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Pair Impurities in Alkali Halides-2:Analytical Expressions

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ABSTRACT

Analytical expressions have been derived for different modes of vibrations using elegant group theoretical tools and Green function technique. Five atom linear molecule having D_{4h} site symmetry has been considered. 15-dimensional representation has been reduced to irreducible representations with the help of point group to which the molecule belongs. The effect of mass changes as well as changes in short range force constants have been taken into account.

Keywords: Green function, Site symmetry

INTRODUCTION

A five atom defect space having D_{4h} symmetry displayed in figure 1 has been considered. The defect atoms 1 and 2 are at $(00\bar{1})$ and (001) and the host atoms 0, 3 and 4 are at (000), $(00\bar{2})$ and (002) locations of Cartesian co-ordinate system.

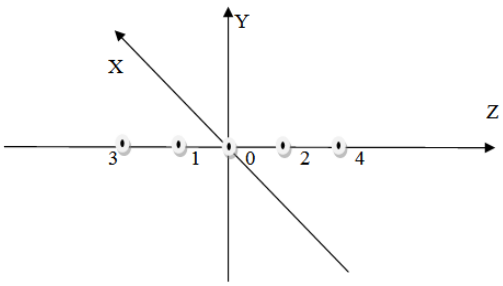

Figure 1. Five atoms linear molecule having D_{4h} point symmetry.

2. METHOD OF DERIVATION AND EXPRESSIONS

The modes of vibrations are obtained from the solution of the determinantal equation [1,2]

$$|I - GJ| = 0 \tag{1}$$

Here I denotes unit matrix, G the perfect lattice Green function matrix and J the perturbation matrix corresponding to the defect space.

Using the normalised symmetry co-ordinates [3], the (15x15) dimensional $|I - GJ|$ matrix was block diagonalized into various irreducible representations. The block diagonalized matrix is written as

$$\tilde{D} = U^{\dagger}|I - GJ|\tilde{U} \tag{2}$$

Where U is the (15x15) matrix formed by the normalized symmetry co-ordinates and $U^{\dagger}$ is the adjoint matrix of U. The various modes, obtained on block-diagonalizing $|\tilde{I} - \tilde{G}\tilde{J}|$, are given by

A_{1g} mode:

$$\begin{vmatrix} 1 - A_{1g}(1,1) & A_{1g}(1,2) \\ A_{1g}(2,1) & 1 - A_{1g}(2,2) \end{vmatrix} = 0 \tag{3}$$

where,

$A_{1g}(1,1) = -2\Delta A g_3 + 2J(g_0 - g_{10})$
$A_{1g}(1,2) = 2\Delta A(-g_0 + g_3 + g_{10})$
$A_{1g}(2,1) = 2\Delta A(-g_1 + g_3)$
$A_{1g}(2,2) = 2\Delta A(g_1 - g_3)$

Similar expressions have been derived for E_g, A_{2u} and E_u modes.
ΔA=A parameter for defect host bond – A parameter for the perfect lattice
$J = \varepsilon M\omega^2 + 2\Delta A$
$\varepsilon M = M_{host} - M_{defect}$

The expression involve following 8 independent Green functions defined below:
$g_0 = G_{xx}(000,-;000,-;\omega^2)$
$g_1 = G_{xx}(000,+;000,+;\omega^2)$
$g_2 = G_{xx}(000,+;001,-;\omega^2)$
$g_3 = G_{zz}(000,+;001,-;\omega^2)$
$g_7 = G_{xx}(000,+;002,+;\omega^2)$
$g_8 = G_{zz}(000,+;002,+;\omega^2)$
$g_9 = G_{xx}(000,-;002,-;\omega^2)$
$g_{10} = G_{zz}(000,-;002,-;\omega^2)$

RESULT

Using the above expression, the modes of vibrations can be computed and compared with the available experimental results. We are in process of computing the

theoretical values.

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