

Dynamical Electric Field Gradient in Face-Centered Cubic Single Crystal

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Abstract

Dynamical electric field gradients due to lattice vibration in face-centered cubic single crystals were calculated using the classical Born-von Kármán model of the thermal vibration of crystals. Numerical tables for several single crystals are shown for some typical directions of propagating wave and at a few temperature.

§1. Introduction

The static electric field gradient at a nucleus of lattice atom of perfect cubic single crystal is expected to be zero, because of the symmetry property of the extra-nuclear fields.

The propagating wave with a definite wave vector in a cubic crystal, however, can produce a electric field gradient at a nucleus of the lattice atom. This kind of propagating wave plays one of the fundamental roles in nuclear acoustic resonance phenomena¹⁻⁴), because it is based on the interaction between the oscillating electric field gradient and the nuclear electric quadrupole moment.

Furthermore, there were some speculative discussions⁵⁻⁶) on the interpretation of the result of angular correlation between the successive gamma-rays in ¹¹¹Cd which was embedded in cubic Ag single crystal. Especially, the discussion by Narumi and Matsuo⁵) stems from the estimation of the dynamical electric field gradient due to thermal vibration, although whether or not it would be possible for the interpretation of the experimental result by Zurich groupe⁶) is still open for demonstration. Considering these situations, it is work while to estimate the order of the dynamical electric field gradient in cubic crystal in classical limit, in connections with the perturbed angular correlation in single cubic crystal and acoustic resonance experiment.

§2. Formulation of the estimation of the dynamical electric field gradient in cubic crystal.

2.1 Vibration of cubic crystal

Here, we take Born-von Kármán theory⁷) to describe the motions of atoms in which each lattice point is occupied by an atom with a mass M and a charge Ze . The face-centered cubic crystal (fcc) is treated throughout this paper, although the extension to body centered cubic (bcc) crystal is quite easy.

Fig. 1 shows the 12 nearest neighbors (n, n) and 6 next nearest neighbors in fcc crystal around the origin. In the figure, symbol "a" denotes the lattice constant and the number at lattice point specify the individual lattice atom.

These lattice atoms oscillate according to the allowed mode of vibrations. The electric field gradient at 0th atom arises mainly from the relative displacements of outer 18 atoms. Using (u_n, v_n, w_n) for the cartesian components of the displacement of nth atom from its equilibrium position, α_1 for the force constant between 0th atom and (n, n) atom, and α_2 for that between 0th atom and next (n, n) atom, the

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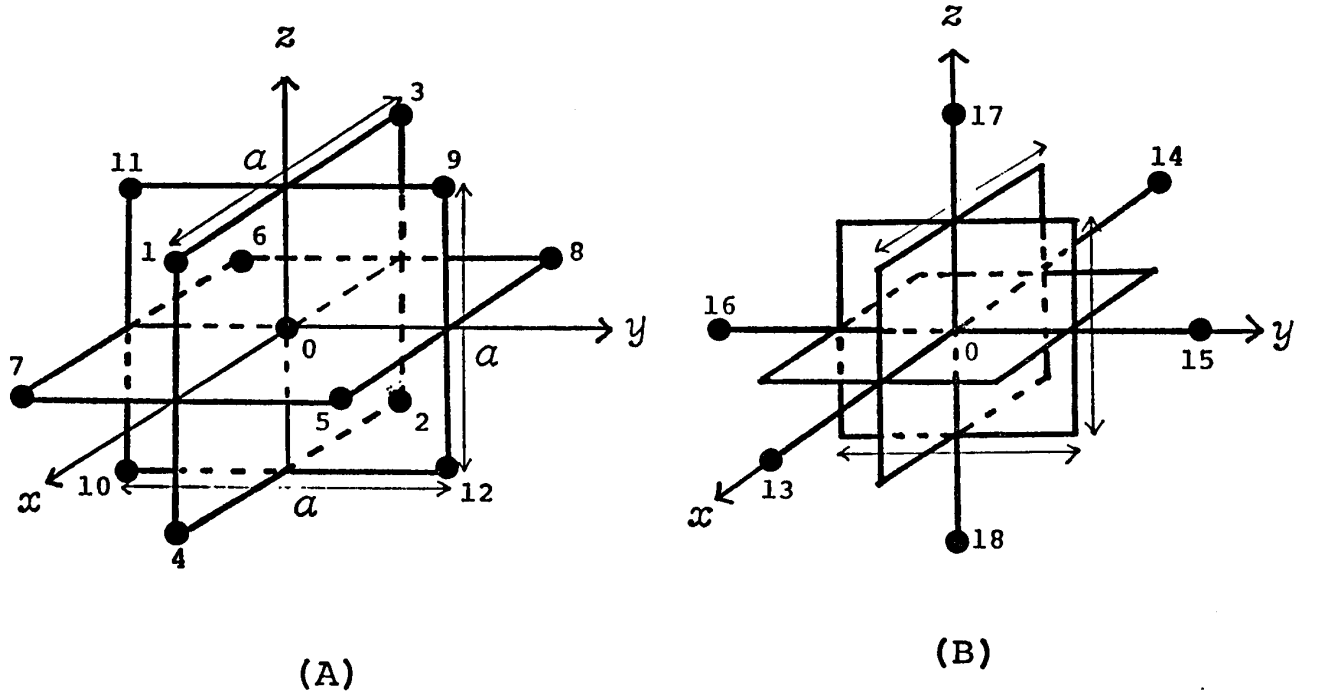


Fig. 1. 12 nearest neighbors (A) and 6 next nearest neighbors (B) in fcc crystal lattice. Symbol "a" denotes the lattice constant and the number at lattice point specify the individual lattice atom.

equations of the motion of 0th atom are described by equation (1)⁸⁾.

$$\begin{aligned}
 M \frac{\partial^2 u_0}{\partial t^2} &= -\frac{\alpha_1}{2} \left(8u_0 - \sum_{j=1}^8 u_j - \sum_{j=5}^6 v_j + \sum_{j=7}^8 v_j - \sum_{j=1}^2 w_j + \sum_{j=3}^4 w_j \right) - \alpha_2 \left(2u_0 - \sum_{j=13}^{14} u_j \right) \\
 M \frac{\partial^2 v_0}{\partial t^2} &= -\frac{\alpha_1}{2} \left(-\sum_{j=5}^6 u_j + \sum_{j=7}^8 u_j + 8v_0 - \sum_{j=5}^{12} v_j - \sum_{j=9}^{10} w_j + \sum_{j=11}^{12} w_j \right) - \alpha_2 \left(2v_0 - \sum_{j=15}^{16} v_j \right) \\
 M \frac{\partial^2 w_0}{\partial t^2} &= -\frac{\alpha_1}{2} \left(-\sum_{j=1}^2 u_j + \sum_{j=3}^4 u_j - \sum_{j=9}^{10} v_j + \sum_{j=11}^{12} v_j - 8w_0 - \sum_{j=1}^4 w_j - \sum_{j=9}^{12} w_j \right) - \alpha_2 \left(2w_0 - \sum_{j=17}^{18} w_j \right) \quad (1)
 \end{aligned}$$

Here, only the central forces between 0th atom and the outer 18 (n, n) atoms were assumed.

The solutions of equation (1) are assumed to be equation (2)

$$\begin{aligned}
 u_n &= A_x \exp 2\pi i (\nu t - \mathbf{k} \cdot \mathbf{r}_n) \\
 v_n &= A_y \exp 2\pi i (\nu t - \mathbf{k} \cdot \mathbf{r}_n) \\
 w_n &= A_z \exp 2\pi i (\nu t - \mathbf{k} \cdot \mathbf{r}_n) \quad (2)
 \end{aligned}$$

,where \mathbf{k} (k_1, k_2, k_3), \mathbf{r}_n and ν are wave vector of propagating wave with $|k|$ being the inverse of the wave length, the position vector of nth atom and the frequency of the oscillation motion. Inserting equation (2) into equation (1), equation (3) follows

$$\begin{aligned}
 [2 - C_1(C_2 + C_3) + 2\beta S_1^2 - \Omega^2] A_x + S_1 S_2 A_y + S_1 S_3 A_z &= 0 \\
 S_1 S_2 A_x + [2 - C_2(C_1 + C_3) + 2\beta S_2^2 - \Omega^2] A_y + S_2 S_3 A_z &= 0 \\
 S_1 S_3 A_x + S_2 S_3 A_y + [2 - C_3(C_1 + C_2) + 2\beta S_3^2 - \Omega^2] A_z &= 0 \quad (3)
 \end{aligned}$$

with

$$\begin{aligned}
 S_i &= \sin(\pi k_i a) \\
 C_i &= \cos(\pi k_i a) \\
 \beta &= \alpha_2 / \alpha_1 \\
 \Omega &= 2\pi \nu^2 M / \alpha_1 \quad (4)
 \end{aligned}$$

In order that the equation (3) is fulfilled for A_x, A_y, A_z except $A_x=A_y=A_z=0$, the value ν is restricted to obey the secular equation (5) for a given wave vector \mathbf{k} .

$$\begin{vmatrix} 2-C_1(C_2+C_3)+2\beta S_1^2-\Omega^2, & S_1S_2, & S_1S_3 \\ S_1S_2, & 2-C_2(C_1+C_3)+2\beta S_2^2-\Omega^2, & S_2S_3 \\ S_1S_3, & S_2S_3, & 2-C_3(C_1+C_2)+2\beta S_3^2-\Omega^2 \end{vmatrix} = 0 \quad (5)$$

The equation (5) is the equation of 3rd degree of ν^2 , so we have three values (ν_1, ν_2, ν_3) for a given wave vector \mathbf{k} . The relative amplitude $\rho_{xl}, \rho_{yl}, \rho_{zl}$ with $\rho_{xl}^2 + \rho_{yl}^2 + \rho_{zl}^2 = 1$ are obtained from the equation (3) in which the value ν is replaced by ν_l ($l=1, 2, 3$).

The displacement of n th atom for the allowed ν_l takes the following form for a given \mathbf{k} ,

$$\begin{aligned} u_n &= A_l \rho_{xl} \cos 2\pi(\nu_l t - \mathbf{k} \cdot \mathbf{r}_n) \\ v_n &= A_l \rho_{yl} \cos 2\pi(\nu_l t - \mathbf{k} \cdot \mathbf{r}_n) \\ w_n &= A_l \rho_{zl} \cos 2\pi(\nu_l t - \mathbf{k} \cdot \mathbf{r}_n) \end{aligned} \quad (6)$$

because u_n, v_n, w_n should be real.

Physically speaking, $A_l \rho_{xl}, A_l \rho_{yl}, A_l \rho_{zl}$ mean the x, y, z projection component of amplitude vector A_l with a specific direction.

The square of amplitude A_l for a given frequency ν_l and temperature T is estimated as follows. The average value of the amplitude of the allowed three dimensional oscillation is expressed as⁹⁾

$$\langle A^2 \rangle = (\hbar / 2M) \int_0^{\omega_D} g(\omega) (1/\omega) \coth(\hbar \omega / 2kT) d\omega \quad (7)$$

where ω, k, \hbar, T are angular frequency of oscillation, Boltzman constant, Plank's constant, absolute temperature of crystal and

$$\begin{aligned} g(\omega) &= (3/\omega_D^3) \omega^2 & \text{for } \omega \leq \omega_D \\ g(\omega) &= 0 & \text{for } \omega > \omega_D \end{aligned}$$

with Debye angular frequency ω_D .

Using Debye temperature T_D which is connected with ω_D by $\hbar \omega_D = kT_D$, and relative frequency $\nu^R = \omega/\omega_D = \nu/\nu_D$, the equation (7) transform to

$$\langle A^2 \rangle = (3h^2 / 8\pi^2 M k T_D) \int_0^1 \nu^R \coth(T_D \nu^R / 2T) d\nu^R \quad (8)$$

Hence, we can take

$$\langle A_l^2 \rangle = (3h^2 / 8\pi^2 M k T_D) \nu^R \coth(T_D \nu^R / 2T) \quad (9)$$

The temperature dependence of electric field gradient comes only from the temperature dependence of A_l shown in the equation (9).

2.2 Electric field gradient due to the displacement of the neighbor lattice atom.

The electric field gradient at 0th atom at rest due to the displacement of n th atom ($\Delta x_n, \Delta y_n, \Delta z_n$) from its equilibrium position (x_n, y_n, z_n) takes the following form,

$$\begin{aligned} V_{ZZ}(n) &= V''_0(n) + V''_{xx}(n) \Delta x_n + V''_{yy}(n) \Delta y_n + V''_{zz}(n) \Delta z_n \\ &+ V''_{xx}(n) (\Delta x_n)^2 + V''_{yy}(n) (\Delta y_n)^2 + V''_{zz}(n) (\Delta z_n)^2 \\ &+ V''_{xy}(n) (\Delta x_n) (\Delta y_n) + V''_{yz}(n) (\Delta y_n) (\Delta z_n) \\ &+ V''_{zx}(n) (\Delta z_n) (\Delta x_n) + \dots \end{aligned} \quad (10)$$

In order to apply this equation to the case of the thermal vibration of crystal, the displacements are to be replaced as follows:

$$\begin{aligned}
\Delta x_n &= u_n(t) - u_0(t) \\
&= A l \rho_x l [\cos 2\pi(\nu l t - \mathbf{k} \cdot \mathbf{r}_n) - \cos 2\pi\nu l t] \\
\Delta y_n &= v_n(t) - v_0(t) \\
&= A l \rho_y l [\cos 2\pi(\nu l t - \mathbf{k} \cdot \mathbf{r}_n) - \cos 2\pi\nu l t] \\
\Delta z_n &= w_n(t) - w_0(t) \\
&= A l \rho_z l [\cos 2\pi(\nu l t - \mathbf{k} \cdot \mathbf{r}_n) - \cos 2\pi\nu l t]
\end{aligned} \tag{11}$$

,using the equation (6).

The electric field gradient \bar{V}_{zz} (\mathbf{k} , l , T) at a given wave vector \mathbf{k} , a specified l value and a temperature T is obtained by the summing up over 18 (n , n) atoms and averaging over time. The 0th order term of the displacement in \bar{V}_{zz} disappear due to the symmetry property of the cubic crystal, summing up on n .

The odd order terms of the displacement in \bar{V}_{zz} is zero also, because the time average of the odd power of the equation (11) equal to zero.

The time average of $(\Delta x_n)^2$ etc. reduces to the following form.

$$\begin{aligned}
\overline{(\Delta x_n)^2} &= A l^2 \rho_x l^2 (1 - \cos 2\pi \mathbf{k} \cdot \mathbf{r}_n) \\
\overline{(\Delta y_n)^2} &= A l^2 \rho_y l^2 (1 - \cos 2\pi \mathbf{k} \cdot \mathbf{r}_n) \\
\overline{(\Delta z_n)^2} &= A l^2 \rho_z l^2 (1 - \cos 2\pi \mathbf{k} \cdot \mathbf{r}_n) \\
\overline{(\Delta x_n)(\Delta y_n)} &= A l^2 \rho_x l \rho_y l (1 - \cos 2\pi \mathbf{k} \cdot \mathbf{r}_n) \\
\overline{(\Delta y_n)(\Delta z_n)} &= A l^2 \rho_y l \rho_z l (1 - \cos 2\pi \mathbf{k} \cdot \mathbf{r}_n) \\
\overline{(\Delta z_n)(\Delta x_n)} &= A l^2 \rho_z l \rho_x l (1 - \cos 2\pi \mathbf{k} \cdot \mathbf{r}_n)
\end{aligned} \tag{12}$$

In the approximation of the neglecting of the 4th order terms of the displacement to the 2nd order term, \bar{V}_{zz} is expressed as

$$\begin{aligned}
\bar{V}_{zz}(\mathbf{k}, l, T) &= \sum_{n=1}^{18} V''_{xx}(n) \overline{(\Delta x_n)^2} + \sum_{n=1}^{18} V''_{yy}(n) \overline{(\Delta y_n)^2} + \sum_{n=1}^{18} V''_{zz}(n) \overline{(\Delta z_n)^2} \\
&\quad + \sum_{n=1}^{18} V''_{xy}(n) \overline{(\Delta x_n)(\Delta y_n)} + \sum_{n=1}^{18} V''_{yz}(n) \overline{(\Delta y_n)(\Delta z_n)} \\
&\quad + \sum_{n=1}^{18} V''_{zy}(n) \overline{(\Delta z_n)(\Delta x_n)}
\end{aligned} \tag{13}$$

,where

$$\begin{aligned}
V''_{xx}(n) &= (3Ze/2r_n^5) [1 - 5(z_n - z_0)^2/r_n^2 - 5(x_n - x_0)^2/r_n^2 + 35(x_n - x_0)^2(z_n - z_0)^2/r_n^4] \\
V''_{yy}(n) &= (3Ze/2r_n^5) [1 - 5(z_n - z_0)^2/r_n^2 - 5(y_n - y_0)^2/r_n^2 + 35(y_n - y_0)^2(z_n - z_0)^2/r_n^4] \\
V''_{zz}(n) &= (3Ze/2r_n^5) [3 - 30(z_n - z_0)^2/r_n^2 + 35(z_n - z_0)^4/r_n^4] \\
V''_{xy}(n) &= -(15Ze/r_n^7) (x_n - x_0) (y_n - y_0) [1 - 7(z_n - z_0)^2/r_n^2] \\
V''_{yz}(n) &= -(15Ze/r_n^7) (y_n - y_0) (z_n - z_0) [3 - 7(z_n - z_0)^2/r_n^2] \\
V''_{zx}(n) &= -(15Ze/r_n^7) (z_n - z_0) (x_n - x_0) [3 - 7(z_n - z_0)^2/r_n^2]
\end{aligned} \tag{14}$$

§ 3. Numerical calculation

3.1 Brillouin zone

In the case of the thermal vibration of fcc crystal, the allowed wave vectors are restricted by a Brillouin zone in reciprocal space (\mathbf{k} space)¹⁰⁾. Fig 2 shows the Brillouin zone (in (A)) for fcc crystal and the 1st octant (in (B)) ($k_1 > 0$, $k_2 > 0$, $k_3 > 0$) of it bounded by 7 sheets in which 3 sheets make 3 characteristic boundary values of k_1 , k_2 and k_3 on k_1 , k_2 and k_3 axis respectively. The point made by 3 planes in \mathbf{k} space is represented in $1/a$ unit.

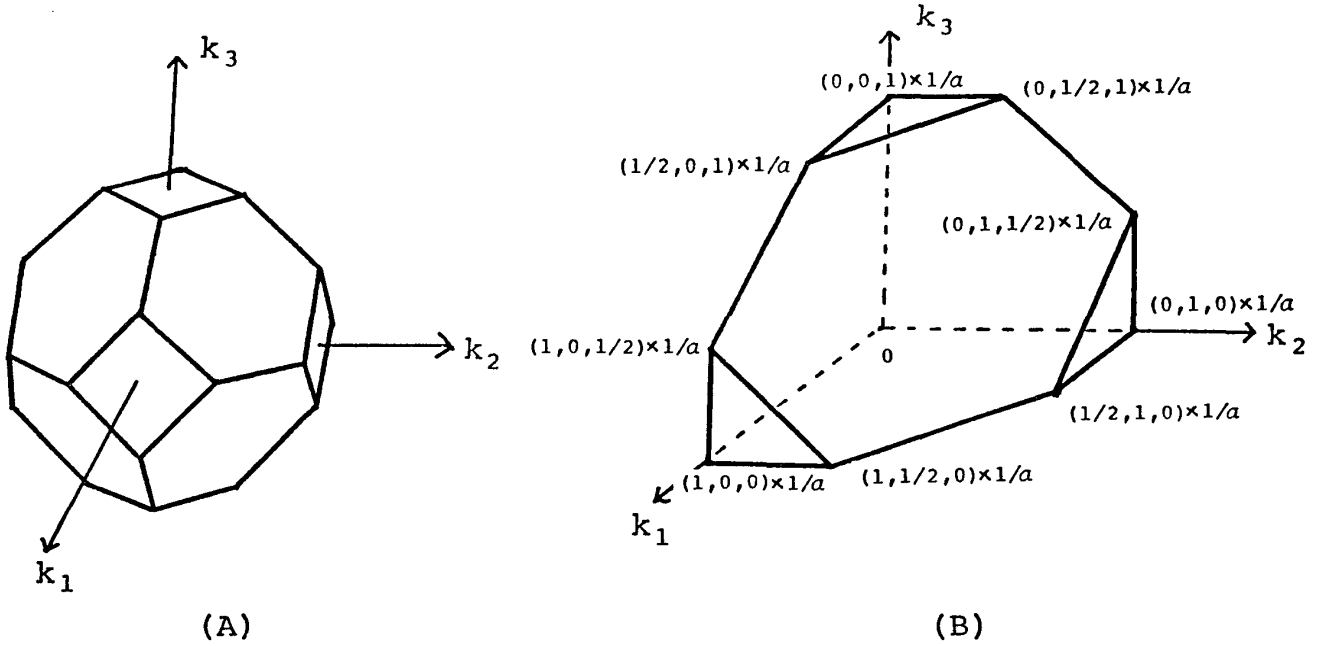


Fig. 2. Brillouin zone of fcc crystal lattice (A) and 1st octant of it (B). The coordinates of a point made by 3 characteristic planes in k space are expressed in $1/a$ unit.

3.2 Flow chart of our computer program

In numerical calculation of \bar{V}_{zz} , the relation between the force constants α_1 , α_2 and the stiffness constants c_{11} , c_{12} , c_{44} was taken into account.

$$\begin{aligned}\alpha_1 &= a \times c_{44} \\ \alpha_2 &= (a/4)(c_{11} - c_{12} - c_{44}) \\ \beta &= \alpha_2/\alpha_1 = (c_{11} - c_{12} - c_{44})/4c_{44}\end{aligned}\quad (15)$$

A computer program was built up following the flow-chart shown in Fig 3, in which input data was lattice constant (a), atomic weight of lattice atom (M), stiffness constants of crystal (c_{11} , c_{12} , c_{44}), assumed effective charge of lattice atom (Ze) and Debye temperature (T_D). The numerical values $\bar{V}_{zz}(\mathbf{k}, l, T)$ were calculated for many allowed values of \mathbf{k} in Brillouin zone and several values of temperatures.

§ 4. Result and Discussion

All kinds of fcc crystal constructed by a simple element were examined following the above-mentioned procedure. The lattice constant (a) was taken from ref.¹¹⁾, the atomic weight of lattice atom (M) from ref.¹²⁾, the stiffness constants of lattice (c_{11} , c_{12} , c_{44}) from ref.¹³⁾ and the Debye temperature (T_D) from ref.¹⁴⁾. For the effective charge of lattice atom (Ze), the valence number¹⁵⁾ adopted in a calculation of Fermi energy of referred crystal was tentatively assumed.

The values of $\bar{V}_{zz}(\mathbf{k}, l, T)$ on a crystal were calculated at 72 representative points in k space which were taken as $\mathbf{k} = (n_1/4, n_2/4, n_3/4) \times 1/a$ in 1st octant of Brillouin zone with integer n_1, n_2, n_3 and $0 \leq n_1, n_2, n_3 \leq 4$. The fcc-crystals examined by the procedure mentioned above were silver (Ag), aluminum (Al), gold (Au), copper (Cu), nickel (Ni), lead (Pb) and palladium (Pd).

The common features of the results of the calculations are as follows.

1. The value of \bar{V}_{zz} at a fixed (\mathbf{k}, l) combination slightly increases with a raise of the temperature.
2. The value of \bar{V}_{zz} at $(n_1=0, n_2=0, n_3=n \neq 0)$ and $l=2$ is always larger than that at $(n_1 \neq 0, n_2 \neq 0, n_3=n)$. Especially, the maximum value of \bar{V}_{zz} appears at $(n_1=0, n_2=0, n_3=4)$ and $l=2$, namely

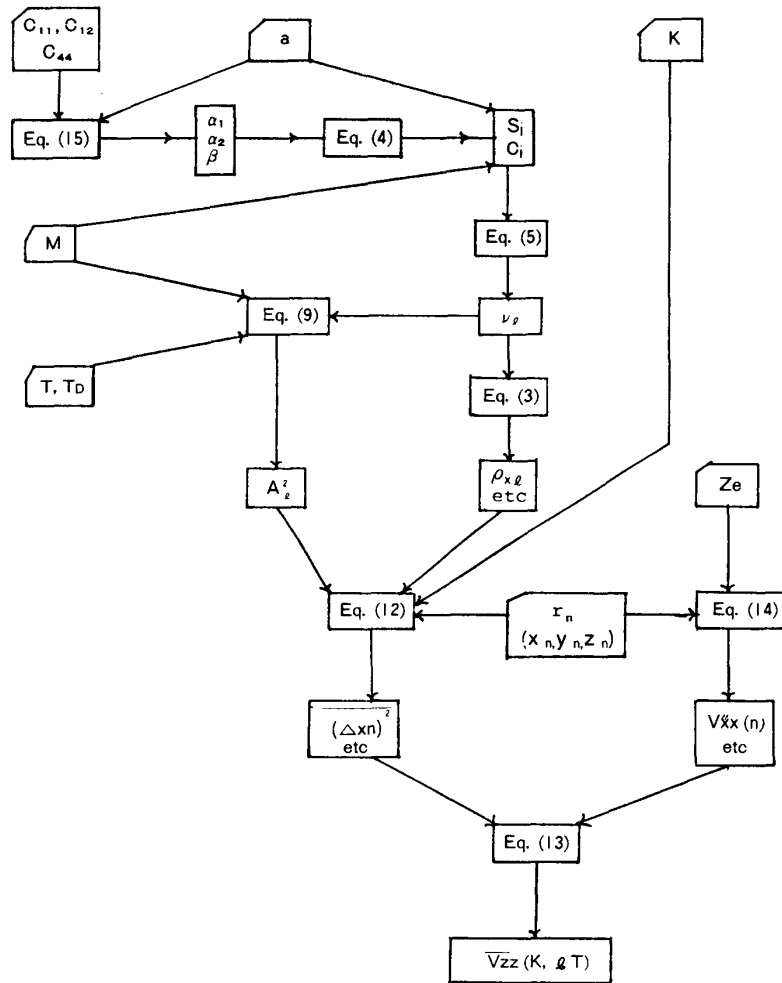


Fig. 3. Flow-chart of the computer program

$k=(0.0, 0.0, 1.0) \times 1/a$ and $l=2$.

3. The values of \bar{V}_{zz} at $(n_1=n, n_2=n, n_3=n)$ always vanish unconcerned with the temperature.

4. The value of \bar{V}_{zz} averaged over all allowed values of k in Brillouin zone and l values is practically zero.

Table 1-7 show the calculated values of \bar{V}_{zz} at $k=(0.0, 0.0, 1.0) \times 1/a$ and $k=(1.0, 0.0, 0.0) \times 1/a$ and at 2 temperatures, namely 300K (room temperature) and 700K, except the case of Pb in which the temperature 500K is substituted for 700K because of the extremely low melting temperature (600K) of Pb. In tables, the number with parentheses p (q) means $p \times 10^q$ and the upper numbers in the row of A_l and \bar{V}_{zz} are for the temperature 300K and the lower ones for 700K with the exception of 500K for Pb. The values at $k=(0.0, 1.0, 0.0) \times 1/a$ are easily obtained by the exchange of the number 1 and 3 in row of and the exchange of the character ρ_{xl} and ρ_{yl} in tables of $k=(1.0, 0.0, 0.0) \times 1/a$. In spite of the simple demonstration of the dependence of \bar{V}_{zz} on k, l and T and the order of the magnitude of \bar{V}_{zz} , these \bar{V}_{zz} values are useful for the estimation of the order of the dynamical electric field gradient experienced for the acoustic resonance experiment and the interpretation of the result of the perturbed angular correlation experiment using crystal in a real state. It is well known that the electric field

Table 1 Ag $a=4.078\text{\AA}$ $M=107.88$ $Ze=1$ $T_D=229\text{K}$
 $c_{11}=1.240 \times 10^{12}$ dyne/cm²
 $c_{12}=0.937 \times 10^{12}$ dyne/cm²
 $c_{44}=0.461 \times 10^{12}$ dyne/cm²

$\mathbf{k}=(0.00, 0.00, 1.00) \times 1/a$			
l	1	2	3
$\nu_l(\text{s}^{-1})$	0.326(13)	0.461(13)	0.326(13)
ρ_{xl}	0.000	0.000	1.000
ρ_{yl}	1.000	0.000	0.000
ρ_{zl}	0.000	1.000	0.000
$A_l(\text{cm})$ 300K	0.888(-9)	0.898(-9)	0.888(-9)
700K	0.135(-8)	0.135(-8)	0.135(-8)
$\bar{V}_{zz}(\text{V}/\text{cm}^2)$ 300K	0.222(15)	-0.455(15)	0.222(15)
700K	0.510(15)	-0.102(16)	0.510(15)
$\mathbf{k}=(1.00, 0.00, 0.00) \times 1/a$			
l	1	2	3
$\nu_l(\text{s}^{-1})$	0.326(13)	0.461(13)	0.326(13)
ρ_{xl}	0.000	1.000	0.000
ρ_{yl}	0.000	0.000	1.000
ρ_{zl}	1.000	0.000	0.000
$A_l(\text{cm})$ 300K	0.888(-9)	0.898(-9)	0.888(-9)
700K	0.135(-8)	0.135(-8)	0.135(-8)
$\bar{V}_{zz}(\text{V}/\text{cm}^2)$ 300K	-0.171(14)	0.227(15)	-0.205(15)
700K	-0.392(14)	0.512(15)	-0.471(15)

Table 2 Al $a=4.0415\text{\AA}$ $M=26.97$ $Ze=3$ $T_D=375\text{K}$
 $c_{11}=1.068 \times 10^{12}$ dyne/cm²
 $c_{12}=0.607 \times 10^{12}$ dyne/cm²
 $c_{44}=0.282 \times 10^{12}$ dyne/cm²

$\mathbf{k}=(0.00, 0.00, 1.00) \times 1/a$			
l	1	2	3
$\nu_l(\text{s}^{-1})$	0.508(13)	0.718(13)	0.508(13)
ρ_{xl}	0.000	0.000	1.000
ρ_{yl}	1.000	0.000	0.000
ρ_{zl}	0.000	1.000	0.000
$A_l(\text{cm})$ 300K	0.110(-8)	0.113(-8)	0.110(-8)
700K	0.165(-8)	0.166(-8)	0.165(-8)
$\bar{V}_{zz}(\text{V}/\text{cm}^2)$ 300K	0.107(16)	-0.226(16)	0.107(16)
700K	0.240(16)	-0.485(16)	0.240(16)
$\mathbf{k}=(1.00, 0.00, 0.00) \times 1/a$			
l	1	2	3
$\nu_l(\text{s}^{-1})$	0.508(13)	0.718(13)	0.508(13)
ρ_{xl}	0.000	1.000	0.000
ρ_{yl}	0.000	0.000	1.000
ρ_{zl}	1.000	0.000	0.000
$A_l(\text{cm})$ 300K	0.110(-8)	0.113(-8)	0.110(-8)
700K	0.165(-8)	0.166(-8)	0.165(-8)
$\bar{V}_{zz}(\text{V}/\text{cm}^2)$ 300K	-0.826(14)	0.113(16)	-0.991(15)
700K	-0.185(15)	0.242(16)	-0.222(16)

Table 3 Au $a=4.0705\text{\AA}$ $M=197.2$ $Z_e=1$ $T_D=164\text{K}$

$c_{11}=1.923 \times 10^{12}$ dyne/cm²

$c_{12}=1.631 \times 10^{12}$ dyne/cm²

$c_{44}=0.420 \times 10^{12}$ dyne/cm²

$\mathbf{k}=(0.00, 0.00, 1.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.230(13)	0.325(13)	0.230(13)
ρ_{xl}	0.000	0.000	1.000
ρ_{yl}	1.000	0.000	0.000
ρ_{zl}	0.000	1.000	0.000
$A_l(\text{cm})$ 300K	0.912(-9)	0.917(-9)	0.912(-9)
700K	0.139(-8)	0.139(-8)	0.139(-8)
$\bar{V}_{zz}(\text{V/cm}^2)$ 300K	0.237(15)	-0.479(15)	0.237(15)
700K	0.548(15)	-0.110(16)	0.548(15)

$\mathbf{k}=(1.00, 0.00, 0.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.230(13)	0.325(13)	0.230(13)
ρ_{xl}	0.000	1.000	0.000
ρ_{yl}	0.000	0.000	1.000
ρ_{zl}	1.000	0.000	0.000
$A_l(\text{cm})$ 300K	0.912(-9)	0.917(-9)	0.912(-9)
700K	0.139(-8)	0.139(-8)	0.139(-8)
$\bar{V}_{zz}(\text{V/cm}^2)$ 300K	-0.182(14)	0.239(15)	-0.219(15)
700K	-0.421(14)	0.549(15)	-0.505(15)

Table 4 Cu $a=3.60775\text{\AA}$ $M=63.54$ $Z_e=1$ $T_D=343\text{K}$

$c_{11}=1.684 \times 10^{12}$ dyne/cm²

$c_{12}=1.214 \times 10^{12}$ dyne/cm²

$c_{44}=0.754 \times 10^{12}$ dyne/cm²

$\mathbf{k}=(0.00, 0.00, 1.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.511(13)	0.723(13)	0.511(13)
ρ_{xl}	0.000	0.000	1.000
ρ_{yl}	1.000	0.000	0.000
ρ_{zl}	0.000	1.000	0.000
$A_l(\text{cm})$ 300K	0.785(-9)	0.805(-9)	0.785(-9)
700K	0.117(-8)	0.118(-8)	0.117(-8)
$\bar{V}_{zz}(\text{V/cm}^2)$ 300K	0.321(15)	-0.674(15)	0.321(15)
700K	0.716(15)	-0.145(16)	0.716(15)

$\mathbf{k}=(1.00, 0.00, 0.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.511(13)	0.723(13)	0.511(13)
ρ_{xl}	0.000	1.000	0.000
ρ_{yl}	0.000	0.000	1.000
ρ_{zl}	1.000	0.000	0.000
$A_l(\text{cm})$ 300K	0.785(-9)	0.805(-9)	0.785(-9)
700K	0.117(-8)	0.118(-8)	0.117(-8)
$\bar{V}_{zz}(\text{V/cm}^2)$ 300K	-0.247(14)	0.337(15)	-0.296(15)
700K	-0.551(14)	0.723(15)	-0.661(15)

Table 5 Ni $a=3.52\text{\AA}$ $M=58.71$ $Ze=2$ $T_D=413\text{k}$
 $c_{11}=2.508 \times 10^{12}$ dyne/cm²
 $c_{12}=1.500 \times 10^{12}$ dyne/cm²
 $c_{44}=1.235 \times 10^{12}$ dyne/cm²

$\mathbf{k}=(0.00, 0.00, 1.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.672(13)	0.951(13)	0.672(13)
ρ_{xl}	0.000	0.000	1.000
ρ_{yl}	1.000	0.000	0.000
ρ_{zl}	0.000	1.000	0.000
$A_l(\text{cm})$ 300K	0.691(-9)	0.719(-9)	0.691(-9)
700K	0.102(-8)	0.103(-8)	0.102(-8)
$\bar{V}_{zz}(\text{V}/\text{cm}^2)$ 300K	0.562(15)	-0.122(16)	0.562(15)
700K	0.122(16)	-0.248(16)	0.122(16)

$\mathbf{k}=(1.00, 0.00, 0.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.672(13)	0.951(13)	0.672(13)
ρ_{xl}	0.000	1.000	0.000
ρ_{yl}	0.000	0.000	1.000
ρ_{zl}	1.000	0.000	0.000
$A_l(\text{cm})$ 300K	0.691(-9)	0.719(-9)	0.691(-9)
700K	0.102(-8)	0.103(-8)	0.102(-8)
$\bar{V}_{zz}(\text{V}/\text{cm}^2)$ 300K	-0.432(14)	0.608(15)	-0.518(15)
700K	-0.937(14)	0.124(16)	-0.112(16)

Table 6 Pb $a=4.9396\text{\AA}$ $M=207.21$ $Ze=4$ $T_D=96.3\text{K}$
 $c_{11}=0.495 \times 10^{12}$ dyne/cm²
 $c_{12}=0.423 \times 10^{12}$ dyne/cm²
 $c_{44}=0.149 \times 10^{12}$ dyne/cm²

$\mathbf{k}=(0.00, 0.00, 1.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.147(13)	0.208(13)	0.147(13)
ρ_{xl}	0.000	0.000	1.000
ρ_{yl}	1.000	0.000	0.000
ρ_{zl}	0.000	1.000	0.000
$A_l(\text{cm})$ 300K	0.151(-8)	0.151(-8)	0.151(-8)
500K	0.195(-8)	0.195(-8)	0.195(-8)
$\bar{V}_{zz}(\text{V}/\text{cm}^2)$ 300K	0.987(15)	-0.198(16)	0.987(15)
500K	0.164(16)	-0.329(16)	0.164(16)

$\mathbf{k}=(1.00, 0.00, 0.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.147(13)	0.208(13)	0.147(13)
ρ_{xl}	0.000	1.000	0.000
ρ_{yl}	0.000	0.000	1.000
ρ_{zl}	1.000	0.000	0.000
$A_l(\text{cm})$ 300K	0.151(-8)	0.151(-8)	0.151(-8)
500K	0.195(-8)	0.195(-8)	0.195(-8)
$\bar{V}_{zz}(\text{V}/\text{cm}^2)$ 300K	-0.759(14)	0.992(15)	-0.911(15)
500K	-0.126(15)	0.164(16)	-0.151(16)

Table 7 Pd

$a=3.88\text{\AA}$ $M=106.4$ $Z_e=2$ $T_D=275\text{K}$
 $c_{11}=2.271 \times 10^{12}$ dyne/cm²
 $c_{12}=1.761 \times 10^{12}$ dyne/cm²
 $c_{44}=0.717 \times 10^{12}$ dyne/cm²

 $\mathbf{k}=(0.00, 0.00, 1.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.399(13)	0.565(13)	0.399(13)
ρ_{xl}	0.000	0.000	1.000
ρ_{yl}	1.000	0.000	0.000
ρ_{zl}	0.000	1.000	0.000
$A_l(\text{cm})$ 300K	0.749(-9)	0.761(-9)	0.749(-9)
700K	0.113(-8)	0.113(-8)	0.113(-8)
$\bar{V}_{zz}(\text{V/cm}^2)$ 300K	0.406(15)	-0.837(15)	0.406(15)
700K	0.921(15)	-0.185(16)	0.921(15)

 $\mathbf{k}=(1.00, 0.00, 0.00) \times 1/a$

l	1	2	3
$\nu_l(\text{s}^{-1})$	0.399(13)	0.565(13)	0.399(13)
ρ_{xl}	0.000	1.000	0.000
ρ_{yl}	0.000	0.000	1.000
ρ_{zl}	1.000	0.000	0.000
$A_l(\text{cm})$ 300K	0.749(-9)	0.761(-9)	0.749(-9)
700K	0.113(-8)	0.113(-8)	0.113(-8)
$\bar{V}_{zz}(\text{V/cm}^2)$ 300K	-0.312(14)	0.419(15)	-0.374(15)
700K	-0.709(14)	0.927(15)	-0.850(15)

gradient at a probe nucleus in non-cubic crystal is enhanced by Sternheimer's antishielding enhancement effect¹⁶⁾. If we can expect some amount of the enhancement of the dynamical electric field gradient by the antishielding effect even in a cubic crystal, the \bar{V}_{zz} value become a detectable order of magnitude for a probe nucleus having the typical value of the nuclear electric quadrupole moment¹⁷⁾.

This work was performed, using the computer system of Data Processing Center of Kyoto University.

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