Numerical and approximate calculation of the generalized susceptibility matrix elements of dislocation segment in nondissipative crystal

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Abstract. Numerical calculation of the generalized susceptibility and the inverse generalized susceptibility matrix elements of the dislocation segment for edge and screw dislocations, different frequencies and different values of the dislocation segment length is performed. Certain regularities have been established. Based on the graphical results of numerical calculations, an approximate calculation of the generalized susceptibility matrix elements was carried out. Expressions for the diagonal and off-diagonal generalized susceptibility matrix elements of the dislocation segment are obtained.

1. Introduction
Earlier, to describe the dynamics of the dislocation segment, Koehler [1] proposed a string model. Further development of Kohler's theory was made by Granato and Lücke [2]. Garcia-Moliner and Thomson [3] used the Fourier transform of the response function to calculate the Granato-Lücke model. In [4], the equation of motion of a dislocation segment was obtained by means of the Lagrange function. The most consistent solution to the problem of a dislocation crystal vibrations using a self-consistent dynamic dislocation theory was carried out in the works of Ninomiya [5-7]. In [9], using the results of [8], a string model with nonlocal dynamic dislocation characteristics was constructed. The generalized susceptibility (the response function) of the dislocation segment, which is a matrix of dislocation oscillators generalized susceptibilities, is found in [10-12] based on the results of [8]. Analytic expressions for the matrix elements $B_{mn}$ of the dislocation oscillators generalized susceptibilities inverse matrix are obtained. Later on, studies of the two adjacent dislocation segments oscillations were started [13, 14] on the basis of papers [8, 10-12]. In this paper, a numerical and approximate calculation of the dislocation oscillators generalized susceptibilities matrix elements $\alpha_{mn} = (B^{-1})_{mn}$ is carried out.

2. Numerical calculation of the matrix elements
In this section, we numerically compute the elements of the matrix $\alpha$ and the inverse matrix $B$ for different types of dislocations (edge and screw), different frequencies $\omega$, and different values of the dislocation segment length $L$. The results of calculations were made in the form of graphs. We use the notation: $k_m$ is the maximum wave number, $c_t$ is the transverse elastic waves velocity, $q_t = \omega L / c_t$ is the normalized frequency.
Figure 1. Modules of matrix elements for edge dislocation, $k_m L = 100$, $q_t = 1$.
  a) $|\text{Re} B_{mn}|$, b) $|\text{Im} B_{mn}|$, c) $|\text{Re} \alpha_{mn}|$, d) $|\text{Im} \alpha_{mn}|$.

Figure 2. Modules of matrix elements for edge dislocation, $k_m L = 1000$, $q_t = 25$.
  a) $|\text{Re} B_{mn}|$, b) $|\text{Im} B_{mn}|$, c) $|\text{Re} \alpha_{mn}|$, d) $|\text{Im} \alpha_{mn}|$. 
Figure 3. Modules of matrix elements for screw dislocation, $k_m L = 100$, $q_t = 1$.

a) $|\text{Re } B_{mn}|$, b) $|\text{Im } B_{mn}|$, c) $|\text{Re } \alpha_{mn}|$, d) $|\text{Im } \alpha_{mn}|$.

Figure 4. Modules of matrix elements for screw dislocation, $k_m L = 1000$, $q_t = 25$.

a) $|\text{Re } B_{mn}|$, b) $|\text{Im } B_{mn}|$, c) $|\text{Re } \alpha_{mn}|$, d) $|\text{Im } \alpha_{mn}|$.

Based on the constructed graphs, we do the following conclusions.

1. The diagonal elements of all matrices are predominant in absolute value over off-diagonal elements.

2. The minimum value of the inverse matrix element $B_{kk}$ corresponds to the maximum value of the corresponding element $\alpha_{kk}$.

3. As the frequency increases, the minimum value of the diagonal elements of the inverse matrix $B$ moves from $B_{11}$ to $B_{NN}$. Simultaneously, the minimum value of the diagonal elements of the matrix $\alpha$ moves from $\alpha_{NN}$ to $\alpha_{11}$.

3. Approximate calculation of the matrix elements

We will carry out an approximate calculation of the matrix elements $\alpha$, using the results of the previous section. Consider the matrix elements $B_{mn}$, which form a matrix of size $N \times N$. This matrix is symmetric, i.e. $B_{mn} = B_{nm}$ [10-12]. We define the vector $b = (B_{1k} / \beta \ B_{2k} / \beta \ \ldots \ b_k = \beta \ B_{Nk} / \beta)^T$ and express the matrix elements in terms of this vector components: $B_{mn} = b_m b_n + B'_{mn}$ or $B = bb^T + B'$. Here, the number $k$ is chosen from the minimum modulus condition of the matrix $B$ diagonal element, i.e. from the resonance condition, the number $\beta$ is defined as $\beta = \sqrt{B_{kk} - \eta}$, $\eta$ is an arbitrary number under the condition $B_{kk} - \eta > 0$, the auxiliary matrix $B'$ has the form
We write the matrix inverse to the matrix $B$ in the form of a sum of a matrix inverse to $B'$ and an additive summand $B^{-1} = (B')^{-1} + CC^T$. We divide the $B'$ into two matrices $B' = B^{(d)} + B^{(nd)}$. In this case, the matrix $B^{(d)}$ consists of the diagonal elements of the matrix $B'$, and the matrix $B^{(nd)}$ consists of off-diagonal elements. It can be seen from the numerical calculations of the previous section that the diagonal elements of the matrix $B'$ substantially predominate over the off-diagonal elements in absolute value, so we seek the inverse to it in the form of the sum of the diagonal matrix with the elements inverse to the corresponding elements of the matrix $B'$ and the matrix $D$ with elements that are significantly smaller in absolute value for the elements of the diagonal matrix, i.e. $(B'^{-1})_{ij} = \delta_{ij}/B'_{ii} + D_{ij}$. After further cumbersome calculations, setting $\eta \to -\infty$, we obtain an elements of the matrix $\alpha = B^{-1}$:

\[
B_{kk}^{-1} = \frac{1}{B_{kk} - \sum_{i(k)} \frac{(B_{kk})^2}{B_{ii}} + \sum_{(i, j \neq k)} \frac{B_{kl}B_{lj}^{(nd)}}{B_{li}B_{lj}}} = \frac{1}{B_{ii} \left( \frac{-B_{ik}}{B_{jj}} + \sum_{j \neq k} \frac{B_{kj}B_{ji}^{(nd)}}{B_{jj}} \right)}, \
\]

\[
B_{ik}^{-1} \approx \frac{1}{B_{kk} - \sum_{m \neq k} \frac{(B_{km})^2}{B_{mm}} + \sum_{m, j \neq k} \frac{B_{km}B_{mj}^{(nd)}}{B_{mm}B_{jj}}} = \frac{1}{B_{ii} \left( \frac{B_{ik}}{B_{jj}} - \sum_{j \neq k} \frac{B_{kj}B_{ji}^{(nd)}}{B_{jj}} \right)^2}, \
\]

\[
B_{lj}^{-1} \approx \frac{1}{B_{ii}} + \frac{1}{B_{ii} \left( \frac{B_{lj}}{B_{jj}} - \sum_{j \neq k} \frac{B_{kj}B_{ji}^{(nd)}}{B_{jj}} \right)^2}, \quad (i \neq k),
\]
Calculations based on these formulas showed good agreement with numerical calculations of the previous section.

4. Conclusion
In this paper, the elements of the generalized susceptibility matrix of dislocation oscillators are found. The results obtained can be used to determine the orientation and size dependence of the dislocation segment vibrational spectrum, the dependence of the dislocation segment vibrational spectrum on the Poisson's ratio.

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