{7}$$

where $(\omega_A)_{max}$ is the maximum frequency of the acoustic band or the bottom of the gap and $(\omega_O)_{min}$ is the minimum frequency of the optic band or the top of the gap. The experimental values of ω_{TO} and ω_{LO} are taken from Burstein[20] and those of $(\omega_A)_{max}$ and $(\omega_O)_{min}$ from the neutron scattering data as compiled by Bäuerle.[21] The values for different systems on which experimental measurements exist are given in Table I. Columns 7 and 8 of Table I give the predicted impurity-mode frequencies and their nature as determined by Eqs. (6) and (7). Columns 9–11 summarize the experimentally observed modes. It can be seen that the theory does not predict a local mode for any of the systems (except for a mode which lies 0.8 cm^{-1} above ω_{LO} in the case of KI:Cl^-Cl^-). In the case of Br^- and Cl^- pairs in KI, the calculated gap-mode frequencies are higher than those obtained from experiment. Moreover in the case of Cl^- pairs, three gap modes are observed as compared to one predicted. These discrepancies between the theory and experiment are due to the neglect of force-constant changes, which are expected to soften for the

lighter-mass impurities like Cl^- and Br^-. In the case of an Na^+ pair in KCl and an F^- pair in NaCl, no gap mode is predicted by the theory, in agreement with the experiment. For an Na^+ pair in KI the predicted gap mode frequency of 81.16 cm^{-1} is in good agreement with one of the two (84.2 cm^{-1}) measured frequencies of 76.18 and 84.2 cm^{-1}. Finally, for the Rb^+ pair in KI the theory does not predict any gap or local modes, whereas a gap mode[22] exists at 86.17 cm^{-1}. It is presumed that substitution of heavy impurities like Rb^+ in a K^+ sublattice may enhance the impurity-host force constant which, when taken into account, may produce the observed gap mode.

In the case of H^-, D^-, and H^-D^- pairs in KCl, the theory does not predict the observed local modes. This is expected in view of the well-known fact that the mass-defect approximation alone, even for single impurities of H^- and D^-, does not give satisfactory results.[14] In all the above-mentioned cases, molecular models[9,10] predict more modes than observed.

This simple mass-defect theory does not provide an explanation for the resonant pair modes observed at 44 and 36 cm^{-1} due to Na^+ pairs in KCl,[1] and Cl^- pairs in KI,[4] respectively, because the theory does not predict resonant modes due to a pair of light-mass impurities. In order to explain these in-band pair modes one has to incorporate in the theory the fact that the force constants around these light-mass impurities are softened considerably. We hope that inclusion of force-constant changes will also improve the agreement between the theoretically predicted and experimentally observed gap and localized-mode frequencies, besides giving the in-band resonant modes. A preliminary calculation[23] including force-constant changes confirms this.

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