LATTICE DYNAMICS OF STRONTIUM OXIDE USING THREE-BODY FORCE SHELL MODEL

S MOHAN* and S DURAI

Division of Applied Sciences, Anna University, Madras Institute of Technology, Madras 600 044, India

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The phonon dispersion relations in SrO at 300 K have been calculated along the three high symmetry directions using the three body force shell model (TSM). This model takes care of the effect of many body interactions in the lattice potential. The main aim of the present work is to treat the various interactions between the ions in a more general way without making them numerically equal. The Sr\(^{2+}\) and O\(^{2-}\) ions are both polarizable. The results are briefly discussed. The values of the phonon frequencies evaluated by the new approach are, in general, in good agreement with the experimental values.

Key Words: Lattice Dynamics; Alkaline Earth Oxides; Strontium Oxide

INTRODUCTION

The alkaline earth oxide crystals are predominantly ionic in character and their lattice dynamics can be studied on the basis of the same theoretical models which are applicable to alkali halides. The shell model developed by Woods et al.\(^1\) for the study of vibrational properties of alkali halides have been improved by Verma and Singh\(^2\) by including the three body forces between ion pairs. This improved model has been refined further by Verma and Agarwal.\(^3\) In the present investigation, we have applied this model with a new modification, and evaluated the phonon frequencies of strontium oxide (Sr\(^{2+}\) O\(^{2-}\)).

THEORY

The TSM equations in the matrix form are given by

\[- m\omega^2 U = (R + ZC'Z) U + (T + ZC'Y) W\]

\[O = (YC'Z + T') U + (YC'Y + S) W\]

with

\[ZC'Z = Z(Z + 12f(a)) + V,\]

where \(R, S, T\) are matrices specifying short range core-core, shell-shell, and core-shell interactions respectively and \(f(a)\) is related to overlap integrals of electron wave functions. \(V\) is the force constant derived from the purely three body part of the lattice potential as expressed by Lundquist.\(^4\) The other terms assume the usual meaning as given by Cowley et al.\(^5\).

*Department of Physics, Pondicherry University, Pondicherry 605 006.
In the earlier approaches\textsuperscript{3,6} the $R$, $S$, $T$ elements have been set equal to one another and hence the phonon frequencies have been evaluated. In the present investigation we have started with a more general approach such that $R \neq S \neq T$. The $R$ and $C$ elements are calculated from the dimensionless coefficients of Kellermann.\textsuperscript{7} The introduction of short range force constants $A_1$, $B_1$, $A_{11}$ and $B_{11}$\textsuperscript{8} enables one to calculate the $T$ matrix elements. Further the variations in $T$ elements with respect to the symmetry directions $-q$, are identical to the corresponding variations in $R$ elements. With this $S$ matrix elements are estimated using the relation $2T - R = S$. The $V$ matrix elements are calculated using the coefficients (revised values) given by Verma and Singh. The secular equation to be solved and other details are the same as those given in our recent communication.\textsuperscript{9}

\textbf{RESULTS, DISCUSSION AND CONCLUSION}

The availability of data such as the Second order Raman Spectrum, neutron scattering measurements, elastic and dielectric properties for SrO makes our investigation a fruitful and interesting one.

Table I presents the input data which are the elastic constants, lattice constant, the long wave optical frequencies and the optical polarizability. The basic equations used for the calculation of the model parameters (Table II) from the elastic constants are the same as given in reference.\textsuperscript{6} The experimental values and the calculated theoretical values of the phonon frequencies are given in Table III. The value of phonon frequencies are reasonable and fall in the expected range, being also in good agreement with the observed values which bears out the significance of the present approach.

\begin{table}[h]
\centering
\caption{Input data}
\begin{tabular}{ll}
Elastic Constants ($10^{11}$ dynes/cm$^2$) & $C_{11} = 17.3$, $C_{12} = 4.5$, $C_{44} = 5.6$
\hline
Lattice constants ($10^{-8}$ cm) & $a_0 = 2.58$
\hline
Longwave optical frequencies ($10^{13}$ rad/sec) & $\omega_L = 9.08$, $\omega_T = 4.40$
\hline
Molecular Polarizability ($10^{-24}$ c.cm) & $\alpha_1 = 0.52$, $\alpha_s = 3.17$
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{Model parameters}
\begin{tabular}{llll}
A & \multicolumn{1}{l}{30.0618} & B & \multicolumn{1}{l}{-3.6078} & $f(a)$ & \multicolumn{1}{l}{-0.0376} \\
$B$ & \multicolumn{1}{l}{$\left( \frac{df}{da} \right)$} & \multicolumn{1}{l}{-0.0495} & $Y_1 =$ & \multicolumn{1}{l}{-3.1386} & $Y_s =$ & \multicolumn{1}{l}{-4.0129}
\end{tabular}
\end{table}
Table III

Vibrational frequencies (10^{12} \text{ C/s})

<table>
<thead>
<tr>
<th>(q)</th>
<th>(q)</th>
<th>(q)</th>
<th>Optical mode</th>
<th>Acoustical mode</th>
<th>Optical mode</th>
<th>Acoustical mode</th>
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<td>0</td>
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<td>7.6105 (7.50)</td>
<td>2.0189 (1.75)</td>
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<td>0</td>
<td>15.2806 (14.00)</td>
<td>4.1334 (4.000)</td>
<td>7.5748 (7.50)</td>
<td>2.8074 (2.30)</td>
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<td>0</td>
<td>0</td>
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<td>4.9545 (5.250)</td>
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<tr>
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<td>0.4</td>
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<tr>
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<td>0.1</td>
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<td>6.4281</td>
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<td>0.2</td>
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<td>8.4482 (8.5)</td>
<td>3.1775 (3.50)</td>
</tr>
</tbody>
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Values in parantheses refer to experimental values.  

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