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Vibrations of off-centre Ag^+ in RbI

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Abstract. A defect model for ⟨111⟩ off-centre substitutional impurities in alkali halide crystals is developed. The model includes changes in the force constant between the impurity and its nearest neighbours in addition to mass changes. The model is applied to calculate the local density of states of ⟨111⟩ off-centre Ag^+ in RbI which is expected to give peaks at the possible resonant mode frequencies.

1. Introduction

Extensive experimental and theoretical work on the vibrational properties of doped alkali halides has been done over the last two decades. Most of the investigations were directed towards the study of the vibrations of 'on-centre' substitutional impurities whose centre of mass occupies the position earlier occupied by the replaced host ion. The theory for the vibrational problem for such impurities is well developed (see, e.g., Lifshitz and Kosevitch 1969, Ludwig 1967, Maradudin *et al* 1971). The off-centre substitutional impurities in alkali halides form an important class of impurity–host systems with electric or elastic dipoles having preferred directions in the host lattice. The work on such systems has been reviewed by Barker and Sievers (1975) and by Bridges (1975). Theoretically an oscillator model with a local potential of lower symmetry than the octahedral symmetry of the lattice gives a good account of different transitions observed in different experiments. Kirby *et al* (1970) have used this approach to discuss the ⟨111⟩ off-centre Li^+ in KCl and ⟨110⟩ off-centre Ag^+ in RbCl in connection with their far-infrared absorption measurements. However, the problem of vibrations of the off-centre defect can best be formulated using the Green function technique.

Mokross and Dick (1977) and Mokross *et al* (1977) have developed a general model for ⟨110⟩ 'off-centre' substitutional impurities in alkali halides and applied the theory for the calculation of infrared absorption and first-order Raman scattering. Recently, Kapphan (1982) has measured ultraviolet absorption and electro-optical behaviour of off-centre Ag^+ in RbI and has concluded that the most probable direction of off-centre displacement should be ⟨111⟩. This and the planned work on infrared lattice absorption (Kapphan 1986) have been the reason for our interest in the theory of resonant vibrations of Ag^+ in RbI. The purpose of the present paper is to present a theoretical treatment of vibrations of ⟨111⟩ off-centre impurities in an alkali halide crystal of NaCl structure and apply it to RbI:Ag^+. In particular, we look for possible resonance modes which may be observed in experiments such as infrared lattice absorption.

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The calculation of impurity-induced infrared absorption and first-order Raman scattering in doped crystals involves essentially the computation of the lattice Green function of the imperfect crystal in different symmetry modes. The occurrence of a resonance mode is signalled by an increase in the density of states near the resonance frequency which is generally observed as resonance-type peaks in the frequency spectrum of the doped crystals. The density of states can be expressed in terms of the Green function of the imperfect lattice. The resonant vibrations of the defect are best described by the defect Green function $G_{ii}^{\mathrm{dd}}(\omega)$ which is the dynamic response of the defect d, i.e. its displacement in the ith direction due to a unit force with frequency ω acting on the defect d in direction i. The imaginary part of the defect Green function represents the local density of states of the defect. Therefore the defect model has been employed to calculate the local density of states of off-centre Ag^+ in RbI.

2. Theory

2.1. *The defect Green function*

The Green function for the defect lattice is defined by

$$(\boldsymbol{\Phi} - \mathbf{M}\omega^2)\mathbf{G}(\omega) = 1 \tag{1}$$

while that of the ideal lattice is given by

$$(\boldsymbol{\Phi}^0 - \mathbf{M}^0\omega^2)\mathbf{G}^0(\omega) = 1 \tag{2}$$

where $\boldsymbol{\Phi}$ and $\mathbf{M}$ are the force constant and mass matrices for the defect lattice, and $\boldsymbol{\Phi}^0$ and $\mathbf{M}^0$ are the force constant and mass matrices for the ideal lattice. For a substitutional defect, the coupling parameters around the defect atom are changed in addition to the mass change at the defect site. Only changes in the coupling parameters between the impurity and its immediate neighbours are considered as the changes in the coupling parameters far away from the impurity site are negligibly small. For the present case of isoelectronic defects, such an approximation is adequate. However, it may be mentioned that changes in long-range Coulombic and dipolar forces would be necessary for defects with a change in charge state (Gillan and Jacobs 1983). The Green function for the defect lattice is evaluated in terms of the ideal lattice Green function and the perturbation which is strongly localised in space. If we assume only one impurity atom, so that in the dilute limit the change in any extensive physical property is to be multiplied by the number of impurities actually present, we can write equation (1) as

$$[\boldsymbol{\Phi}^0 - \mathbf{M}^0\omega^2 + \mathbf{V}(\omega)]\mathbf{G}(\omega) = 1 \tag{3a}$$

or

$$\mathbf{G}(\omega) = \mathbf{G}^0(\omega) - \mathbf{G}^0(\omega)\mathbf{V}(\omega)\mathbf{G}(\omega) \tag{3b}$$

where

$$\mathbf{V}(\omega) = \boldsymbol{\Phi} - \boldsymbol{\Phi}^0 - (\mathbf{M} - \mathbf{M}^0)\omega^2 = \boldsymbol{\Phi} - \Delta\mathbf{M}\omega^2 \tag{4}$$

is the change in the force constant matrix for a single impurity. Therefore, from equation (3), we obtain

$$\mathbf{G}(\omega) = [1/(1 + G^0\mathbf{V})]\mathbf{G}^0 = \mathbf{G}^0/(1 + \mathbf{V}\mathbf{G}^0). \tag{5}$$

An equivalent expression for $\mathbf{G}(\omega)$ can be written in terms of the $\mathbf{t}$ matrix by inserting equation (5) into the right-hand side of (3*b*) as

$$\mathbf{G}(\omega) = \mathbf{G}^0 - \mathbf{G}^0\mathbf{t}(\omega)\mathbf{G}^0 \qquad \text{with } \mathbf{t}(\omega) = \mathbf{V}/(1 + \mathbf{G}^0\mathbf{V}). \tag{6}$$

In order to evaluate the $\mathbf{t}$ matrix we have to deal with the finite matrices of dimension $3n$, if n is the number of atoms affected by the perturbation. The use of group theory exploiting the point group symmetry of the impurity further simplifies the calculation (see § 2.3).

The elements of the ideal lattice Green function matrix are explicitly given by

$$G^0_{ij}(lK, l'K', \omega) = \frac{1}{N(M^0_k M^0_{k'})^{1/2}} \sum_{k\sigma} \frac{e_i(K, k\sigma) \cdot e_j(K', k\sigma)}{\omega^2_{k\sigma} - (\omega + \mathrm{i}\varepsilon)^2} \times \exp[\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{R}(lK) - \boldsymbol{R}(l'K'))] \tag{7}$$

where $\omega_{k\sigma}$ and $\boldsymbol{e}(K, k\sigma)$ are the eigen-frequencies and polarisation vectors corresponding to the wavevector $\boldsymbol{k}$ and branch index σ; $\boldsymbol{R}(lK)$ is the equilibrium position of the ion (lK). The infinitesimal positive quantity $\varepsilon(\rightarrow 0^+)$ in equation (7) ensures the causality, i.e. that retarded Green functions are used.

2.2. Perturbation model

We assume a nearest-neighbour perturbation model in which the short-range force constants between the impurity and its nearest neighbours are taken to be different from the force constants between two ions in the perfect crystal in addition to the change in mass at the impurity sites. The long-range Coulomb forces are assumed to be unchanged. We assume that the impurity occupies a ⟨111⟩ off-centre equilibrium position with the same electric charge as the ion that it replaces. The defect is characterised by four force constant changes, i.e. $\Delta f^1_\parallel$ and $\Delta f^1_\perp$ between the impurity and ions 1, 2, 3, and $\Delta f^2_\parallel$ and $\Delta f^2_\perp$ between the impurity and ions $\bar{1}, \bar{2}, \bar{3}$ (figure 1). Evidently the defect space consists of 21 Cartesian displacements of the impurity and its six nearest neighbours.

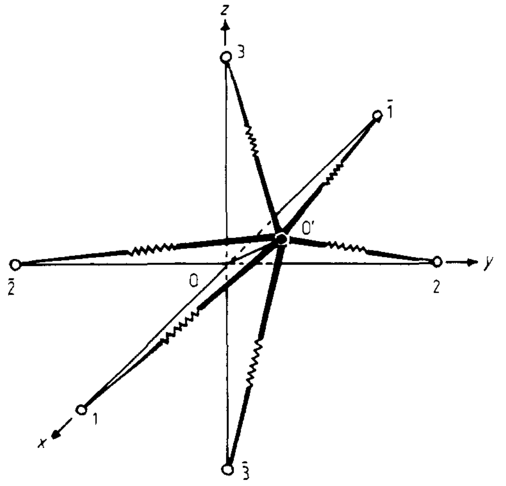

Figure 1. Impurity space for an off-centre ⟨111⟩ defect: ●, Ag^+; ○, I^-; $OO' = d$; $O'1 = O'2 = O'3 = a$; $O'\bar{1} = O'\bar{2} = O'\bar{3} = b$. $\Delta f^1_\parallel$ and $\Delta f^1_\perp$ are central and non-central force constant changes, respectively, between the impurity and host ions 1, 2, 3, and $\Delta f^2_\parallel$ and $\Delta f^2_\perp$ are force constants changes between the impurity and host ions $\bar{1}, \bar{2}, \bar{3}$.

In order to calculate the force constant change matrix $\Delta\mathbf{\Phi}$ use is made of the formula (Maradudin *et al* 1971)

$$\varphi_{\alpha\beta}(lK, l'K') = \{(x_\alpha x_\beta/r^2)[\varphi''_{KK'}(r) - (1/r)\varphi'_{KK'}(r)] + (\delta_{\alpha\beta}/r)\varphi'_{KK'}(r)\}|_{r=x(lK,l'K')} \tag{8a}$$

$$\Phi_{\alpha\beta}(lK, l'K') = -\varphi_{\alpha\beta}(lK, l'K')$$
$$\Phi_{\alpha\beta}(lK, lK) = \sum_{l'K'}{}' \varphi_{\alpha\beta}(lK, l'K') \tag{8b}$$

for interaction betwen two ions (lK) and $(l'K')$ separated by the equilibrium distance $x(lK, l'K')$. Here $f_\parallel = \varphi''_{KK'}(r)$ and $f_\perp = (1/r)\varphi'_{KK'}(r)$ are the central and non-central force constants, respectively. For example the xx component of the change $\Delta\mathbf{\Phi}(0, 1)$ in force constants between ions 0 and 1 is given by

$$\Delta\Phi_{xx}(0, 1) = -(r_0 - d/3^{1/2})^2(\Delta f_\parallel^1 - \Delta f_\perp^1)/[(r_0 - d/3^{1/2})^2 + d^2/3 + d^2/3] - \Delta f_\perp^1 \tag{9}$$

where d is the static off-centre displacement of the impurity and r_0 is the nearest-neighbour distance in the host lattice. The mass change matrix $\Delta\mathbf{M}$ is a 21×21 diagonal matrix with only three non-zero elements referring to coordinates of the impurity ion. This completes the 21×21 perturbation matrix $\mathbf{V}(\omega) = \Delta\mathbf{\Phi} - \Delta\mathbf{M}\,\omega^2$.

The elements of the perfect lattice Green function matrix $\mathbf{G}^0$ follow the symmetry of the ideal lattice (O_h in this case) which restricts the number of non-zero distinct elements. The elements of $\mathbf{G}^0$ needed in the present defect model are $G_{xx}^{++}(0,0,0)$, $G_{xx}^{--}(0,0,0)$, $G_{xx}^{--}(2,0,0)$, $G_{yy}^{--}(2,0,0)$, $G_{xx}^{+-}(1,0,0)$, $G_{yy}^{+-}(1,0,0)$, $G_{xx}^{--}(1,1,0)$, $G_{xy}^{--}(1,1,0)$ and $G_{zz}^{--}(1,1,0)$, where the difference in lattice vectors is denoted by (n_1, n_2, n_3); n_i is in units of nearest-neighbour distance r_0. Here $++$ or $+-$ indicates that the Green function elements are taken between cation and cation or between cation and anion.

2.3. *Symmetry coordinates*

Apart from destroying the translational symmetry of the lattice an off-centre impurity causes a reduction in the site symmetry from the cubic (O_h) to some group of lower order. For the present case of $\langle 111\rangle$ off-centre impurities the point group symmetry is C_{3v}. The Cartesian components of the amplitudes of the displacements of the ions from their equilibrium positions in the defect space provide basis functions for the reducible representation of the point group C_{3v}. We form a 21-dimensional column vector $U(n)$ taking these amplitudes as its elements. The components of vector $U(n)$ can be expressed in terms of Cartesian or symmetry coordinates. The symmetry coordinates provide basis functions for irreducible representations of the point group C_{3v} and are obtained by standard projection technique (Maradudin 1969). The total representation is broken as

$$\Gamma_{C_{3v}} = 5A_1 + 2A_2 + 7E. \tag{10}$$

The required symmetry coordinates are presented in table 1. In addition to simplifying the calculations the symmetry coordinates are useful in identifying the impurity modes (resonant and localised modes) according to different irreducible representations.

If the symmetry coordinates are utilised, the perturbation matrix $\mathbf{V}(\omega)$ and the Green function matrix $\mathbf{G}^0(\omega)$ are block diagonalised according to different irreducible representations to get a 5 × 5 matrix in the A_1 mode, a 2 × 2 matrix in the A_2 mode and a 7 × 7 matrix in the E mode. It may be observed that the impurity moves only in the A_1 and E modes which are infrared active. The possible resonance modes are expected in these irreducible representations.

3. Calculation for RbI : Ag^+

3.1. *Local density of states*

As pointed out earlier, the resonant vibrations of the defect are best described by the defect Green function $G_{ii}^{dd}(\omega)$. The imaginary part of the defect Green function represents the local density of states of the defect. We define local density of states of the defect by (Ram and Dederichs 1981a, b).

$$Z^{d}(\omega) = \tfrac{1}{3}\sum_{i=1}^{3} Z_i^{d}(\omega) = \frac{2\omega M}{3\pi}\sum_{i} \mathrm{Im}[G_{ii}^{dd}(\omega)]. \tag{11}$$

The defect Green function can be projected in different subspaces of the defect space:

$$G_{ii}^{dd} = \langle \mathrm{d}i|G|\mathrm{d}i\rangle = \sum_{\Gamma}\sum_{jj'=1}^{\sigma_\Gamma}\sum_{\mu=1}^{d_\Gamma} \langle \mathrm{d}i|\Gamma j\mu\rangle\langle \Gamma j\mu|G|\Gamma j'\mu\rangle\langle \Gamma j'\mu|\mathrm{d}i\rangle \tag{12}$$

where σ_Γ gives the number of times that the Γth irreducible representation with dimension d_Γ occurs in the total representation $\Gamma_{C_{3v}}$. With the help of the symmetry coordinates $U(\Gamma j\mu) = |\Gamma j\mu\rangle$ the coefficients $\langle \mathrm{d}i|\Gamma j\mu\rangle$ are readily evaluated, facilitating

Table 1. Symmetry coordinates in the impurity space. $U(li)$ is the amplitude of displacement of the lth ion in the ith direction.

Representation	Symmetry coordinates
A_1	$U(A_1, 1) = (1/3^{1/2})[U(0x) + U(0y) + U(0z)]$
	$U(A_1, 2) = (1/3^{1/2})[U(1x) + U(2y) + U(3z)]$
	$U(A_1, 3) = (1/3^{1/2})[U(\bar{1}x) + U(\bar{2}y) + U(\bar{3}z)]$
	$U(A_1, 4) = (1/6^{1/2})[U(2x) + U(3x) + U(1y) + U(3y) + U(1z) + U(2z)]$
	$U(A_1, 5) = (1/6^{1/2})[U(\bar{2}x) + U(\bar{3}x) + U(\bar{1}y) + U(\bar{3}y) + U(\bar{1}z) + U(\bar{2}z)]$
A_2	$U(A_2, 1) = (1/6^{1/2})[(U(2x) - U(3x) + U(3y) - U(1y) + U(1z) - U(2z)]$
	$U(A_2, 2) = (1/6^{1/2})[U(\bar{2}x) - U(\bar{3}x) + U(\bar{3}y) - U(\bar{1}y) + U(\bar{1}z) - U(\bar{2}z)]$
E	$U(E1, 1) = (1/6^{1/2})[2U(0x) - U(0y) - U(0z)]$
	$U(E1, 2) = (1/6^{1/2})[2U(1x) - U(2y) - U(3z)]$
	$U(E1, 3) = (1/6^{1/2})[2U(\bar{1}x) - U(\bar{2}y) - U(\bar{3}z)]$
	$U(E1, 4) = (1/12^{1/2})[U(2x) + U(3x) - 2U(1y) + U(3y) - 2U(1z) + U(2z)]$
	$U(E1, 5) = \tfrac{1}{2}[U(2x) + U(3x) - U(2z) - U(3y)$
	$U(E1, 6) = (1/12^{1/2})[U(\bar{2}x) + U(\bar{3}x) - 2U(\bar{1}y) + U(\bar{3}y) - 2U(\bar{1}z) + U(\bar{2}z)]$
	$U(E1, 7) = \tfrac{1}{2}[U(\bar{2}x) + U(\bar{3}x) - U(\bar{3}y) - U(\bar{2}z)]$
	$U(E2, 1) = (1/2^{1/2})[U(0y) - U(0z)]$
	$U(E2, 2) = (1/2^{1/2})[U(2y) - U(3z)]$
	$U(E2, 3) = (1/2^{1/2})[U(\bar{2}y) - U(\bar{3}z)]$
	$U(E2, 4) = \tfrac{1}{2}[-U(2x) + U(3x) + U(3y) - U(2z)]$
	$U(E2, 5) = (1/12^{1/2})[U(2x) - U(3x) + 2U(1y) + U(3y) - 2U(1z) - U(2z)]$
	$U(E2, 6) = \tfrac{1}{2}[-U(\bar{2}x) + U(\bar{3}x) + U(\bar{3}y) - U(\bar{2}z)]$
	$U(E2, 7) = (1/12^{1/2})[U(\bar{2}x) - U(\bar{3}x) + 2U(\bar{1}y) + U(\bar{3}y) - 2U(\bar{1}z) - U(\bar{2}z)]$

the calculation of the defect Green function:

$$G^{\mathrm{dd}}_{xx} = G^{\mathrm{dd}}_{yy} = G^{\mathrm{dd}}_{zz} = \tfrac{1}{3}G_{11}(\mathrm{A}_1) + \tfrac{2}{3}G_{11}(\mathrm{E}) \tag{13}$$

where $G_{11}(\Gamma)$ is 11 element of $G(\Gamma)$. The local density of states of the defect is given by

$$Z^{\mathrm{d}}(\omega) = (2\omega M/3\pi)\mathrm{Im}[G_{11}(\mathrm{A}_1) + 2G_{11}(\mathrm{E})]. \tag{14}$$

Using equations (6) and (12), we can write

$$\begin{aligned} G_{11}(\mathrm{A}_1) &= G^0_{11}(\mathrm{A}_1) - \sum_{ij=1}^{5} G^0_{12}(\mathrm{A}_1)t_{ij}(\mathrm{A}_1)G^0_{j1}(\mathrm{A}_1) \\ G_{11}(\mathrm{E}) &= G^0_{11}(\mathrm{E}) - \sum_{ij=1}^{7} G^0_{1i}(\mathrm{E})t_{ij}(\mathrm{E})G^0_{ji}(\mathrm{E}). \end{aligned} \tag{15}$$

3.2. *Numerical results*

In order to calculate the local density of states of the ⟨111⟩ off-centre Ag^+ in RbI, the perfect lattice is described in terms of shell model phonons. To calculate the required perfect lattice Green functions of RbI, a modified method of Gilat and Raubenheimer (1966) is used. The lattice phonons used in the present calculation are calculated on the basis of the shell model parameters (model 2) of Raunio and Rolandson (1970). The model is derived on the basis of fits to the measured results in neutron scattering experiments.

Usually in such a Green function treatment the force constant changes are treated as free parameters in the theory and are determined by fitting to experiment. Sometimes they are estimated from a knowledge of interaction potential in the crystal and relaxations of atoms around the defect. In that case the potential should be consistent with the force constant model used to generate the perfect lattice Green functions. However, in the present work, we seek an alternative because the potential function corresponding to shell model parameters used for perfect lattice description is not known. Catlow *et al* (1977) and Sangster and Atwood (1978) have developed potentials for alkali halides which are based on a shell model description and are quite successful in giving defect energies in the case of intrinsic defects and the displacements of off-centre impurities (Catlow *et al* 1976, 1978, 1979, Rowell and Sangster 1981, Sangster 1980). In the calculation that follows, we use the potential due to Catlow *et al* (1977) because the perfect lattice force constants calculated from it compare favourably with the force constants appearing in the shell model. Catlow *et al* (1977) used a Born–Mayer-type potential $V(r) = A\exp(-r/\rho)$ for the nearest-neighbour cation–anion interaction and the second-nearest-neighbour cation–cation and anion–anion interactions plus a van der Waals type of term for the second-neighbour interaction. Since we are interested in force constant changes between the impurity and its first neighbours, we have considered the potential with only first-neighbour interactions. For RbI, we used the potential parameter set 1 of Catlow *et al* (1977): $A_{+-} = 5282.0\,\mathrm{eV}$ and $\rho_{+-} = 0.3431\,\text{Å}$. For RbI : Ag^+, we find A by putting A equal to $b\exp[(r_+ + r_-)/\rho]$; r_+ and r_- are the ionic radii of cations and anions, respectively, and on the assumption that, because of the presence of Ag^+, only r_+ changes from 1.47 Å (Rb^+) to 1.26 Å (Ag^+) and r_- and b remain unchanged. The static off-centre displacement d of Ag^+ is 0.916 Å which is deduced from the observed value of the electric dipole moment p of Ag^+ in RbI of 2.0 e Å (Kapphan 1982). It is assumed that the local field is given by the Lorentz local field $E_{\mathrm{loc}} = [(\varepsilon_0 + 2)/3]\mathrm{E}$, ε_0 being the static dielectric constant, and the charge on the Ag^+ ion is equal to the electronic charge e. The calculated force constant changes are as follows:

$\Delta f^1_{\parallel} = 1.74953 \times 10^4$ dyn cm^{-1} $\qquad \Delta f^1_{\perp} = -0.21207 \times 10^4$ dyn cm^{-1}

$\Delta f^2_{\parallel} = -1.65722 \times 10^4$ dyn cm^{-1} $\qquad \Delta f^2_{\perp} = 0.15901 \times 10^4$ dyn cm^{-1}.

It is pertinent to point out that the calculated force constant changes may not be the best choice and, as indicated earlier, the usual course in such a situation is to compare the calculated spectrum with some experimental spectrum such as infrared lattice absorption and to adjust the force constant changes in the process. This type of procedure would have been quite natural especially when the model assumes changes only in the repulsive force constants between the impurity and its nearest neighbours and all other possible force constant changes are ignored. Unfortunately, as yet, no reasonable spectra for RbI : Ag^+ are available.

The problem of calculating force constant changes around defects within a shell model has been thoroughly discussed by Sangster and co-workers (1981, 1982). Their method consists in examining the energy changes for small static displacements of ion cores in both the perfect and the defect crystals. The force constant changes thus obtained are entirely consistent with the treatment based on Green functions obtained from core eigenvectors (the shell coordinates being eliminated by using the adiabatic approximation). Sangster *et al* (1981) conclude that the force constant changes obtained from direct calculations from interaction potentials do not conform to the constraints imposed by the localised nearest-neighbour defect model. Although the second-neighbour force constant changes are small, the simple localised defect models normally used in Green function methods for defect dynamics are likely to be in error (Sangster and Rowell 1982). Moreover, except for the off-centre position of the impurity ion itself, the present defect model ignores any relaxation of ions from their perfect lattice equilibrium positions and therefore the calculated force constant changes should be used with some caution.

We use the calculated perfect lattice Green function and the force constant changes $\Delta f^1_{\parallel}$, $\Delta f^1_{\perp}$, $\Delta f^2_{\parallel}$ and $\Delta f^2_{\perp}$ to evaluate the local density of states of Ag^+ in RbI with the help of equations (14) and (15). The calculated result is presented in figure 2. In the actual calculation, we have considered only those symmetry modes in which the impurity moves, namely $U(A_1, 1)$ and $U(E, 1)$. These are the modes in which resonance may be expected. This suggestion is borne out by the vibrational behaviour of off-centre Ag^+ in RbCl where almost the entire intensity of low-frequency resonant peaks in the infrared lattice absorption comes from those symmetry modes which involve defect motion (Mokross and Dick 1977).

From figure 2, it is clear that we obtain four peaks at 40.0, 62.5, 72.5 and 82.5 cm^{-1}. However, it is not clear whether the peaks correspond to activated resonance modes of the impurity or the projected peaks (critical points) of the density of states of the host as the calculated phonon spectrum of the host crystal does have peaks in the vicinity of the obtained frequencies. As regards experiments, preliminary infrared results obtained by Kapphan (1986) show only one peak at about 70 cm^{-1} in both pure and doped RbI. Future experimental measurements should clarify the situation.

4. Conclusion

We have developed an impurity model for the ⟨111⟩ off-centre substitutional impurity in an alkali halide crystal of rocksalt structure. We have used the static off-centre

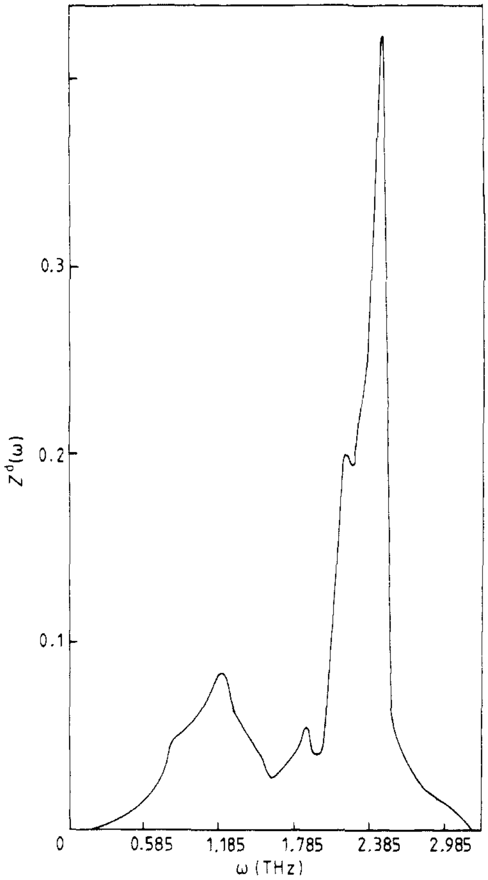

Figure 2. Local density of states of off-centre ⟨111⟩ Ag^+ in RbI.

displacement of the impurity determined from ultraviolet absorption and electro-optical measurements of Kapphan (1982) and the short-range potential developed by Catlow *et al* (1977) to estimate the force constant changes between the impurity and its nearest neighbours. The model is applied to calculate the local density of states of Ag^+ in RbI. We obtain resonance-like peaks at 40, 62.5, 72.8 and 82.5 cm^{-1}.

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