Effect of electric field on the lattice viscosity of doped displacive ferroelectrics

R. P. Gairola and M. K. Gupta
Physics Department, University of Garhwal, Postal Box 21, Srinagar 246174, Garhwal, India
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A general expression for the lattice viscosity in doped displacive ferroelectrics, in the presence of an external electric field, is obtained using the double-time thermal Green's-function technique. The mass and force-constant changes between the impurity and host-lattice atoms are taken into account in the Silverman Hamiltonian augmented with higher-order anharmonic and electric moment terms. The defect-dependent, electric-field-dependent, and anharmonic contributions to the lattice viscosity are discussed separately. It is shown that the lattice viscosity tensor, which is the sum of two terms arising from acoustical and optical phonons, can be further separated into diagonal and nondiagonal parts. The nondiagonal contribution vanishes in the absence of defects. The frequency and temperature dependences of the viscosity tensor are also discussed.

I. INTRODUCTION

In the past there has been considerable interest in investigating the physical properties[1-3] of displacive ferroelectrics doped with impurities. These properties reveal interesting applications in ceramic industry, optoelectric devices, and in Masers and waveguides where these crystals doped with specific impurities are of great importance because of their response to applied electric and magnetic fields. In displacive ferroelectrics the soft transverse-optic mode of vibration is responsible for most of the temperature-dependent properties of these solids, and it is the anharmonic interaction which stabilizes this mode in the paraelectric phase.[4] So the anharmonic interactions cannot be neglected in discussing the physical properties of these crystals. The phenomenological theory of lattice viscosity due to De Vault and McLennan[5,6] is extended for displacive ferroelectrics by Goyal and Sharma,[7] considering up to quartic anharmonic terms in the Silverman Hamiltonian.[4] However, the lattice viscosity for displacive ferroelectrics doped with isotopic impurities has not been considered so far in the literature.

In the present study we have obtained a general expression for the lattice viscosity of doped displacive ferroelectrics in the paraelectric phase by augmenting the Silverman Hamiltonian with the terms responsible for mass change and force-constant changes between the impurity and host-lattice atoms. The effect of higher-order electric moment terms, due to the deformation of electronic shells in an external electric field, is also taken into account. We have also retained anharmonic terms up to fourth order in the Hamiltonian owing to the vital role played by the anharmonicity, as mentioned earlier. It is, therefore, also the aim of this paper to study the interaction of defect and anharmonic parameters in discussing the internal friction in ferroelectric solids.

The Hamiltonian for the problem is described in detail in Sec. II, and Sec. III deals with the evaluation of required Green's functions. The expression for lattice viscosity is obtained in Sec. IV, and Sec. V is left for discussion.

II. HAMILTONIAN

The modified Silverman Hamiltonian[4] of displacive ferroelectrics in the paraelectric phase which includes defects, dominant third- and fourth-order anharmonicity, and higher-order electric moment terms in an external electric field $\vec{E}$ can be conveniently written as

$$H=H_h+H_a-\vec{E}\cdot\vec{M}\ , \tag{2.1}$$

where H_h is the modified harmonic part involving the effect of mass change and harmonic-force-constant change between the impurity and host-lattice atoms due to substitutional defects, which is given by

$$H_h=\sum_k \hbar\omega_k^a(a_k^{a\dagger}a_k^a+\tfrac{1}{2})+\sum_k{}' \hbar\omega_k^o(a_k^{o\dagger}a_k^o+\tfrac{1}{2})-\left[\frac{\hbar\omega_0^o}{4}\right](A_0^oA_0^o+B_0^oB_0^o)-\hbar B_0^oX+\hbar A_0^oY+\hbar Z \ , \qquad (2.2)$$

with

$$X=\sum_{k,\lambda} C(k^\lambda,0)B_k^\lambda \ , \qquad (2.3)$$

$$Y=\sum_{k,\lambda} D(k^\lambda,0)A_k^\lambda \ , \qquad (2.4)$$

$$Z=\sum_{k_1,k_2,\lambda}[D(k_1^\lambda,k_2^\lambda)A_{k_1}^\lambda A_{k_2}^\lambda-C(k_1^\lambda,k_2^\lambda)B_{k_1}^\lambda B_{k_2}^\lambda]+\sum_{k_1,k_2}[D(k_1^ak_2^o)A_{k_1}^aA_{k_2}^o-C(k_1^ak_2^o)B_{k_1}^aB_{k_2}^o] \ . \qquad (2.5)$$

Here $\lambda=a,o$, for acoustic and optic modes, respectively, $A_k=a_k+a_{-k}^\dagger$, $B_k=a_k-a_{-k}^\dagger$, $a_k^\dagger$ and a_k being the usual creation and destruction operators. The defect parameters $C(k_1,k_2)$ and $D(k_1,k_2)$, depending upon the mass change and force-constant changes between impurity and host-lattice atoms, respectively, are given by[8]

$$C(k_1,k_2)=(\tfrac{1}{2}\mu^{-1})(M_0/2N)(\omega_{k_1}\omega_{k_2})^{1/2}\vec{e}(k_1)\cdot\vec{e}(k_2)\left[\sum_{l=1}^{N} f\exp[i(\vec{k}_1+\vec{k}_2)\cdot\vec{R}(l)]-\sum_{i=1}^{n}\exp[i(\vec{k}_1+\vec{k}_2)\cdot\vec{R}(i)]\right] , \qquad (2.6)$$

$$D(k_1k_2)=(\tfrac{1}{4}N^{-1})(\omega_{k_1}\omega_{k_2})^{-1/2}\sum_{l,\alpha}\sum_{l',\beta}[\Delta\phi_{\alpha\beta}(ll')/M_0]\vec{e}(k_1)\cdot\vec{e}(k_2)\exp\{i[\vec{k}_1\cdot\vec{R}(l)+\vec{k}_2\cdot\vec{R}(l')]\} \ , \qquad (2.7)$$

where $\vec{e}(k)$ is the polarization vector, $\vec{R}(l)$ is the equilibrium position vector of the lth atom, $\Delta\phi_{\alpha\beta}$ denotes the force-constant change, l and l' refer to the impurity and its nearest neighbors, and $\mu=MM'/(M'-M)$. M_0 is the weighted harmonic mean of the masses of all atoms defined by the relation

$$(1/M_0)=(f/M')+(1-f)/M \ , \qquad (2.8)$$

where $f=n/N$. Here N is the total number of atoms in the crystal whose $(N-n)$ lattice sites are occupied by atoms of mass M, and n sites are occupied by randomly distributed substitutional impurities each of mass M'. In Eq. (2.6) above, $C(k_1,k_2)$ vanishes when n is either zero or N and the prime on the summation in Eq. (2.2) excludes $k=0$.

In Eq. (2.1), H_a is the anharmonic part which includes the effect of third- and fourth-order anharmonicity and $-\vec{E}\cdot\vec{M}$ is the contribution to the lattice potential energy due to the electric moment $\vec{M}$ developed in the crystal when placed in an external electric field $\vec{E}$. These contributions are given by

$$H_a=\hbar A_0^oP+\hbar(A_0^o)^2Q+\hbar A_0^oR+\hbar A_0^oS \ , \qquad (2.9)$$

$$-\vec{E}\cdot\vec{M}=\hbar E(-\alpha A_0^o+qA_0^o+p+r+s) \ , \qquad (2.10)$$

with

$$P=\sum_k \alpha(k)A_k^oA_k^{a\dagger}, \quad p=\sum_k A(k)A_k^oA_k^{a\dagger} \ , \qquad (2.11)$$

$$Q=\sum_{k,\lambda}\beta^\lambda(k)A_k^{\lambda\dagger}A_k^\lambda, \quad q=\sum_{k,\lambda}B^\lambda(k)A_k^{\lambda\dagger}A_k^\lambda \ , \qquad (2.12)$$

$$R=\sum_{k_1,k_2,k_3}\gamma(k_1,k_2,k_3)A_{k_1}^oA_{k_2}^aA_{k_3}^a \ ,$$
$$r=\sum_{k_1,k_2,k_3}C(k_1,k_2,k_3)A_{k_1}^oA_{k_2}^aA_{k_3}^a \ , \qquad (2.13)$$

and

$$S=\sum_{k_1,k_2,k_3}\mu(k_1,k_2,k_3)A_{k_1}^oA_{k_2}^oA_{k_3}^o \ ,$$
$$s=\sum_{k_1,k_2,k_3}D(k_1,k_2,k_3)A_{k_1}^oA_{k_2}^oA_{k_3}^o \ . \qquad (2.14)$$

Here $\alpha(k)$, $\beta^\lambda(k)$, $\gamma(k_1,k_2,k_3)$, and $\mu(k_1,k_2,k_3)$ are related[9] to the Fourier transforms of the third- and fourth-order derivatives of the lattice potential energy. α, $A(k)$,$B^\lambda(k)$, and $C(k_1,k_2,k_3)$,$D(k_1,k_2,k_3)$ represent the linear, second-, and third-order electric moment coefficients, respectively.

We now transform the Hamiltonian (2.1) with the help of a transformation operator $T=-igEB_0^o$, according to the following scheme[10]:

$$H_T=\exp(-iT)H\exp(iT)$$
$$=H+i[H,T]-\tfrac{1}{2}[[H,T],T]+\cdots \ , \qquad (2.15)$$

where the value of coefficient g is chosen in such a way that it eliminates the linear term $(-\hbar\alpha EA_0^o)$ in A_0^o from the Hamiltonian (2.1). This gives $g=(\alpha/\omega_0^o)$. This transformation is necessary,[9] whenever the effect of electric field on some physical properties of displacive ferroelectrics is sought through Hamiltonian (2.1). Without this transformation, the dominant electric-field-dependent term $(-\hbar\alpha EA_0^o)$ gives rise to a zero Green's function and so the electric field effects, through the dominant first-order electric moment coefficient, are not obtained in the final results. With the aid of the above transformation, the transformed Hamiltonian operator becomes

$$H_T=H_h+H_a+\hbar A_0^o qE+\hbar E(p+r+s)$$
$$-2\hbar gE(P+R+S+qE+Y)$$
$$-4\hbar gEA_0^oQ+4\hbar g^2E^2Q \ . \qquad (2.16)$$

III. GREEN'S FUNCTIONS

Consider the following Green's functions for the optical ($\lambda=o$) and acoustical ($\lambda=a$) phonons:

$$G_{kk'}^{\lambda}(t-t')=\langle\langle A_k^{\lambda}(t);A_{k'}^{\lambda\dagger}(t')\rangle\rangle$$
$$=-i\Theta(t-t')\langle[A_k^{\lambda}(t),A_{k'}^{\lambda\dagger}(t')]\rangle \ , \qquad (3.1)$$

where $\Theta(t)$ is the Heaviside unit step function. By differentiating Eq. (2.17) for $\lambda=a$ with respect to t and Fourier transforming, the equation of motion of acoustical Green's function via the transformed Hamiltonian (2.16) is given by

$$[\omega^2-(\bar{\omega}_k^a)^2]G_{kk'}^a(\omega)=(\omega_k^a\delta_{kk'}/\pi)+4C(-k^a,k'^a)/\pi+(\omega_k^a/\pi)\langle\langle L_k^a(t);A_{k'}^{a\dagger}(t')\rangle\rangle_\omega \ , \qquad (3.2)$$

where

$$L_k^a(t)=\bar{F}_k^a(t)+\sum_{k_1}[4C(-k^a,k_1^a)/\omega_{k_1}^a]\bar{F}_{k_1}^a(t)+4\pi\sum_{k_1}\alpha(-k^a,k_1^a)A_{k_1}^a(t) \ , \qquad (3.3)$$

$$\bar{F}_k^a(t)=F_k^a(t)+E\left\{[A(k)-2g\alpha(k)]A_k^o+2[B^a(k)-4g\beta^a(k)]A_0^oA_k^a + 2\sum_{k_1,k_2}[C(k_1,k_2-k)-2g\gamma(k_1,k_2-k)]A_{k_1}^oA_{k_2}^a\right\} \ , \qquad (3.4)$$

$$\alpha(k^a,k_1^a)=\left\{D(k^a,k_1^a)+[(\omega_{k_1}^a)^2/\omega_{k_1}^a\omega_k^a]C(k^a,k_1^a)+(4/\omega_k^a)\sum_{k_2}C(-k^a,k_2^a)D(-k_2^a,k_1^a)\right\} \ , \qquad (3.5)$$

$$(\bar{\omega}_k^a)^2=(\omega_k^a)^2+8g[2g\beta^a(k)-B^a(k)]E^2\omega_k^a \ . \qquad (3.6)$$

The treatment for the evaluation of the Green's functions adopted here is similar to that considered elsewhere.[7,9] Here $F_k^a(t)$ is given by Eq. (16) of Ref. 7 (hereafter referred to as I), and $F_{k_1}^a(t)$ can be obtained from it by replacing k with k_1. If we now write the equation of motion of the Green's function $\langle\langle L_k^a(t);A_{k'}^{a\dagger}(t')\rangle\rangle$, appearing in Eq. (3.2) with respect to time argument t' and substituting the resulting expression in Eq. (3.2) the Green's function $G_{kk'}^a(\omega)$ can be written in the form of Dyson's equation

$$G_{kk'}^a(\omega)=\tilde{G}_k^a(\omega)\delta_{kk'}+\tilde{G}_k^a(\omega)\tilde{P}^a(k,k',\omega)\tilde{G}_k^a(\omega)+4g_k^aC(-k^a,k'^a)$$
$$=\tilde{G}_k^a(\omega)\delta_{kk'}+\tilde{G}_k^a(\omega)\Pi^a(k,\omega)G_{kk'}^a(\omega)+4g_k^a(\omega)C(-k^a,k'^a) \ , \qquad (3.7)$$

where

$$\tilde{G}_k^a(\omega)=\omega_k^a\{\pi[\omega^2-(\bar{\omega}_k^a)^2]\}^{-1}, \quad g_k^a(\omega)=\{\pi[\omega^2-(\bar{\omega}_k^a)^2]\}^{-1} \qquad (3.8)$$

and the polarization operator $\Pi^a(k,\omega)$ are given by

$$\Pi^a(k,\omega)=\tilde{P}^a(k,k',\omega)[1+\tilde{G}_k^a(\omega)\tilde{P}^a(k,k',\omega)+4C(-k^a,k'^a)/\omega_k^a]^{-1} \ , \qquad (3.9)$$

with

$$\tilde{P}^a(k,k',\omega)=\frac{1}{2}\left[\langle[L_k^a(t),B_{k'}^{a\dagger}(t')]\rangle+(\omega/\omega_k^a)\langle[L_k^a(t),A_{k'}^{a\dagger}(t')]\rangle + (4/\omega_k^a)\sum_{k_1}C(-k^a,k_1^a)\langle[L_k^a(t),B_{k'}^{a\dagger}(t')]\rangle\right]_{t=t'} +\frac{1}{2}\langle\langle L_k^a(t);L_{k'}^{a\dagger}(t')\rangle\rangle \,. \tag{3.10}$$

If the frequencies ω are far from the zeros of the denominator in Eq. (3.9), one may expand the right-hand side in powers of $\tilde{P}(k,k',\omega)$, and retaining only the dominant[7,11] first term, i.e., $\Pi^a(k,\omega)\simeq P^a(k,k',\omega)$, the Green's function can be written as

$$G_{kk'}^a(\omega)=\frac{\omega_k^a[\delta_{kk'}+4C(-k^a,k'^a)/\omega_k^a]}{\pi[\omega^2-(\hat{\omega}_k^a)^2-2\omega_k^a P^a(k,\omega)]}\,, \tag{3.11}$$

where $\hat{\omega}_k^a$, the renormalized frequency of the mode k, which depends both on defect and electric field, is given by

$$(\hat{\omega}_k^a)^2=(\bar{\omega}_k^a)^2+(\omega_k^a/2\pi)\left[\langle[L_k^a(t),B_{k'}^{a\dagger}(t')]\rangle+(\omega/\omega_k^a)\langle[L_k^a(t),A_{k'}^{a\dagger}(t')]\rangle + (4/\omega_k^a)\sum_{k_1}C(-k^a,k_1^a)\langle[L_k^a(t),B_{k_1}^{a\dagger}(t')]\rangle\right]_{t=t'} \tag{3.12a}$$

$$=(\bar{\omega}_k^a)^2+W^a(k,k')+(4/\omega_k^a)\sum_{k_1}C(-k^a,k_1^a)W^a(k,k_1)\,, \tag{3.12b}$$

with

$$W^a(k,k')=4\left[\omega_k^a+4\sum_{k_1}C(-k^a,k_1^a)\right]\left[\beta^a(k)\langle A_0^oA_0^o\rangle+\sum_{k_1}\gamma(k_1,k',-k)\langle A_0^oA_{k_1}^o\rangle\right] +4\omega_k^a\{D(-k^a,k'^a)+[(\bar{\omega}_{k_1}^a)^2/\omega_k^a]C(-k^a,k'^a)\}+16\sum_{k_2}C(-k^a,k_2^a)D(-k^a,k_2^a) \tag{3.13}$$

and

$$P^a(k,\omega)=(2\pi)^{-1}\langle\langle L_k^a(t);L_{k'}^{a\dagger}(t')\rangle\rangle_\omega\,. \tag{3.14}$$

The response function (3.14) can be evaluated in the lowest-order approximation of perturbation theory via the following zeroth-order renormalized Hamiltonian

$$H_{\text{ren}}^0=(\hbar/4)\sum_k\{[(\hat{\omega}_k^a)^2/\omega_k^a]A_k^{a\dagger}A_k^a+\omega_k^aB_k^{a\dagger}B_k^a\}+(\hbar/4)\sum_k\{[(\hat{\omega}_k^o)^2/\omega_k^o]A_k^{o\dagger}A_k^o+\omega_k^oB_k^{o\dagger}B_k^o\} +(\hbar\hat{\Omega}/4)(A_0^oA_0^o+B_0^oB_0^o)\,, \tag{3.15}$$

where $\hat{\omega}_k^o$ and $\hat{\Omega}$ are the defect and electric-field-dependent renormalized frequencies for the optic ($k\neq0$) and low-lying transverse optic mode ($k=0$), respectively; the latter can be obtained by starting with Green's function $\langle\langle A_0^o(t);A_0^o(t')\rangle\rangle$ and writing its equation of motion in the above manner. We thus obtain

$$\hat{\Omega}^2=-(\omega_0^o)^2+4\omega_0^oD(0,0)+4\omega_0^o\sum_{k,\lambda}\beta^\lambda(k)\langle A_k^{\lambda\dagger}A_k^\lambda\rangle+\Delta(\hat{\Omega})\,, \tag{3.16}$$

where $\Delta(\hat{\Omega})$ is the shift in frequency $\hat{\Omega}$. In Eq. (3.16) it is assumed that all modes, other than the soft mode, remain hard (mean-field approximation). Replacing ω by $\omega+i\epsilon(\epsilon\to+0)$ in Eq. (3.14) and recalling $\hat{\Delta}_k^a(\omega)$ and $\hat{\Gamma}_k^a(\omega)$ as the real and imaginary parts of the response function $P^a(k,\omega+i\epsilon)$, we can write Eq. (3.11) as

$$G_{kk'}^a(\omega+i\epsilon)=\omega_k^a\xi_{kk'}^a\pi^{-1}[\omega^2-(\hat{\nu}_k^a)^2+2i\omega_k^a\hat{\Gamma}_k^a(\omega)]^{-1}\,, \tag{3.17}$$

where

$$(\hat{\nu}_k^a)^2=(\hat{\omega}_k^a)^2+2\omega_k^a\hat{\Delta}_k^a(\omega)\ , \tag{3.18}$$

$$\xi_{kk'}^a=\delta_{kk'}+4C(-k^a,k'^a)/\omega_k^a\ . \tag{3.19}$$

After evaluating the values of various two- and three-particle Green's functions appearing in Eq. (3.14) via the Hamiltonian (3.15), one finds the values of shift $\hat{\Delta}_k^a(\omega)$ and width $\hat{\Gamma}_k^a(\omega)$ of the response function as

$$\hat{\Delta}_k^a(\omega)=[\Delta_k^a(\omega)+\phi_k^aE^2]+\sum_{k_1}[4C(-k^a,k_1^a)/\omega_k^a]^2[\Delta_{k_1}^a(\omega)+\phi_{k_1}^aE^2]$$
$$+16\,\mathrm{Re}\sum_{k_1}\alpha(-k^a,k_1^a)\alpha^\dagger(k'^a,k_1^a)\omega_{k_1}^a[\omega^2-(\hat{\omega}_{k_1}^a)^2]^{-1} \tag{3.20}$$

and

$$\hat{\Gamma}_k^a(\omega)=[\Gamma_k^a(\omega)+\psi_k^aE^2]+\sum_{k_1}[4C(-k^a,k_1^a)/\omega_k^a]^2[\Gamma_{k_1}^a(\omega)+\psi_{k_1}^aE^2]$$
$$+8\pi\sum_{k_1}\alpha(-k^a,k_1^a)\alpha^\dagger(k'^a,k_1^a)(\omega_k^a/\hat{\omega}_{k_1}^a)[\delta(\omega-\hat{\omega}_{k_1}^a)-\delta(\omega+\hat{\omega}_{k_1}^a)]\ , \tag{3.21}$$

where

$$\phi_k^a=2[A(k)-2g\alpha(k)]^2\omega_k^o\delta_{kk'}[\omega^2-(\hat{\omega}_k^o)^2]^{-1}$$
$$+4[B^a(k)-4g\beta^a(k)]^2(\omega_k^a/\hat{\omega}_k^a)\sum_{l=\pm1}(\hat{N}_k^a+l\hat{N}_0)(\hat{\Omega}+l\hat{\omega}_k^a)[\omega^2-(\hat{\Omega}+l\omega_k^a)^2]^{-1}$$
$$+4\sum_{k_1,k_2}[C(k_1,k_2,-k)-2g\gamma(k_1,k_2,-k)](\omega_{k_1}^o\omega_{k_2}^a/\hat{\omega}_{k_1}^o\hat{\omega}_{k_2}^a)$$
$$\times\sum_{l=\pm1}(\hat{N}_{k_2}^a+l\hat{N}_{k_1}^o)(\hat{\omega}_{k_1}^o+l\omega_{k_2}^a)[\omega^2-(\hat{\omega}_{k_1}^o+l\hat{\omega}_{k_2}^a)^2]^{-1}\ , \tag{3.22}$$

$$\psi_k^a=2\pi[A(k)-2g\alpha(k)]^2(\omega_k^o/\hat{\omega}_k^o)[\delta(\omega-\hat{\omega}_k^o)-\delta(\omega+\hat{\omega}_k^o)]$$
$$+4\pi[B^a(k)-4g\beta^a(k)]^2(\omega_k^a/\hat{\omega}_k^a)\sum_{l=\pm1}(\hat{N}_k^a+l\hat{N}_0)[\delta(\omega-\hat{\Omega}-l\hat{\omega}_k^a)-\delta(\omega+\hat{\Omega}+l\hat{\omega}_k^a)]$$
$$+4\pi\sum_{k_1,k_2}[C(k_1,k_2,-k)-2g\gamma(k_1,k_2,-k)]^2(\omega_{k_1}^o\omega_{k_2}^a/\hat{\omega}_{k_1}^o\hat{\omega}_{k_2}^a)$$
$$\times\sum_{l=\pm1}(\hat{N}_{k_2}^a+l\hat{N}_{k_1}^o)[\delta(\omega-\hat{\omega}_{k_1}^o-l\hat{\omega}_{k_2}^a)-\delta(\omega+\hat{\omega}_{k_1}^o+l\hat{\omega}_{k_2}^a)]\ , \tag{3.23}$$

$$\hat{N}_k^\lambda=\langle A_k^{\lambda\dagger}A_k^\lambda\rangle=\coth(\tfrac{1}{2}\beta\hbar\hat{\omega}_k^\lambda),\quad \hat{N}_0=\langle A_0^oA_0^o\rangle=\coth(\tfrac{1}{2}\hat{\beta}\hbar\hat{\Omega})\ . \tag{3.24}$$

In the above equations $\Delta_k^a(\omega)$ and $\Gamma_k^a(\omega)$ are given[11] by the same expressions (32) and (33) of I, except for the replacement of Ω and ω_k^λ by $\hat{\Omega}$ and $\hat{\omega}_k^\lambda$, which arises in our case due to the effect of complete renormalization of phonon frequencies by the defect and electric moment parameters. Starting again with Eq. (3.1) for $\lambda=0$ and proceeding as above, we obtain the following equations for the shift and width of optical phonons:

$$\hat{\Delta}_k^o(\omega)=[\Delta_k^o(\omega)+\phi_k^oE^2]+\sum_{k_1}[4C(-k^o,k_1^o)/\omega_k^o]^2[\Delta_{k_1}^o(\omega)+\phi_{k_1}^oE^2]$$
$$+16\,\mathrm{Re}\sum_{k_1}\alpha(-k^o,k_1^o)\alpha^\dagger(k'^o,k_1^o)\omega_{k_1}^o[\omega^2-(\hat{\omega}_{k_1}^o)^2]^{-1}\ , \tag{3.25}$$

$$\hat{\Gamma}_k^o(\omega)=[\Gamma_k^o(\omega)+\psi_k^oE^2]+\sum_{k_1}[4C(-k^o,k_1^o)/\omega_k^o]^2[\Gamma_{k_1}^o(\omega)+\psi_{k_1}^oE^2]$$
$$+8\pi\sum_{k_1}\alpha(-k^o,k_1^o)\alpha^\dagger(k'^o,k_1^o)(\omega_k^o/\hat{\omega}_{k_1}^o)[\delta(\omega-\hat{\omega}_{k_1}^o)-\delta(\omega+\hat{\omega}_{k_1}^o)]\ , \tag{3.26}$$

with

$$\phi_k^o = 2[A(k)-2g\alpha(k)]^2\omega_k^a\delta_{kk'}[\omega^2-(\hat{\omega}_k^a)^2]^{-1}$$
$$+4[B^o(k)-4g\beta^o(k)]^2\left[(\omega_k^o/\hat{\omega}_k^o)\delta_{kk'}\sum_{l=\pm 1}(\hat{N}_k^o+l\hat{N}_0)(\hat{\Omega}+l\hat{\omega}_k^o)[\omega^2-(\hat{\Omega}+l\hat{\omega}_k^o)^2]^{-1}\right]+4\hat{N}_0\hat{\Omega}(\omega^2-4\hat{\Omega}^2)^{-1}$$
$$+\sum_{k_2,k_3}[C(-k,k_2,k_3)-2g\gamma(-k,k_2,k_3)]^2$$
$$\times(\omega_{k_2}^a\omega_{k_3}^a/\hat{\omega}_{k_2}^a\hat{\omega}_{k_3}^a)\left[\sum_{l=\pm 1}(\hat{N}_{k_3}^a+l\hat{N}_{k_2}^a)\delta^2(\hat{\omega}_{k_2}^o+l\hat{\omega}_{k_3}^a)[\omega^2-(\hat{\omega}_{k_2}^a+l\hat{\omega}_{k_3}^a)^2]^{-1}\right]$$
$$+9\sum_{k_2,k_3}[D(-k,k_2,k_3)-2g\mu(-k,k_2,k_3)]^2$$
$$\times(\omega_{k_2}^o\omega_{k_3}^o/\hat{\omega}_{k_2}^o\hat{\omega}_{k_3}^o)\left[\sum_{l=\pm 1}(\hat{N}_{k_3}^o+l\hat{N}_{k_2}^o)\delta^2(\hat{\omega}_{k_2}^o+l\hat{\omega}_{k_3}^o)[\omega^2-(\hat{\omega}_{k_2}^0+l\hat{\omega}_{k_3}^o)]^{-1}\right], \tag{3.27}$$

$$\psi_k^o = 2\pi[A(k)-2g\alpha(k)]^2(\omega_k^a/\hat{\omega}_k^a)[\delta(\omega-\hat{\omega}_k^a)-\delta(\omega+\hat{\omega}_k^a)]$$
$$+4\pi[B^0(k)-4g\beta^o(k)]^2\left[\delta_{kk'}(\omega_k^o/\hat{\omega}_k^o)\sum_{l=\pm 1}(\hat{N}_k^o+l\hat{N}_0)[\delta(\omega-\hat{\Omega}-l\hat{\omega}_k^o)-\delta(\omega+\hat{\Omega}+l\hat{\omega}_k^o)]\right.$$
$$\left.+2\hat{N}_0[\delta(\omega-2\hat{\Omega})-\delta(\omega+2\hat{\Omega})]\right]$$
$$+\pi\sum_{k_2,k_3}[C(-k,k_2,k_3)-2g\gamma(-k,k_2,k_3)]^2(\omega_{k_2}^a\omega_{k_3}^a/\hat{\omega}_{k_2}^a\hat{\omega}_{k_3}^a)$$
$$\times\left[\sum_{l=\pm 1}(\hat{N}_{k_3}^a+l\hat{N}_{k_2}^a)\delta^2[\delta(\omega-\hat{\omega}_{k_2}^a-l\omega_{k_3}^a)-\delta(\omega+\hat{\omega}_{k_2}^a+l\hat{\omega}_{k_3}^a)]\right]$$
$$+2\pi\sum_{k_2,k_3}[D(-k,k_2,k_3)-2g\mu(-k,k_2,k_3)]^2(\omega_{k_2}^o\omega_{k_3}^o/\hat{\omega}_{k_2}^o\hat{\omega}_{k_3}^o)$$
$$\times\left[\sum_{l=\pm 1}(\hat{N}_{k_3}^o+l\hat{N}_{k_2}^o)\delta^2[\delta(\omega-\hat{\omega}_{k_2}^o-l\hat{\omega}_{k_3}^o)-\delta(\omega+\hat{\omega}_{k_2}^o+l\hat{\omega}_{k_3}^o)]\right], \tag{3.28}$$

where

$$\delta^2=\delta_{k_2,-k_2'}\delta_{k_3,-k_3'}+\delta_{k_2,-k_3'}\delta_{k_3,-k_2'} \tag{3.29}$$

and $\Delta_k^o(\omega)$ and $\Gamma_k^o(\omega)$ are given by Eqs. (4.2) and (4.3) of I, except for the replacement of ω_k^λ and Ω by $\hat{\omega}_k^\lambda$ and $\hat{\Omega}$, respectively. The value of the optical-phonon Green's function is

$$G_{kk'}^o(\omega+i\epsilon)=\omega_k^o\xi_{kk'}^o\pi^{-1}[\omega^2-(\hat{\nu}_k^o)^2+2i\omega_k^o\hat{\Gamma}_k^o(\omega)]^{-1}, \tag{3.30}$$

where

$$\xi_{kk'}^o=\delta_{kk'}+4C(-k^o,k'^o)/\omega_k^o, \tag{3.31}$$

$$(\hat{\nu}_k^o)^2=(\hat{\omega}_k^o)^2+2\omega_k^o\hat{\Delta}_k^o(\omega), \tag{3.32}$$

$$(\hat{\omega}_k^o)^2=(\overline{\omega}_k^o)^2+W^o(k,k')+(4/\omega_k^o)\sum_{k_1}C(-k^o,k_1^o)W^o(k,k_1), \tag{3.33}$$

with

$$(\overline{\omega}_k^o)^2=(\omega_k^o)^2+8\omega_k^o gE^2[2g\beta^o(k)-B^o(k)], \tag{3.34}$$

$$W^o(k,k')=4\omega_k^o\left[\beta^o(k)\langle A_0^oA_0^o\rangle+\sum_{k_1}3\mu(k_1,k',-k)\langle A_0^oA_{k_1}^o\rangle\right]$$
$$+16\sum_{k_1}C(-k^o,k_1^o)\left[\beta^o(k)\langle A_0^oA_0^o\rangle+3\sum_{k_1}\mu(k_1,k',-k)\langle A_0^oA_{k_1}^o\rangle\right]$$
$$+4\omega_k^o\{D(-k^o,k'^o)+[(\bar{\omega}_k^o)^2/\omega_k^o]C(-k^o,k'^o)\}$$
$$+16\sum_{k_2}C(-k^o,k_2^o)D(-k^o,k_2^o)\;. \quad (3.35)$$

IV. LATTICE VISCOSITY

The lattice viscosity tensor due to DeVault and McLennan, as extended by Goyal and Sharma, for displacive ferroelectrics can be written as[7]

$$\eta_{ijlm}=\sum_\lambda \eta_{ijlm}^\lambda\;, \quad (4.1)$$

with

$$\eta_{ijlm}^\lambda=(\beta\hbar^2/V)\lim_{\epsilon\to 0}\int_0^\infty dt\,\epsilon^{-\epsilon t}\sum_{k,k'}\omega_k^\lambda\omega_{k'}^\lambda\gamma_k^{ij\lambda}(\gamma_{k'}^{lm\lambda}-\gamma^{lm\lambda})\langle a_k^{\lambda\dagger}(t)a_{k'}^\lambda(0)\rangle\langle a_k^\lambda(t)a_{k'}^{\lambda\dagger}(0)\rangle\;, \quad (4.2)$$

where $\gamma_k^{ij\lambda}$ is the generalized Grüneisen parameter of the phonon for wave vector k, V is the volume of crystal, and $\beta^{-1}=k_BT$. By substituting the value of correlation functions appearing in Eq. (4.2) with the help of following relations,

$$\langle a_k^{\lambda\dagger}(t)a_{k'}^\lambda(0)\rangle=\tfrac{1}{4}\int_{-\infty}^\infty[1+(\omega/\omega_k^\lambda)]^2J_{kk'}^\lambda(\omega)\exp(i\omega t)d\omega\;, \quad (4.3)$$

$$J_{kk'}^\lambda(\omega)=\lim_{\epsilon\to 0}i(e^{\beta\hbar\omega}-1)^{-1}[G_{kk'}^\lambda(\omega+i\epsilon)-G_{kk'}^\lambda(\omega-i\epsilon)]\;, \quad (4.4)$$

and carrying out the integration, one finds that the lattice viscosity for the mode λ is given by

$$\eta_{ijlm}^\lambda=(\eta_{ijlm}^\lambda)_1+(\eta_{ijlm}^\lambda)_2\;, \quad (4.5)$$

where

$$(\eta_{ijlm}^\lambda)_1=\left[\frac{\beta\hbar^2}{V}\right]\sum_k(\omega_k^\lambda)^2\gamma_k^{ij\lambda}(\gamma_k^{lm\lambda}-\gamma^{lm\lambda})\frac{e^{\beta\hbar\hat{\nu}_k^\lambda}}{(e^{\beta\hbar\hat{\nu}_k^\lambda}-1)^2}\left[\frac{\omega_k^\lambda+\hat{\nu}_k^\lambda}{2\omega_k^\lambda}\right]^4[\Gamma_k^\lambda(\hat{\nu}_k^\lambda)]^{-1}\;, \quad (4.6)$$

$$(\eta_{ijlm}^\lambda)_2=\left[\frac{\beta\hbar^2}{V}\right]\sum_{k,k'}\omega_k^\lambda\omega_{k'}^\lambda\gamma_k^{ij\lambda}(\gamma_k^{lm\lambda}-\gamma^{lm\lambda})\frac{e^{\beta\hbar\hat{\nu}_k^\lambda}}{(e^{\beta\hbar\hat{\nu}_k^\lambda}-1)^2}\left[\frac{\omega_k^\lambda+\hat{\nu}_k^\lambda}{2\omega_k^\lambda}\right]^4[\Gamma_k'^\lambda(\hat{\nu}_k^\lambda)]^{-1}\;, \quad (4.7)$$

and

$$[\Gamma_k'^\lambda(\omega)]^{-1}=16\,|\,C(-k^\lambda,k'^\lambda)/\omega_k^\lambda\,|^2[\Gamma_k^\lambda(\omega)]^{-1}\;. \quad (4.8)$$

The lattice viscosity given by $(\eta_{ijlm}^\lambda)_1$ has a similar form to that given by Eq. (4.9) of I, which has also been discussed elsewhere.[5,12] Our result (4.6) is modified due to the effect of complete renormalization of phonon frequencies by defect and electric moment parameters besides the anharmonic parameters. The viscosity given by $(\eta_{ijlm}^\lambda)_2$ involves a parameter $C(-k^\lambda,k'^\lambda)$, which contributes only when $k\neq k'$ [cf. Eq. (2.6)]. Hence this contribution given by η_2^λ can be termed as the nondiagonal contribution. In the absence of isotopic impurities this nondiagonal contribution vanishes.

Let us now discuss the following cases:

(i) *Chemically pure crystal.* In the absence of isotopic impurities, the electric-field-dependent perturbed normal-mode frequency $\hat{\nu}_k^\lambda$ (which we now write as $\bar{\nu}_k^\lambda$) is given by

$$(\bar{\nu}_k^\lambda)^2=(\omega_k^\lambda)^2+4\omega_k^\lambda\beta^\lambda(k)\langle A_0^o A_0^o\rangle+4\omega_k^\lambda\sum_{k_1}\zeta^\lambda(k_1,k',-k)\langle A_0^o A_{k_1}^o\rangle+2\omega_k^\lambda\Delta_k^\lambda(\omega)$$
$$+2\omega_k^\lambda[\phi_k^\lambda+8g^2\beta^\lambda(k)-4gB^\lambda(k)]E^2\ . \tag{4.9}$$

Here $\zeta^\lambda(k_1,k',-k)$ is equal to $\gamma(k_1,k',-k)$ for $\lambda=a$, and $\mu(k_1,k',-k)$ for $\lambda=o$. The electric field dependence of the phonon width can be expressed as

$$\bar{\Gamma}_k^\lambda(\omega)=\Gamma_k^\lambda(\omega)+\psi_k^\lambda E^2\ , \tag{4.10}$$

where $\Gamma_k^\lambda(\omega)$ is the temperature-dependent anharmonic contribution and $\psi_k^\lambda E^2$ gives the electric-field-dependent contribution to the phonon widths, besides the field dependence of renormalized frequencies. For chemically pure ferroelectrics, the lattice viscosity contributed by a particular mode λ is given by the first term η_1^λ of Eq. (4.5). It can be seen using Eqs. (4.6)–(4.10) that this contribution to lattice viscosity increases with the applied electric field E because of the dominant effect of $\bar{\nu}_k^\lambda$ occurring in fourth power in the numerator of Eq. (4.6).

(ii) *Doped harmonic crystal.* Anharmonicity is often neglected as a good approximation at low temperatures. So with an isotopically disordered harmonic crystal, we find following expressions for the perturbed phonon frequency and the width of phonons,

$$(\hat{\nu}_k^\lambda)^2=(\omega_k^\lambda)^2+4\omega_k^\lambda D(-k^\lambda,k'^\lambda)+(4\omega_k^\lambda)^2C(-k^\lambda,k'^\lambda)+16\sum_{k_2}C(-k^\lambda,k_2^\lambda)D(-k^\lambda,k_2^\lambda)$$
$$+32\omega_k^\lambda\mathrm{Re}\sum_{k_1}\alpha(-k^\lambda,k_1^\lambda)\alpha^\dagger(k'^\lambda,k_1^\lambda)\omega_{k_1}^\lambda[\omega^2-(\hat{\omega}_{k_1}^\lambda)^2]^{-1} \tag{4.11}$$

and

$$\hat{\Gamma}_k(\omega)=8\pi\sum_{k_1}\alpha(-k^\lambda,k_1^\lambda)\alpha^\dagger(k'^\lambda,k_1^\lambda)(\omega_k^\lambda/\hat{\omega}_{k_1}^\lambda)[\delta(\omega-\hat{\omega}_{k_1}^\lambda)-\delta(\omega+\hat{\omega}_{k_1}^\lambda)]\ . \tag{4.12}$$

Analysis shows[13,14] that the relaxation rate $(\tau_k^\lambda)^{-1}$ $(=\Gamma_k^\lambda)$ given by Eq. (4.12) gives the usual Rayleigh scattering law $[(\omega_k^\lambda)^4$ dependence] when only the mass-change parameter $C(k_1,k_2)$ is retained, but the modification of force-constant changes through the parameter $D(k_1,k_2)$ gives the scattering rate proportional to $(\omega_k^\lambda)^2$ besides a frequency-independent term and would give rise to a non-Rayleigh scattering, which is also responsible,[13] for the experimental asymmetry in the peak of thermal conductivity curves. It can be shown[2] that for small values of $(M'-M)$ and $\Delta\phi_{\alpha\beta}$, the mass change and force-constant change make reinforcing or cancelling contributions to latttice viscosity $(\eta_{ijlm}^\lambda)_1$, through the term $\Gamma_k^\lambda(\omega)$, depending on whether they are of similar or opposite signs. Now at lower concentration of impurities one may neglect[13] the effect of force-constant changes and can consider the dominant mass change. Equation (4.12) is then simplified[14] as

$$\hat{\Gamma}_k^\lambda(\omega)=(\omega^4/12\pi NC^3)(M_0/\mu)^2(\omega_k^\lambda/\hat{\omega}_k^\lambda)f(1-f)\ , \tag{4.13}$$

C being the sound velocity, which shows that $\hat{\Gamma}_k^\lambda$ increases and hence the lattice viscosity $(\eta_{ijlm}^\lambda)_1$ decreases due to the scattering and phonons by defect atoms in the crystal. It is interesting to note that the effect of electric field (due to the deformation of electron shells) through the electric moment parameters cannot be revealed in the framework of harmonic theory, even if the defect parameters are accounted. For the electric field effects, anharmonic interactions are necessary.

(iii) *Doped anharmonic crystal in the absence of electric field.* In this case the perturbed normal-mode frequency and phonon width are given by

$$(\hat{\nu}_k^\lambda)^2 = (\omega_k^\lambda)^2 + W^\lambda(k,k') + (4/\omega_k^\lambda)\sum_{k_1} C(-k^\lambda,k_1^\lambda)W^\lambda(k,k_1)$$
$$+2\omega_k^\lambda \left[\Delta_k^\lambda(\omega) + \sum_{k_1}[4C(-k^\lambda,k_1^\lambda)/\omega_k^\lambda]\Delta_{k_1}^\lambda(\omega) \right.$$
$$\left. + 16\,\mathrm{Re}\sum_{k_1}\alpha(-k^\lambda,k_1^\lambda)\alpha^\dagger(k^\lambda,k_1^\lambda)\frac{\omega_{k_1}^\lambda}{\omega^2-(\omega_k^\lambda)^2} \right] \tag{4.14}$$

and

$$\hat{\Gamma}_k^\lambda(\omega) = \Gamma_k^\lambda(\omega) + \sum_{k_1}[4C(-k^\lambda,k_1^\lambda)/\omega_k^\lambda]\Gamma_{k_1}^\lambda(\omega)$$
$$+8\pi\sum_{k_1}\alpha(-k^\lambda,k_1^\lambda)\alpha^\dagger(k'^\lambda,k_1^\lambda)(\omega_k^\lambda/\hat{\omega}_{k_1}^\lambda)[\delta(\omega-\hat{\omega}_{k_1}^\lambda)-\delta(\omega+\hat{\omega}_{k_1}^\lambda)] \,. \tag{4.15}$$

In Eq. (4.15) the first term $\Gamma_k^\lambda(\omega)$ is the phonon width for a pure crystal arising due to anharmonic interactions only, the second term is the interaction term of anharmonicity with defect parameters, and the third term arises due to defect parameters alone which we have already discussed in (ii). It can be shown that at high temperature $\Gamma_k^\lambda(\omega) \sim (\omega_k^\lambda)^2 T + (\omega_k^\lambda)^2 T^2$, where $(\omega_k^\lambda)^2 T$ dependence is due to three-phonon scattering while $(\omega_k^\lambda)^2 T^2$ variation arises due to four-phonon interactions. The relaxation rate given by the second term in Eq. (4.12) varies as $\sim(\omega_k^\lambda)^4 T$. The lattice viscosity is the sum of both diagonal η_1^λ and nondiagonal η_2^λ terms in Eq. (4.5).

So far we have discussed the lattice viscosity for three different situations, but for doped displacive ferroelectrics placed in an external field, the lattice viscosity, in general, can be expressed as the sum of the two parts corresponding to the optical and acoustical contributions given by Eq. (4.1). Each of these contributions (η^a and η^o) can be further expressed as the sum of diagonal (η_1^λ) and nondiagonal (η_2^λ) contributions given by Eqs. (4.6) and (4.7), respectively. The nondiagonal contribution, however, vanishes in the absence of isotopic impurities and is approximately $|4C(-k^\lambda,k'^\lambda)/\omega_k^\lambda|^2$ times the diagonal contribution.

Now at a given temperature the electric field dependence of the phonon width can be expressed as $\hat{\Gamma}_k^\lambda(\omega) \sim K_1 + K_2 E^2$, where K_1 and K_2 are the field-independent coefficient in Eqs. (3.21) and (3.25) besides the field dependence of renormalized frequencies. Similarly, the variation of perturbed normal-mode frequency $\hat{\nu}_k^\lambda(\omega)$ with electric field can be expressed in the form $(\hat{\nu}_k^\lambda)^2(\omega) \simeq (\hat{\omega}_k^\lambda)^2(K_3 + K_4 E^2)$, where the field-independent coefficients K_3 and K_4 can be read from Eqs. (3.18), (3.20), (3.25), and (3.32). With these variations one finds the lattice viscosity η_1^λ as given by Eq. (4.6) increases with applied electric field, which may be compared with the increase in thermal conductivity of displacive ferroelectrics with electric field as observed elsewhere.[15,16]

V. DISCUSSION

In this paper we have obtained a general expression for the lattice viscosity of doped displacive ferroelectrics, placed in an external electric field, as a function of defect, anharmonic, and electric moment parameters in the paraelectric phase. The consideration of anharmonic terms gives the temperature dependence of lattice viscosity as $\alpha T + \beta T^2$ as discussed earlier.[7] The anomalous temperature dependence of lattice viscosity near the Curie temperature is due to the soft optical-mode frequency $\hat{\Omega}$ which tends to zero, making $\hat{N}_0$ anomalously large and hence the lattice viscosity (through the term $\hat{\nu}_k^\lambda$). The soft-mode frequency $\hat{\Omega}$ is responsible for most of the temperature-dependent properties of the displacive ferroelectrics. This frequency, which is imaginary in the harmonic approximation [cf. Eq. (3.16)], is stabilized in the paraelectric phase due to the anharmonic interactions, which in this way play an important role as does the stability of the system. In discussing the phonon viscous effects in doped ferroelectrics it is, therefore, necessary to retain the anharmonic term along with the defect parameters in the Hamiltonian. This leads us to a cross term [second term in Eq. (4.15)] of defect with anharmonic parameters in the phonon relaxation rate which varies as $\omega^4 T$. The consideration of mass change and force-constant change between impurity and host-lattice atoms leads to a Rayleigh (ω^4 scattering) and non-Rayleigh scattering behavior, respectively, in the expression for inverse relaxation time. This variation can be expressed as $\sim a\omega^4 + b\omega^2 + C$, which has been discussed in case (ii) above and is also represented by the last term in Eq. (4.15). The dependence of the scattering rate arising due to anharmonic interactions is of the form $\sim \omega^2 T + \omega^2 T^2$.

In order to consider the effect of electric field on the lattice viscosity, one has to consider the electric moment terms (due to the deformation of electron shells) along with the anharmonic and defect terms in the Hamiltonian. For a doped crystal this leads to a cross term of defect with anharmonic and electric field parameters in the expression for acoustical- and optical-phonon widths given by the second term on the right-hand side of expressions (3.21) and (3.26), respectively. It is seen that the lattice viscosity increases with the applied electric field. This effect is similar to the increase in lattice thermal conductivity of ferroelectric perovskites[15,16] with the applied electric field.

The expression (4.6) for lattice viscosity is similar in form to that for thermal conductivity,[16] particularly in the sense in which the inverse relaxation time (phonon width) occurring in both the expressions is concerned. One may even replace[5] the relaxation time occurring in the lattice-viscosity expression with the effective relaxation time found from lattice thermal conductivity experiments. Conversely, it should be remarked here that the interaction term of defect with anharmonic parameters (which varies as $\omega^4 T$) appearing in the relaxation rate for the lattice viscosity of doped ferroelectrics also appears[14] in the thermal conductivity expressions. This cross term is, in general, not obtained in thermal conductivity expressions because whenever isotopic impurities are accounted in the Hamiltonian, the anharmonicity is not considered.[13,17,18] With doped displacive ferroelectrics, we cannot ignore the anharmonicity which stabilizes[7] the system, and so the cross term appears. It is interesting to analyze the lattice thermal conductivity of displacive ferroelectrics employing a Callaway model with a relaxation time including the cross term ($\sim A\omega^4 T$). It is hoped that this term shall be responsible for a dip in the thermal conductivity of displacive ferroelectrics beyond the low-temperature maximum.[19] The sound attenuation constant[20] $\hat{a}(\omega)(=\Gamma_k^a(\omega)/C)$, where $\Gamma_k^a(\omega)$ is given by Eq. (3.21), can also be analyzed using our results.

[1]R. Bahadur and P. K. Sharma, Phys. Rev. B 12, 448 (1975).

[2]U. C. Naithani, R. P. Gairola, and B. S. Semwal, J. Phys. Soc. Jpn. 43, 204 (1977).

[3]B. D. Silverman, Phys. Rev. 125, 1921 (1962).

[4]B. D. Silverman and R. I. Joseph, Phys. Rev. 129, 2062 (1963).

[5]G. P. De Vault, Phys. Rev. 155, 875 (1967); 149, 624 (1966).

[6]J. A. McLennan, in *Advances in Chemical Physics,* edited by I. Prigogine (Interscience, New York, 1968), Vol. 5, pp. 261–318.

[7]V. K. Goyal and P. K. Sharma, Phys. Rev. B 23, 1252 (1981).

[8]B. S. Semwal and P. K. Sharma, Phys. Rev. B 7, 868 (1973).

[9]R. P. Gairola and B. S. Semwal, J. Phys. Soc. Jpn. 42, 975 (1977).

[10]S. Tani, Prog. Theor. Phys. 11, 190 (1954).

[11]R. P. Gairola and B. S. Semwal, J. Phys. Soc. Jpn. 42, 608 (1977).

[12]M. J. Rice, Proc. Phys. Soc. London 89, 373 (1966).

[13]P. K. Sharma and R. Bahadur, Phys. Rev. B 12, 1522 (1975).

[14]R. P. Gairola, Acta. Phys. Pol. 62, 59 (1982).

[15]E. F. Steigmeir, Phys. Rev. 168, 523 (1968).

[16]R. P. Gairola and B. S. Semwal, J. Phys. Soc. Jpn. 43, 954 (1977).

[17]A. A. Maradudin, J. Am. Chem. Soc. 86, 3405 (1964).

[18]B. S. Semwal and P. K. Sharma, J. Math. Phys. 15, 648 (1974).

[19]A. J. Sievers and R. O. Pohl, *Proceedings of the Conference on Thermal Conductivity* (U. S. Naval Radiological Laboratory, San Francisco, California, 1964).

[20]K. Tani and N. Tsuda, J. Phys. Soc. Jpn. 26, 113 (1969).