The generalized susceptibility of dislocation segment in nondissipative crystal

I L Bataronov and V V Dezhin
Voronezh State Technical University, Moskovsky prospect 14, Voronezh 394026, Russian Federation
E-mail: viktor.dezhin@mail.ru

Abstract. Oscillations of a dislocation segment dependence on the external forces are considered. Expressions are obtained for matrix elements which are expressed by means of the generalized susceptibilities matrix of dislocation oscillators. Elimination of non-physical features in the range of large wave numbers was made within the Peierls dislocation model. An expression was obtained describing the low-frequency asymptotic behavior of the diagonal and non-diagonal elements of the generalized susceptibilities matrix of dislocation oscillators.

1. Introduction
The important role of dislocations in the formation of mechanical, thermodynamic, electrical and other properties of crystals is a well known fact nowadays. Therefore, the vibrations of a crystal having dislocations are of considerable practical interest. For a crystals with a simple lattice the problem of vibrations of crystal dislocation and the phonon scattering by dislocations was solved in [1-3] using self-consistent dynamic theory of dislocations. In [4-7] generalized susceptibility endless dislocation for different types of crystals was found, which determines the response of dislocations to an external force. In this paper we describe the obtained the generalized susceptibility inverse matrix and its analysis.

2. Calculation of the generalized susceptibility dislocation oscillators
Neglecting the elastic fields of defects that perpetuate this dislocation, the equation of dislocation motion can be obtained by putting the respective boundary conditions on the displacement of the points in the dislocation line \( \xi(l,t) \) in the pinning points, where \( l \) is the coordinate along the dislocation line, \( t \) is time. In the case of a dislocation pinning under consideration we require that \( \xi(l,t) = 0 \) for \( l \in (-\infty, -L/2] \cup [L/2, \infty) \), where \( L \) is the length of a dislocation segment. Under these conditions, the equation oscillations dislocation [5] after the conversion which eliminates the divergence, will take the form

\[
\int_{-L/2}^{L/2} dz' G_0(z-z', \omega) \xi(z', \omega) = f(z, \omega).
\]  

(1)

Here \( z \) is axis extending along of the dislocation line, \( \omega \) is frequency. Function \( \xi(z, \omega) \) and external disturbance \( f(z, \omega) \) will be sought in the form of trigonometric series satisfying the boundary conditions at the points of attachment \( z = \pm L/2 \):
\[ \xi(z, \omega) = \sum_{n=1}^{\infty} Q_n(\omega) \varphi_n(z), \quad f(z, \omega) = \sum_{n=1}^{\infty} F_n(\omega) \varphi_n(z), \] (2)

where is indicated \( \varphi_n(z) = \begin{cases} \cos(mz/L), & n = 1, 3, 5, \ldots \\ \sin(mz/L), & n = 2, 4, 6, \ldots \end{cases} \). Substituting expressions (2) to the equation (1), we obtain, after some transformations, the matrix equation

\[ \sum_n B_{mn}(\omega) Q_n(\omega) = F_m(\omega), \] (3)

where the matrix elements \( B_{mn} \) are defined as:

\[ B_{mn}(\omega) = \frac{2}{L} \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} dz' G_0(z - z', \omega) \varphi_n(z') \varphi_m(z). \] (4)

According to the linear response theory, we write down

\[ Q_n(\omega) = \sum_m \alpha_{mn}(\omega) F_m(\omega), \] (5)

where \( \hat{\alpha} \) is the generalized susceptibilities matrix of dislocation oscillators. Comparing equations (3) and (5), we obtain \( \hat{\alpha}(\omega) = \hat{B}^{-1}(\omega) \).

Integral (4) calculation result in

\[ B_{mn} = (-1)^{[m/2]+[n/2]} \frac{\pi m n}{2 L^2} \int_{0}^{L} \left\{ 3 b_s^2 L_{mn}^{11} + 2 \gamma (b_e^2 - b_s^2) L_{mn}^{10} - b^2 q_i^2 L_{mn}^{10} - \gamma \xi^2 q_i^2 L_{mn}^{10} - \frac{4 b_s^2 - b_e^2}{q_i^2} L_{mn}^{2(2)} \right\}. \] (6)

Here \( \mu \) is the shear modulus of the crystal, \( b \) is Burgers vector of the dislocation, \( b_e \) and \( b_s \) are edge and screw components of the Burgers vector, \( q_i = \omega L / c_i \), \( q_i = \omega L / c_l \), \( c_l \) and \( c_i \) are the transverse and longitudinal sound velocities, \( \gamma = c_l^2 / c_i^2 \). For \( m \neq n \) case we have

\[ L_{mn}^{(1)} = \frac{1}{2} q_n^2 \left\{ \frac{1}{q_m^2} \left[ \mathrm{Ein}(-i(q_a - q_n)) - \mathrm{Ein}(-i(q_a + q_n)) \right] - q_m^{2k-1} \left[ \mathrm{Ein}(-i(q_a - q_m)) - \mathrm{Ein}(-i(q_a + q_m)) \right] - (-1)^m \exp(iq_a) \delta_{k,2} \right\}, \]

\[ L_{mn}^{(2)} = t_{mn}^{12} - t_{mn}^{11} + i(q_i - q_l), \]

where \( q_m = m L, \quad q_n = n L, \quad \mathrm{Ein}(z) = \int_{0}^{1 - \exp(-t)/t} dt \) is the integer part of the integral exponential function [8], \( \delta_{k,2} \) is Kronecker’s symbol. For \( m = n \) case we have

\[ L_{mn}^{(1)} = \frac{q_n^{2k-2}}{4} \left\{ 2C + 2 \ln(k_D L) + 2iq_a \frac{1 - (-1)^n \exp(iq_a)}{q_n^2 - q_a^2} - \left[ \mathrm{Ein}(-i(q_a + q_n)) + \mathrm{Ein}(-i(q_a - q_n)) \right] \right\} \]

\[ + \frac{1}{4} t_{mn}^{12} \left[ \mathrm{Ein}(-i(q_a + q_n)) - \mathrm{Ein}(-i(q_a - q_n)) \right], \]

where \( k_D \) is the Debye wave number, \( C \approx 0.577 \) is Euler's constant,

\[ L_{mn}^{(2)} = t_{mn}^{12} - t_{mn}^{11} + i(q_i - q_l) - (-1)^n \left[ \exp(iq_i) - \exp(iq_l) \right]. \]

3. Matrix elements in the Peierls model

Expressions (6) obtained in section 2 are characterized by the fact that they lead to nonphysical features in the linear dislocation model in the range of wave numbers in approximation to \( k_D \). These features can be eliminated by means of calculations within the frame of Peierls dislocation model which can taken into account with the respective analytic continuation of generalized susceptibility expressions of the infinite dislocation beyond \( k_D \). In the process of calculation of the matrix elements
for dislocation oscillators it leads to the necessity to single out and specify the $\Delta$ amendments. For non-diagonal elements ($m \neq n$) we have

\[
\Delta_{mn} = i \int_{k_{iL}}^{\infty} d(q_{i} + i\varepsilon)[1 - (-1)^m \exp(i(q_{i} + i\varepsilon))] \frac{\gamma}{(q_{i} + i\varepsilon - q_{m}^{n})^2 - q_{m}^{n^2}} \frac{[(q_{i} + i\varepsilon)^2 - q_{m}^{n^2}][(q_{i} + i\varepsilon)^2 - q_{n}^{n^2}]}{[\gamma - (q_{i} + i\varepsilon)^2 - q_{m}^{n^2}][(q_{i} + i\varepsilon)^2 - q_{n}^{n^2}]}.
\]

Integrating (7) and taking into account the main summands, we obtain

\[
\Delta_{mn} \approx \frac{1}{2} \sqrt{\frac{2\gamma}{q_{m}^{n^2} - q_{n}^{n^2}}} \left[ -(3 - 4\gamma)b_{e}^{n} + 2\gamma b_{e}^{n} \right] \left( q_{m} \arctg \frac{2g_{n}}{k_{D}L} - q_{m} \arctg \frac{2g_{m}}{k_{D}L} \right)
\]

\[+ (b^{2} + \gamma^{2} b_{e}^{n}) q_{m}^{n^2} \left( \frac{1}{q_{n}} \arctg \frac{2g_{n}}{k_{D}L} - \frac{1}{q_{m}} \arctg \frac{2g_{m}}{k_{D}L} \right) \].

Thus, the expression for the elements of inverse matrix generalized susceptibility in case of $m \neq n$ will be shown here:

\[
(\alpha^{-1})_{mn} = -(1)^{m/2} \approx \frac{\pi \mu \gamma}{4L} \left[ 3b_{e}^{n} L_{mn}^{11} + 2\gamma (b_{e}^{n} - 2b_{e}^{n^2}) L_{mn}^{11} - b_{e}^{n} q_{m}^{n^2} L_{mn}^{10} - \gamma b_{e}^{n^2} q_{m}^{n^2} L_{mn}^{10} \right]
\]

\[- (4b_{e}^{n} - b_{e}^{n^2}) L_{mn}^{(2)} - q_{m}^{n^2} - \Delta_{mn} \].

(8)

Let us now consider the diagonal elements of the generalized susceptibility inverse matrix ($m = n$). In this case, the integrals should be calculated:

\[
\Delta_{nn} = i \int_{k_{iL}}^{\infty} d(q_{i} + i\varepsilon)[1 - (-1)^m \exp(i(q_{i} + i\varepsilon))] \frac{\gamma}{(q_{i} + i\varepsilon - q_{m}^{n})^2 - q_{m}^{n^2}} \frac{[(q_{i} + i\varepsilon)^2 - q_{m}^{n^2}][(q_{i} + i\varepsilon)^2 - q_{n}^{n^2}]}{[\gamma - (q_{i} + i\varepsilon)^2 - q_{m}^{n^2}][(q_{i} + i\varepsilon)^2 - q_{n}^{n^2}]}.
\]

Integrating (9) and taking into account the main components, we obtain

\[
\Delta_{nn} \approx - \frac{1}{2} \sqrt{\frac{2\gamma}{q_{m}^{n^2} - q_{n}^{n^2}}} \left[ -(3 - 4\gamma)b_{e}^{n} + 2\gamma b_{e}^{n} \right] \left( \frac{1}{2q_{n}} \arctg \frac{2g_{n}}{k_{D}L} + \frac{k_{D}L}{(k_{D}L)^2 + q_{n}^{n^2}} \right)
\]

\[+ (b^{2} + \gamma^{2} b_{e}^{n}) q_{n}^{n^2} \left( \frac{1}{2q_{n}} \arctg \frac{2g_{n}}{k_{D}L} - \frac{k_{D}L}{(k_{D}L)^2 + q_{n}^{n^2}} \right) \].

Thus, the expression for the elements of the generalized susceptibility inverse matrix in case of $m = n$ takes the form shown here:

\[
(\alpha^{-1})_{nn} = \frac{\pi \mu \gamma}{4L} \left[ 3b_{e}^{n} L_{nn}^{11} + 2\gamma (b_{e}^{n} - 2b_{e}^{n^2}) L_{nn}^{11} - b_{e}^{n} q_{m}^{n^2} L_{nn}^{10} - \gamma b_{e}^{n^2} q_{m}^{n^2} L_{nn}^{10} \right]
\]

\[- \frac{4b_{e}^{n} - b_{e}^{n^2}}{q_{n}^{n^2}} L_{nn}^{(2)} - \Delta_{nn} \].

(10)

The requirement to use the second summand in (10) was established in [9].

4. Matrix elements in the low-frequency limit

Is of practical interest to consider the low-frequency asymptotic formulas (8) and (10). For this purpose, we transform the expressions $L_{mn}^{(2)}$ and expand them to powers of $q_{m}$. Then, for the non-diagonal elements ($m \neq n$) we have:
Here in the real parts, summands \( \sim q_\alpha^3 \) can be neglected, and all imaginary parts have the same order of \( \sim q_\alpha^3 \). Therefore we may write down the expression (8) explicitly in the low-frequency limit:

\[
B_{mn} = (\alpha^{-1})_{mn} = (-1)^{\lfloor m/2 \rfloor + \lfloor n/2 \rfloor} \frac{\mu}{4\pi L} \left( C_{mn} - M_{mn} q_\alpha^2 + i \Gamma_{mn} q_\alpha^3 \right),
\]

(11)

where we have introduced the reciprocal rigidity matrix \( C_{mn} \), mass coefficient \( M_{mn} \) and damping coefficients \( \Gamma_{mn} \) of the dislocation oscillators, respectively:

\[
C_{mn} = \left[ (3 - 4\gamma)b_c^2 + 2\gamma b_c^2 \right] q_m q_n \left[ q_m \frac{\text{Si}(q_m) - q_n \text{Si}(q_n)}{q_m} + \frac{1}{2} \left( q_m \arctg \frac{2q_m}{k_D L} - q_n \arctg \frac{2q_n}{k_D L} \right) \right],
\]

\[
M_{mn} = (b^2 + \gamma^2 b_c^2) q_m q_n \left[ \frac{\text{Si}(q_m) - \text{Si}(q_n)}{q_m} + \frac{1}{2} \left( \frac{1}{q_n} \arctg \frac{2q_n}{k_D L} - \frac{1}{q_m} \arctg \frac{2q_m}{k_D L} \right) \right],
\]

\[
\Gamma_{mn} = -\frac{4}{5} \frac{1 - (-1)^n}{q_m q_n} b_c^2 \left( 1 + \frac{2}{3} \gamma^{5/2} \right).
\]

Now we shall define the low-frequency asymptotic behavior of diagonal elements \((m = n)\). To do this, we use the expansions of functions with \( q_\alpha \) powers. With these expansions we obtain:

\[
q_\alpha^2 L_{\alpha mn} = \frac{1}{4} \left[ 2 \ln(k_D L e^C) - 2 \text{Ci}(q_n) - 2 \frac{\text{Si}(q_n)}{q_n} q_\alpha^2 + 4i \frac{1 - (-1)^n}{q_\alpha^3} q_\alpha^3 \right],
\]

\[
L_{\alpha mn} = \frac{1}{4} \left[ 2 \ln(k_D L e^C) - 2 \text{Ci}(q_n) - 2 \frac{\text{Si}(q_n)}{q_n} q_\alpha^2 + 4i \frac{1 - (-1)^n}{q_\alpha^3} q_\alpha^3 \right],
\]

\[
\frac{L_{\alpha n}^{(2)}}{q_\alpha^2} = \frac{1 - \gamma + \gamma^2 q_\alpha^2}{8} q_\alpha^2 + i \frac{1 - (-1)^n}{5q_\alpha^4} (1 - \gamma^{5/2}) q_\alpha^3.
\]

Then the low-frequency asymptotic behavior of elements \( B_{nn} \) is expressed by formula (11) for the non-diagonal elements \( B_{nn} = (\alpha^{-1})_{nn} = \frac{\mu}{4\pi L} \left( C_{nn} - M_{nn} q_\alpha^2 + i \Gamma_{nn} q_\alpha^3 \right) \), where we have now

\[
C_{nn} = \frac{1}{2} \left( 2b_c^2 + (3 - 4\gamma)b_c^2 \right) \left( C + \ln(k_D L) - \text{Ci}(q_n) - \frac{\text{Si}(q_n)}{q_n} + \frac{1}{2q_n} \arctg \frac{2q_n}{k_D L} + \frac{k_D L}{(k_D L)^2 + q_n^2} \right) q_n^2,
\]

\[
M_{nn} = \frac{1}{2} \left( b^2 + \gamma^2 b_c^2 \right) \left( C + \ln(k_D L) - \text{Ci}(q_n) + \frac{\text{Si}(q_n)}{q_n} + \frac{1}{2q_n} \arctg \frac{2q_n}{k_D L} - \frac{k_D L}{(k_D L)^2 + q_n^2} \right),
\]

\[
\Gamma_{nn} = -\frac{4}{5} \frac{1 - (-1)^n}{q_n^2} b_c^2 \left( 1 + \frac{2}{3} \gamma^{5/2} \right).
\]
It is obvious from the recorded expressions that $C_{nn}$ and $M_{nn}$ unlike $C_{mn}$ and $M_{mn}$ contain summands $\ln(k_D L e^C)$, so the diagonal matrix elements exceed significantly the non-diagonal ones in their absolute value.

5. Conclusion
The results obtained in this paper can be used to find the oscillation eigenfrequencies of dislocation segment and their damping coefficients, for the calculation of dynamic characteristics of a dislocation segment and the dislocation internal friction.

References
[1] Ninomiya T and Ishioka Sh 1967 *J. Phys. Soc. Japan* 23 361
[2] Ninomiya T 1968 *J. Phys. Soc. Japan* 25 830
[3] Ninomiya T 1970 *Fundamental Aspects of Dislocations Theory*, ed J A Simmons, R de Wit and R Bullough (Nat. Bur. Stand. (U.S.) Spec. Publ. 317) p 315
[4] Dezhin V V, Nechaev V N and Roshchupkin A M 1989 *Ferroelectrics Letters* 10 155
[5] Bataronov I L, Dezhin V V and Roshchupkin A M 1993 *Bulletin of the Russian Academy of Sciences - Physics*, 57 1947
[6] Roshchupkin A M, Bataronov I L and Dezhin V V 1995 *Bulletin of the Russian Academy of Sciences - Physics*, 59 1648
[7] Bataronov I L, Dezhin V V and Roshchupkin A M 1995 *Bulletin of the Russian Academy of Sciences - Physics*, 59 1690
[8] *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables*, ed Abramowitz M and Stegun I A 1964 (Nat. Bur. Stand. Applied Mathematics Series 55)
[9] Bataronov I L, Nadeina T A, Dezhin V V and Roshchupkin A M 2002 *Interaction of Defects and Inelastic Phenomena in Solids: Proc. 10th Int. Conf.* (Tula: Tula State University) p 179