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Equations of anisotropic elastodynamics in 3D quasicrystals as a symmetric hyperbolic system: Deriving the time-dependent fundamental solutions

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ABSTRACT

The fundamental solution (FS) of the time-dependent differential equations of anisotropic elasticity in 3D quasicrystals are studied in the paper. Equations of the time-dependent differential equations of anisotropic elasticity in 3D quasicrystals are written in the form of a symmetric hyperbolic system of the first order. Using the Fourier transform with respect to the space variables and matrix transformations we obtain explicit formulae for Fourier images of the FS columns; finally, the FS is computed by the inverse Fourier transform. As a computational example applying the suggested approach FS components are computed for icosahedral QCs.

1. Introduction

The quasicrystal as a new structure of solids has been first discovered in 1984 by Schechtman et al. [1]. The physical properties, such as the structural, electronic, magnetic, optical and thermal properties, of QCs have been investigated intensively. Most of these properties combine effectively to give technologically interesting applications which have been protected recently by several patents [2–4]. For instance, the combination of such kind of properties as high hardness, low friction and corrosive resistance of QCs gives almost ideal material for motor-car engines. The application of QCs in motor-car engines would be undoubtedly result in reduced air pollution and increase engine lifetimes. The same set of associated properties (hardness, low friction, corrosive resistance) combined with bio-compatibility is also very promising for introducing QCs in surgical applications as parts used for bone repair and prostheses.

Dynamic analysis of elasticity problems of quasicrystals is very limited. In addition to the difficulty of mathematical analysis for dynamic problems in quasicrystals, a possible reason is that the physical mechanism of phase is not very clear. As is well-known, phonon excitations lead to wave propagations. However, for phason excitations, there are several kinds of different points of views [5–14].

Elasticity is one of the interesting properties of QCs. Equations of anisotropic elastodynamics in 3D QCs are more complicated than those of 1D and 2D QCs. For this reason most authors consider only elastic plane problems for QCs [15–17], i.e. they suppose that the elastic fields induced in QCs are independent of the variable z. In the last several years many works have been devoted to the construction of general solutions of static and plane elasticity in QCs. The plane elasticity problems of 3D and 2D quasicrystals has been studied for static case in [18]. Based on the stress potential function general solution of the plane elasticity problems of icosahedral quasicrystals has been studied for static case in [19]. Gao [20] has established

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general solutions for plane elastostatic of cubic quasicrystals using an operator method. Fan and Guo [21] has developed the potential function theory for plane elastostatic of 3D icosahedral quasicrystals. Using PS method related with polynomial presentation of data 3D elastodynamic problems in 3D QCs have been solved in [22]. The method for the derivation of the time-dependent fundamental solution with three space variables in 2D and 3D QCs with arbitrary system of anisotropy have been studied in [23,24].

In the present paper a method for computation of the time-dependent fundamental solution (FS) of three-dimensional elastodynamics in 3D QCs is studied. This method was proposed for elastodynamic problems of normal crystals in [25]. The method has been applied equations of anisotropic dynamic elasticity for 2D and 3D QCs to obtain fundamental solutions of phonon and phason displacements [23,24]. However, in this paper the phonon displacements, phason displacements, phonon displacement speeds, phason displacement speeds, phonon stresses, phason stresses arising from pulse point source for dynamic elasticity of 3D QCs are computed.

Originality of this paper is the reduction of the second order differential equations of elastodynamics of 3D quasicrystals to a first order symmetric hyperbolic system. This allows us to simplify of a quite complex problem and to obtain phonon and phason elements at the same time with a small number of calculations. Applying the Fourier transform with respect to the space variables to the symmetric hyperbolic system, system of ordinary differential equations with respect to the time variable whose coefficients depend on the Fourier parameters is obtained. Using the some matrix computations a solution of the obtained system is computed with respect to Fourier parameters. Applying the inverse Fourier transform to the resulting formula the time-dependent FS of elasticity for 3D QCs is computed. The obtained time-dependent FS is a vector with components 21 whose are 3 phonon displacement speeds, 6 phonon stresses, 3 phason displacements and 9 phason stresses arising from an arbitrary force. Integrating of phonon and phason displacement speeds give phonon and phason displacement arising from an arbitrary force. Consequently, the phonon displacement speed, phason displacement speed, phonon stress, phason stress arising from pulse point source in time dependent 3D QCs is computed. The method is suitable for computer programming. Using the MATLAB programming the values of the FS in 3D QCs is computed and the wave propagation in these crystals is simulated.

The paper is organized as follows. The basic equations of elastodynamics for 3D QCs are written in Section 2. In Section 3 equations of anisotropic elastodynamics in 3D QCs are written in the form of the symmetric hyperbolic system containing twenty-one partial differential equations of the first order. The time-dependent FS of elasticity for 3D QCs and vector partial differential equation for FS columns are given in Section 4. The method of computing FS columns is described in the Section 5. Computational examples with the description of input data and results of computations are written in Section 6. The conclusion, appendix and a collection of computational images of phonon and phason displacements, displacement speeds and stresses for anisotropic elasticity of QCs with icosahedral structure are given at the end of the paper.

2. The basic equations for 3D QCs

Let $x = (x_1, x_2, x_3) \in R^3$ be a space variable, $t \in R$ be a time variable. The generalized Hooke's laws of the elasticity problem of 3D QCs are given by (see, for example, [15,26,27])

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} + R_{ijkl}w_{kl}, \tag{1}$$

$$H_{ij} = R_{klij}\varepsilon_{kl} + K_{ijkl}w_{kl}, \tag{2}$$

where the subscripts $i, j, k, l = 1, 2, 3$. The equations of deformation geometry are given by

$$\varepsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right), \quad w_{kl} = \frac{\partial w_k}{\partial x_l}, \quad k, l = 1, 2, 3. \tag{3}$$

Here u_k and $w_k, k = 1, 2, 3$ are the phonon and phason displacements; $\varepsilon_{kl}(x, t), w_{kl}(x, t), k, l = 1, 2, 3$ are phonon and phason strains, respectively.

C_{ijkl} are the phonon elastic constants and they satisfy the symmetry property (see, for example, [15,26,27])

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}. \tag{4}$$

K_{ijkl} are the phason elastic constants and they satisfy the symmetry property (see, for example, [15,26,27])

$$K_{ijkl} = K_{klij}. \tag{5}$$

R_{ijkl} are the phonon–phason coupling elastic constants and they satisfy the symmetry property (see, for example, [15,26,27])

$$R_{ijkl} = R_{jikl}. \tag{6}$$

The positivity of elastic strain energy density requires that the elastic constant tensors $C_{ijkl}, K_{ijkl}, R_{ijkl}$ must be positive definite. Namely, when the strain tensors ε_{ij}, w_{ij} are not zero entirely, the elastic constant tensors satisfy the following inequality (see, for example [27])

$$\sum_{i,j,k,l=1}^{3} C_{ijkl}\varepsilon_{ij}\varepsilon_{kl} > 0, \quad \sum_{i,j,k,l=1}^{3} K_{ijkl}w_{ij}w_{kl} > 0, \quad \sum_{i,j,k,l=1}^{3} R_{ijkl}\varepsilon_{ij}w_{kl} > 0. \tag{7}$$

The dynamic equilibrium equations can be written in the following form

$$\rho \frac{\partial^2 u_i(x,t)}{\partial t^2} = \sum_{j=1}^{3} \frac{\partial \sigma_{ij}(x,t)}{\partial x_j} + f_i(x,t), \tag{8}$$

$$\rho \frac{\partial^2 w_i(x,t)}{\partial t^2} = \sum_{j=1}^{3} \frac{\partial H_{ij}(x,t)}{\partial x_j} + g_i(x,t), \qquad i = 1,2,3,\ x \in R^3,\ t \in R, \tag{9}$$

where the constant $\rho > 0$ is the density; σ_{ij} and $H_{ij}, i,j = 1,2,3$ are phonon and phason stresses; $f_i(x,t)$ and $g_i(x,t), i = 1,2,3$ are body forces for the phonon and phason displacements, respectively.

3. Reduction of time-dependent anisotropic elastodynamics in 3D QCs to a symmetric hyperbolic system

From the symmetry property (4) it is convenient to describe the phonon elastic constants in terms of a 6×6 matrix according to the following conventions relating pairs of indices (ij) and (kl) to single indices α and β:

$$(11) \leftrightarrow 1, \quad (22) \leftrightarrow 2, \quad (33) \leftrightarrow 3, \quad (23),(32) \leftrightarrow 4, \quad (13),(31) \leftrightarrow 5, \quad (12),(21) \leftrightarrow 6. \tag{10}$$

The obtained matrix $C = (c_{\alpha\beta})_{6\times 6}$ of all moduli, where $\alpha = (ij), \beta = (kl)$, is symmetric.

Using the symmetry properties (4), (6) and the rule (10) the phonon stresses σ_{ij} can be written in the form

$$\begin{aligned}\sigma_\alpha = {} & C_{\alpha,1}\varepsilon_{11} + C_{\alpha,2}\varepsilon_{22} + C_{\alpha,3}\varepsilon_{33} + 2C_{\alpha,4}\varepsilon_{23} + 2C_{\alpha,5}\varepsilon_{13} + 2C_{\alpha,6}\varepsilon_{12} + R_{\alpha,11}w_{11} + R_{\alpha,22}w_{22} + R_{\alpha,33}w_{33} + R_{\alpha,23}w_{23} \\ & + R_{\alpha,31}w_{31} + R_{\alpha,12}w_{12} + R_{\alpha,32}w_{32} + R_{\alpha,13}w_{13} + R_{\alpha,21}w_{21}, \quad \alpha = 1,2,3,4,5,6.\end{aligned} \tag{11}$$

Using the symmetry property (6) and the rule (10) the phason stresses H_{ij} can be written in the form

$$\begin{aligned}H_{ij} = {} & R_{1,ij}\varepsilon_{11} + R_{2,ij}\varepsilon_{22} + R_{3,ij}\varepsilon_{33} + 2R_{4,ij}\varepsilon_{23} + 2R_{5,ij}\varepsilon_{13} + 2R_{6,ij}\varepsilon_{12} + K_{ij,11}w_{11} + K_{ij,22}w_{22} + K_{ij,33}w_{33} + K_{ij,23}w_{23} \\ & + K_{ij,31}w_{31} + K_{ij,12}w_{12} + K_{ij,32}w_{32} + K_{ij,13}w_{13} + K_{ij,21}w_{21}, \quad i,j = 1,2,3.\end{aligned} \tag{12}$$

The relations (11) and (12) can be written in the matrix form

$$\mathbf{T} = \bar{C}\mathbf{Y}. \tag{13}$$

Here

$$\mathbf{T} = (\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5, \sigma_6, H_{11}, H_{22}, H_{33}, H_{23}, H_{31}, H_{12}, H_{32}, H_{13}, H_{21})^*,$$

$$\mathbf{Y} = (\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, 2\varepsilon_{23}, 2\varepsilon_{13}, 2\varepsilon_{12}, w_{11}, w_{22}, w_{33}, w_{23}, w_{31}, w_{12}, w_{32}, w_{13}, w_{21})^*,$$

$$\bar{C} = \begin{pmatrix} C & R \\ R^* & K \end{pmatrix}_{15\times 15}, \quad C = (C_{\alpha,\beta})_{6\times 6}, \quad \alpha,\beta = 1,2,3,4,5,6, \tag{14}$$

$$R = \begin{pmatrix} R_{1,11} & R_{1,22} & R_{1,33} & R_{1,23} & R_{1,31} & R_{1,12} & R_{1,32} & R_{1,13} & R_{1,21} \\ R_{2,11} & R_{2,22} & R_{2,33} & R_{2,23} & R_{2,31} & R_{2,12} & R_{2,32} & R_{2,13} & R_{2,21} \\ R_{3,11} & R_{3,22} & R_{3,33} & R_{3,23} & R_{3,31} & R_{3,12} & R_{3,32} & R_{3,13} & R_{3,21} \\ R_{4,11} & R_{4,22} & R_{4,33} & R_{4,23} & R_{4,31} & R_{4,12} & R_{4,32} & R_{4,13} & R_{4,21} \\ R_{5,11} & R_{5,22} & R_{5,33} & R_{5,23} & R_{5,31} & R_{5,12} & R_{5,32} & R_{5,13} & R_{5,21} \\ R_{6,11} & R_{6,22} & R_{6,33} & R_{6,23} & R_{6,31} & R_{6,12} & R_{6,32} & R_{6,13} & R_{6,21} \end{pmatrix}_{6\times 9},$$

$$K = \begin{pmatrix} K_{11,11} & K_{11,22} & K_{11,33} & K_{11,23} & K_{11,31} & K_{11,12} & K_{11,32} & K_{11,13} & K_{11,21} \\ K_{22,11} & K_{22,22} & K_{22,33} & K_{22,23} & K_{22,31} & K_{22,12} & K_{22,32} & K_{22,13} & K_{22,21} \\ K_{33,11} & K_{33,22} & K_{33,33} & K_{33,23} & K_{33,31} & K_{33,12} & K_{33,32} & K_{33,13} & K_{33,21} \\ K_{23,11} & K_{23,22} & K_{23,33} & K_{23,23} & K_{23,31} & K_{23,12} & K_{23,32} & K_{23,13} & K_{23,21} \\ K_{31,11} & K_{31,22} & K_{31,33} & K_{31,23} & K_{31,31} & K_{31,12} & K_{31,32} & K_{31,13} & K_{31,21} \\ K_{12,11} & K_{12,22} & K_{12,33} & K_{12,23} & K_{12,31} & K_{12,12} & K_{12,32} & K_{12,13} & K_{12,21} \\ K_{32,11} & K_{32,22} & K_{32,33} & K_{32,23} & K_{32,31} & K_{32,12} & K_{32,32} & K_{32,13} & K_{32,21} \\ K_{13,11} & K_{13,22} & K_{13,33} & K_{13,23} & K_{13,31} & K_{13,12} & K_{13,32} & K_{13,13} & K_{13,21} \\ K_{21,11} & K_{21,22} & K_{21,33} & K_{21,23} & K_{21,31} & K_{21,12} & K_{21,32} & K_{21,13} & K_{12,21} \end{pmatrix}_{9\times 9}$$

and $*$ is the sign of the transposition. Since the matrix C is symmetric and the phason elastic constants K_{ijkl} satisfy the symmetry property (5) the matrix $\bar{C}$ is symmetric. From the conditions (7) the matrix $\bar{C}$ is positive definite (see, Appendix).

Differentiating (13) with respect to t and multiplying the left hand side of the resulting formula by the inverse of $\bar{C}$, denoted $\bar{C}^{-1}$, we find the following matrix representation

$$\bar{C}^{-1}\frac{\partial \mathbf{T}}{\partial t}+\sum_{j=1}^{3}\begin{pmatrix}(A_j^1)^* & 0_{6,3}\\ 0_{9,3} & (A_j^2)^*\end{pmatrix}\frac{\partial}{\partial x_j}\begin{pmatrix}\mathbf{U}\\ \mathbf{W}\end{pmatrix}=0_{15,1}, \tag{15}$$

where

$$A_1^1=\begin{pmatrix}-1&0&0&0&0&0\\0&0&0&0&0&-1\\0&0&0&0&-1&0\end{pmatrix},\quad A_2^1=\begin{pmatrix}0&0&0&0&0&-1\\0&-1&0&0&0&0\\0&0&0&-1&0&0\end{pmatrix},$$
$$A_3^1=\begin{pmatrix}0&0&0&0&-1&0\\0&0&0&-1&0&0\\0&0&-1&0&0&0\end{pmatrix};\quad A_1^2=\begin{pmatrix}-1&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&-1\\0&0&0&0&-1&0&0&0&0\end{pmatrix}, \tag{16}$$
$$A_2^2=\begin{pmatrix}0&0&0&0&0&-1&0&0&0\\0&-1&0&0&0&0&0&0&0\\0&0&0&0&0&0&-1&0&0\end{pmatrix},\quad A_3^2=\begin{pmatrix}0&0&0&0&0&0&0&-1&0\\0&0&0&-1&0&0&0&0&0\\0&0&-1&0&0&0&0&0&0\end{pmatrix};$$
$$\mathbf{U}=(U_1,U_2,U_3),\quad \mathbf{W}=(W_1,W_2,W_3),\quad U_i(x,t)=\frac{\partial u_i(x,t)}{\partial t},\quad W_i(x,t)=\frac{\partial w_i(x,t)}{\partial t},\quad i=1,2,3$$

and $0_{l,n}$ is the zero matrix of the order $l\times n$.

Using symmetry properties (4) and (6) and the rule (10) Eqs. (8) and (9) can be written as

$$\rho\frac{\partial}{\partial t}\begin{pmatrix}\mathbf{U}\\ \mathbf{W}\end{pmatrix}+\sum_{j=1}^{3}\begin{pmatrix}A_j^1 & 0_{3,9}\\ 0_{3,6} & A_j^2\end{pmatrix}\frac{\partial \mathbf{T}}{\partial x_j}=\mathcal{F}, \tag{17}$$

where $\mathcal{F}=(f_1,f_2,f_3,g_1,g_2,g_3)^*$.

The relations (15) and (17) can be presented by the following system

$$A_0\frac{\partial \mathbf{V}}{\partial t}+\sum_{j=1}^{3}A_j\frac{\partial \mathbf{V}}{\partial x_j}=\mathbf{F},\quad x\in R^3,\ t\in R, \tag{18}$$

where $\mathbf{F}=(f_1,f_2,f_3,g_1,g_2,g_3,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)^*$,

$$\mathbf{V}=(U_1,U_2,U_3,W_1,W_2,W_3,\sigma_1,\sigma_2,\sigma_3,\sigma_4,\sigma_5,\sigma_6,H_{11},H_{22},H_{33},H_{23},H_{31},H_{12},H_{32},H_{13},H_{21})^*,$$

$$A_0=\begin{pmatrix}\rho I_6 & 0_{6,15}\\ 0_{15,6} & \bar{C}^{-1}\end{pmatrix}_{21\times 21},\quad A_j=\begin{pmatrix}0_{3,6} & A_j^1 & 0_{3,9}\\ 0_{3,6} & 0_{3,6} & A_j^2\\ (A_j^1)^* & 0_{6,3} & 0_{6,15}\\ 0_{9,3} & (A_j^2)^* & 0_{9,15}\end{pmatrix}_{21\times 21}, \tag{19}$$

Here I_6 is the unit matrix of the order 6×6 and $0_{l,n}$ is the zero matrix of the order $l\times n$, matrices $A_j^1, A_j^2, j=1,2,3$, are defined by (16).

We note that the matrices $A_j, j=1,2,3$, are symmetric. Since $\bar{C}$ is positive definite and symmetric, $\rho>0$ the matrix A_0 is symmetric and positive definite. Therefore system (18) is a symmetric hyperbolic system (see, for example, [28]).

4. Fundamental solution (FS) of anisotropic elastodynamics in 3D QCs

Let m run values $1,2,3,4,5,6$. The time-dependent FS of elasticity for 3D QCs is a 21×6 matrix whose mth column is a vector function

$$\mathbf{V}^m(x,t)=(U_1^m(x,t),U_2^m(x,t),U_3^m(x,t),W_1^m(x,t),W_2^m(x,t),W_3^m(x,t),\sigma_1^m(x,t),\sigma_2^m(x,t),\sigma_3^m(x,t),\sigma_4^m(x,t),$$
$$\sigma_5^m(x,t),\sigma_6^m(x,t),H_{11}^m(x,t),H_{22}^m(x,t),H_{33}^m(x,t),H_{23}^m(x,t),H_{31}^m(x,t),H_{12}^m(x,t),H_{32}^m(x,t),H_{13}^m(x,t),H_{21}^m(x,t))^*$$

satisfying the following initial value problem (IVP)

$$A_0\frac{\partial \mathbf{V}^m}{\partial t}+\sum_{j=1}^{3}A_j\frac{\partial \mathbf{V}^m}{\partial x_j}=\mathbf{E}^m\delta(x,t),\quad x\in R^3,\ t\in R, \tag{20}$$
$$\mathbf{V}^m(x,t)|_{t<0}=0. \tag{21}$$

Here $\mathbf{E}^m=(\delta_1^m,\delta_2^m,\delta_3^m,\delta_4^m,\delta_5^m,\delta_6^m,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)^*$, $m=1,2,3,4,5,6$; δ_n^m be the Kronecker symbol i.e. $\delta_n^m=1$ if $n=m$ and $\delta_n^m=0$ if $n\neq m$; $n,m=1,2,3,4,5,6$; $\delta(x)=\delta(x_1)\delta(x_2)\delta(x_3)$ is the Dirac delta function of the space variable concentrated at $x_1=0,x_2=0,x_3=0$; $\delta(t)$ is the Dirac delta function of the time variable concentrated at $t=0$.

The computation of mth column for the time-dependent FS of 3D QCs is the main problem of this paper. This problem is related with finding a vector function $\mathbf{V}^m(x,t)$ satisfying (20) and (21).

5. Computation of FS of anisotropic elastodynamics in 3D QCs

In this section we compute mth column of the FS $\mathbf{V}^m(x,t)$. Firstly, IVP (20) and (21) are written in terms of the Fourier transform with respect to $x \in R^3$. Then, a solution of the obtained IVP is derived by matrix transformations and the ordinary differential equations technique. Finally, an explicit formula for mth column of the FS is found by the inverse Fourier transform.

Equations for mth column of FS in terms of Fourier images. Let

$$\begin{aligned}\tilde{\mathbf{V}}^m(\nu,t) = (&\tilde{U}_1^m, \tilde{U}_2^m, \tilde{U}_3^m, \tilde{W}_1^m, \tilde{W}_2^m, \tilde{W}_3^m, \tilde{\sigma}_1^m, \tilde{\sigma}_2^m, \tilde{\sigma}_3^m, \tilde{\sigma}_4^m, \tilde{\sigma}_5^m, \tilde{\sigma}_6^m, \tilde{H}_{11}^m(x,t), \tilde{H}_{22}^m(x,t), \tilde{H}_{33}^m(x,t),\\ &\tilde{H}_{23}^m(x,t), \tilde{H}_{31}^m(x,t), \tilde{H}_{12}^m(x,t), \tilde{H}_{32}^m(x,t), \tilde{H}_{13}^m(x,t), \tilde{H}_{21}^m(x,t))^*,\end{aligned}$$

be the Fourier image of $\mathbf{V}^m(x,t)$ with respect to $x = (x_1, x_2, x_3) \in R^3$ (see, for example [29]), i.e.

$$\begin{aligned}&\tilde{V_j}^m(\nu,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} V_j^m(x,t) e^{ix\cdot\nu} dx_1 dx_2 dx_3,\\ &\nu = (\nu_1,\nu_2,\nu_3) \in R^3, \quad x\cdot\nu = x_1\nu_1 + x_2\nu_2 + x_3\nu_3, \quad i^2 = -1,\ j = 1,\dots 21,\ m = 1,\dots 6.\end{aligned}$$

The IVP (20) and (21) can be written in terms of $\tilde{\mathbf{V}}^m(\nu,t)$ as follows

$$A_0 \frac{\partial \tilde{\mathbf{V}}^m}{\partial t} - iB(\nu)\tilde{\mathbf{V}}^m = \mathbf{E}^m \delta(t), \tag{22}$$

$$\tilde{\mathbf{V}}^m(\nu,t)|_{t<0} = 0,, \tag{23}$$

where $B(\nu) = (\nu_1 A_1 + \nu_2 A_2 + \nu_3 A_3)$.

Diagonalization A_0 and $B(\nu)$ simultaneously. The matrix A_0 is symmetric positive definite and $B(\nu)$ is symmetric. We can construct a non-singular matrix $\mathcal{T}(\nu)$ and a diagonal matrix $D(\nu) = diag(d_k(\nu), k = 1,2,\dots,21)$ with real valued elements such that (see, for example, [25])

$$\mathcal{T}^*(\nu) A_0 \mathcal{T}(\nu) = I, \tag{24}$$

$$\mathcal{T}^*(\nu) B(\nu) \mathcal{T}(\nu) = D(\nu), \tag{25}$$

where I is the identity matrix, $\mathcal{T}^*(\nu)$ is the transposed matrix to $\mathcal{T}(\nu)$.

MATLAB commands of constructing $D(\nu), \mathcal{T}(\nu)$ are listed below.

$$\begin{aligned}&Input : C_{ijkl}, R_{ijkl}, K_{ijkl}, \nu_1, \nu_2, \nu_3\\ &[EigVecA_0, EigValA_0] = eig(A_0);\\ &P = EigVecA_0;\\ &PT = P';\\ &M = EigValA_0;\\ &Ms = sqrt(M);\\ &SqrA_0 = P * Ms * PT;\\ &InvSqrA_0 = inv(SqrA_0);\\ &B = v1 * A1 + v2 * A2 + v3 * A3;\\ &H = InvSqrA_0 * B * InvSqrA_0;\\ &[EigVecH, EigValH] = eig(H);\\ &D(\nu) = EigValH;\\ &Q(\nu) = EigVecH;\\ &\mathcal{T}(\nu) = simplify(InvSqrA0 * Q);\\ &Output : D(\nu), \mathcal{T}(\nu).\end{aligned}$$

Computation of mth column of FS in terms of Fourier images. Consider the following transformation

$$\tilde{\mathbf{V}}^m(\nu,t) = \mathcal{T}(\nu)\mathbf{Y}^m(\nu,t), \tag{26}$$

where $\mathbf{Y}^m(\nu,t)$ is unknown vector function. Substituting (26) into (22) and (23) and then multiplying the obtained vector differential equation by $\mathcal{T}^*(\nu)$ and using (24) and (25) we find

$$\frac{\partial \mathbf{Y}^m}{\partial t} - iD(\nu)\mathbf{Y}^m = \mathcal{T}^*(\nu)\mathbf{E}^m\delta(t), \quad t \in R \tag{27}$$

$$\mathbf{Y}^m(\nu,t)|_{t\leqslant 0} = 0. \tag{28}$$

Using the ordinary differential equations technique (see, for example, [30]), a solution of the IVP (27) and (28) is given by

$$\mathbf{Y}^m(\nu,t) = \theta(t)[\cos(D(\nu)t) + i\sin(D(\nu)t)]\mathcal{T}^*(\nu)\mathbf{E}^m,$$

where $\theta(t)$ is the Heaviside function, i.e. $\theta(t) = 1$ for $t \geqslant 0$ and $\theta(t) = 0$ for $t < 0$; $\cos(D(\nu)t)$ and $\sin(D(\nu)t)$ are diagonal matrices whose diagonal elements are $\cos(d_k(\nu)t)$ and $\sin(d_k(\nu)t), k = 1,2,\ldots,21$, respectively.

Finally, a solution of (22) and (23) is determined by

$$\tilde{\mathbf{V}}^m(\nu,t) = \theta(t)\mathcal{T}(\nu)[\cos(D(\nu)t) + i\sin(D(\nu)t)]\mathcal{T}^*(\nu)\mathbf{E}^m. \tag{29}$$

Computation for mth column of FS. Noting that every solution of (20) and (21) is a real valued vector function. Therefore, applying the inverse Fourier transform to (29) we obtain (see, for example, [25])

$$\mathbf{V}^m(x,t) = \frac{\theta(t)}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathcal{T}(\nu)\cos\left(D(\nu)t - \mathbf{I}(\nu\cdot x)\right)\mathcal{T}^*(\nu)\mathbf{E}^m d\nu_1 d\nu_2 d\nu_3,$$
$$\mathbf{V}^m(x,t) = (V_1(x,t), V_2(x,t), V_3(x,t),\ldots,V_{21}(x,t))^*, \tag{30}$$

where $\cos\left(D(\nu)t - \mathbf{I}(\nu\cdot x)\right)$ is the diagonal matrix with diagonal elements $\cos\left(d_k(\nu)t - \nu\cdot x\right), k = 1,2,\ldots,9$.

Remark: Let us point out the physical sense of $\mathbf{V}^m(x,t)$ components. The first three components of $\mathbf{V}^m(x,t)$ are components of the phonon displacement speed $\mathbf{u}^m(x,t) = (u_1(x,t), u_2(x,t), u_3(x,t))$, i.e. $U_n^m(x,t) = \frac{\partial u_n^m}{\partial t}(x,t), n = 1,2,3$; the second three components of $\mathbf{V}^m(x,t)$ are components of the phason displacement speed $\mathbf{w}^m(x,t) = (w_1(x,t), w_2(x,t), w_3(x,t))$, i.e. $W_n^m(x,t) = \frac{\partial w_n^m}{\partial t}(x,t), n = 1,2,3$; the third six components of $\mathbf{V}^m(x,t)$ are the phonon stresses $\sigma_{ij}^m(x,t)$; the fourth nine components of $\mathbf{V}^m(x,t)$ are the phason stresses $H_{ij}^m(x,t)$ of the considered anisotropic medium arising from the source $\mathbf{E}^m\delta(x)\delta(t)$. Integrating the first six components of $\mathbf{V}^m(x,t)$ with respect to t the FS for phonon and phason displacements of elastodynamics of 3D QCs can be found in the following form

$$u_n^m(x,t) = \int_0^t \mathbf{V}_n^m(x,\tau)d\tau, \quad w_n^m(x,t) = \int_0^t \mathbf{V}_{n+3}^m(x,\tau)d\tau, \quad n = 1,2,3,$$

or

$$u_n^m(x,t) = \frac{\theta(t)}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}[\mathcal{T}(\nu)S(\nu,t,x)\mathcal{T}^*(\nu)\mathbf{E}^m]_n d\nu_1 d\nu_2 d\nu_3,$$
$$w_n^m(x,t) = \frac{\theta(t)}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}[\mathcal{T}(\nu)S(\nu,t,x)\mathcal{T}^*(\nu)\mathbf{E}^m]_{n+3} d\nu_1 d\nu_2 d\nu_3, \tag{31}$$

where elements of the matrix $S(\nu,t,x)$ are found by formulae (see, for example, [25])

$$S_{kk}(\nu,t) = \begin{cases} \frac{\sin(d_k(\nu)t - \nu\cdot x)}{d_k(\nu)} + \frac{\sin(\nu x)}{d_k(\nu)}, & \text{if } d_k(\nu) \neq 0, \\ t\cos(\nu\cdot x), & \text{if } d_k(\nu) = 0; \end{cases} \quad S_{kj}(\nu,t,x) = 0, \quad j \neq k, \; k,j = 1,\ldots,21.$$

$[\mathcal{T}(\nu)S(\nu,t,x)\mathcal{T}^*(\nu)\mathbf{E}^m]_n$ is the nth component of the vector $\mathcal{T}(\nu)S(\nu,t,x)\mathcal{T}^*(\nu)\mathbf{E}^m$.

6. Computational experiment

This method was proposed for elastodynamic problems of normal crystals in [25]. [25] is a special case of this paper for $R_{klij} = K_{ijkl} = 0, i,j,k,l = 1,2,3$. The robustness and correctness of the suggested method has been shown on the examples of isotropic crystals in [25].

The aim of the computational experiment is to derive values of elements for the FS of anisotropic elastodynamics in icosahedral QC Al-Mn-Pd (see, for example, [15,31]) and present results in the form of 3D graphs. The elastic constants for Al-Mn-Pd are taken from [31]. We choose $\rho = 1(10^3 kg/m^3)$. Using MATLAB code in Section 5 the matrices $\mathcal{T}(\nu)$ and $D(\nu)$ have been obtained. Substituting $\mathcal{T}(\nu)$ and $D(\nu)$ into formula (30) we have computed a solution $\mathbf{V}^m(x,t) = (V_1^m(x,t), V_2^m(x,t), V_3^m(x,t),\ldots,V_{21}^m(x,t))$ of (20) and (21) for $m = 3$. The computed vector-functions $\mathbf{V}^m(x,t)$ are columns of the FS of elastodynamics in Al-Mn-Pd. We note that the first three components of the vector function $\mathbf{V}^m(x,t)$ are the phonon displacement speed $\mathbf{U}^m(x,t) = (U_1^m(x,t), U_2^m(x,t), U_3^m(x,t))$; the second three components of $\mathbf{V}^m(x,t)$ are the phason displacement speed $\mathbf{W}^m(x,t) = W_1^m(x,t), W_2^m(x,t), W_3^m(x,t))$; the third six components of $\mathbf{V}^m(x,t)$ are the phonon stresses; the fourth nine components of $\mathbf{V}^m(x,t)$ are the phason stresses arising from forces $\mathbf{E}^m\delta(x)\delta(t)$. Substituting $\mathcal{T}(\nu)$ and $D(\nu)$ into formula (31) we have computed fundamental solution of the phonon displacement $\mathbf{u}^m = (u_1^m, u_2^m, u_3^m)$ and the phason displacement $\mathbf{w}^m = (w_1^m, w_2^m, w_3^m)$ arising from pulse point forces $\mathbf{E}^3\delta(x)\delta(t)$ have been computed.

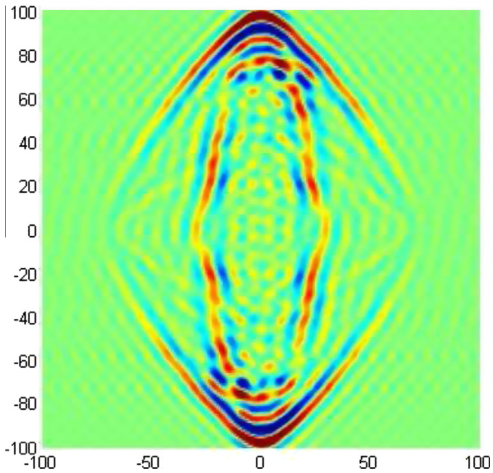

Fig. 1. The third component of the phonon displacement speed $U_3^3(0, x_2, x_3, t)$ at the time $t = 0.1$ in Al-Mn-Pd.

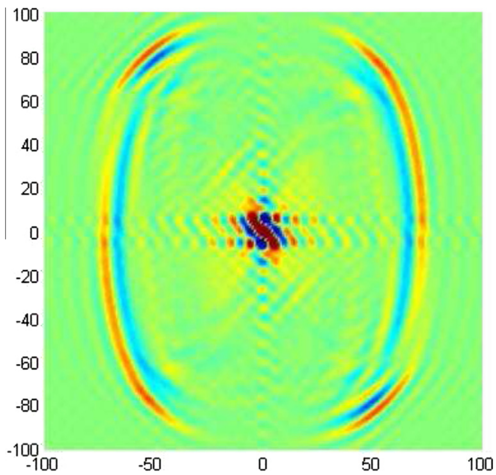

Fig. 2. The second component of the phason displacement speed $W_2^3(x_1, 0, x_3, t)$ at the time $t = 0.1$ in Al-Mn-Pd.

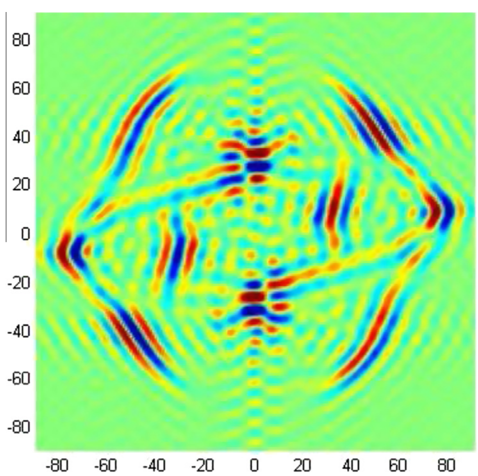

Fig. 3. The sixth component of the phonon stress $\sigma_6^3(x_1, x_2, 0, t)$ at time $t = 0.1$ in Al-Mn-Pd.

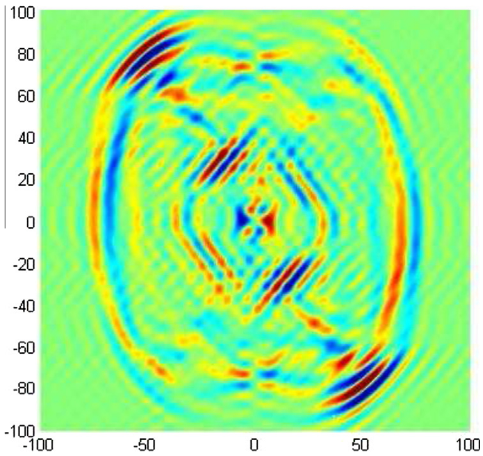

Fig. 4. The ninth component of the phason stress $H_{21}^3(x_1, 0, x_3, t)$ at time $t = 0.1$ in Al-Mn-Pd.

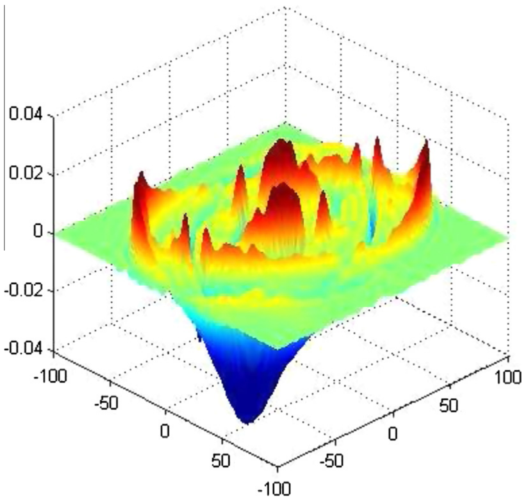

Fig. 5. The first component of the phonon displacement $u_1^3(x_1, 0, x_3, t)$ at time $t = 0.1$ in Al-Mn-Pd.

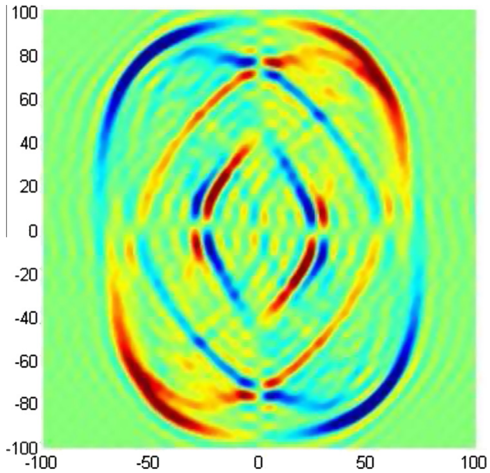

Fig. 6. The first component of the phonon displacement $u_1^3(x_1, 0, x_3, t)$ at time $t = 0.1$ in Al-Mn-Pd.

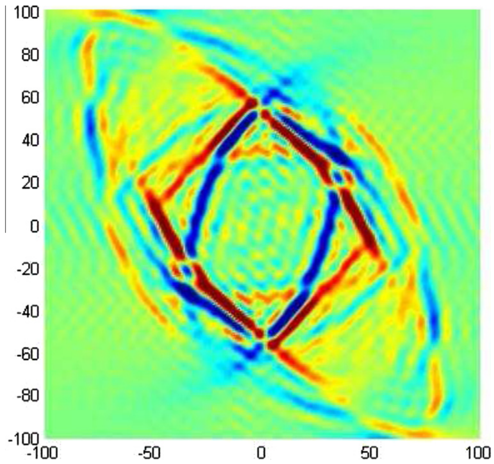

Fig. 7. The second component of the phason displacement $w_2^3(x_1, x_2, 0, t)$ at time $t = 5$ in Al-Mn-Pd.

The result of the computational experiment is presented in Figs. 1–7. Fig. 1 presents the third phonon displacement speed $V_3^3(0, x_2, x_3, 0.1) = U_3^3(0, x_2, x_3, 0.1)$ on the plane $x_1 = 0$ corresponding to source $\mathbf{E}^3\delta(x)\delta(t)$. Fig. 2 presents the second phason displacement speed $V_5^3(x_1, 0, x_3, 0.1) = W_2^3(x_1, 0, x_3, 0.1)$ on the plane $x_2 = 0$ corresponding to source $\mathbf{E}^3\delta(x)\delta(t)$. These images are the view from the top of the magnitude axis V_3^3 (i.e. the view of the surface $z = V_3^3(0, x_2, x_3, 0.1)$) and V_5^3 (i.e. the view of the surface $z = V_5^3(x_1, 0, x_3, 0.1)$), respectively.

Fig. 3 shows 2D level plot of dynamic distribution for the sixth component of the phonon stress $\sigma_6^3(x_1, x_2, 0, t)$ in the Al-Mn-Pd at $t = 0.1$, i.e. $V_{12}^3(x_1, x_2, 0, 0.1)$. Fig. 4 shows 2D level plot of dynamic distribution for the ninth component of the phason stress $H_{21}^3(x_1, 0, x_3, t)$ in the Al-Mn-Pd at $t = 0.1$, i.e. $V_{21}^3(x_1, 0, x_3, 0.1)$.

Figs. 5 and 6 present dynamic distribution of the first component of phonon displacement $u_1^3(x_1, 0, x_3, 0.1)$. Fig. 5 is the graph of the 3-D surface $u_1^3(x_1, 0, x_3, t)$ for $t = 0.1$. Here the horizontal axes are x_1 and x_3. The vertical axis is the magnitude of $u_1^3(x_1, 0, x_3, 0.1)$. Fig. 6 contain screen shot of 2-D level plot of the same surface $u_1^3(x_1, 0, x_3, 0.1)$, i.e. a view from the top of the magnitude axis u_1^3 (i.e. the view of the surface $z = u_1^3(x_1, 0, x_3, 0.1)$). Fig. 7 is 2D level plot of the second phason displacement $w_2^3(x_1, x_2, 0, t)$ at $t = 5$. This figure presents a view from the top of the magnitude axis $w_2^3(x_1, x_2, 0, 5)$ (i.e. the view of the surface $z = w_2^3(x_1, x_2, 0, 5)$).

7. Conclusion

In this paper dynamical equations of homogeneous anisotropic elastic media in 3D QCs have been written in the form of the symmetric hyperbolic system of the first order. To obtain FS of the phonon and phason displacements, displacement speeds and stresses the method which was proposed for elastodynamic problems of normal crystals in [25] has been applied. The robustness and correctness of the suggested method has been shown on the examples of isotropic crystals [25]. This method is based on the modern achievements of computational algebra which allows us to make computer applications. Using our method the simulations of phonon and phason displacements, displacement speeds and stresses of anisotropic elasticity in 3D QCs has been made at the same time. The results of simulation give a possibility to observe and analyze the elastic wave propagation in 3D QCs arising from pulse point sources of the form $E^m\delta(x_1)\delta(x_2)\delta(x_3)\delta(t)$.

Appendix

The matrix $\bar{C}$, defined by (14), is symmetric with real valued elements. Let us show that $\bar{C}$ is positive definite, i.e. the matrix $\bar{C}$ has to satisfy

$$\mathcal{V}^*\bar{C}\mathcal{V} > 0 \tag{32}$$

for arbitrary nonzero vectors $\mathcal{V} = (\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5, \varepsilon_6, w_{11}, w_{22}, w_{33}, w_{23}, w_{31}, w_{12}, w_{32}, w_{13}, w_{21}) \in R^{15}$.

We assume in Section 2 that $C_{ijkl}, R_{ijkl}, K_{ijkl}$ satisfy conditions (7) when the strain tensors ε_{ij}, w_{ij} are not zero entirely.

Using symmetry properties (4) and (6) and the rule (10) the first and third conditions in (7) can be written in the form

$$\sum_{i,j,k,l=1}^{3} C_{ijkl}\varepsilon_{ij}\varepsilon_{kl} = \sum_{\alpha,\beta=1}^{6} C_{\alpha,\beta}\varepsilon_\alpha\varepsilon_\beta > 0, \quad \sum_{i,j,k,l=1}^{3} R_{ijkl}\varepsilon_{ij}w_{kl} = \sum_{\alpha=1}^{6}\sum_{i,j=1}^{3} R_{\alpha,ij}\varepsilon_\alpha w_{ij} > 0, \tag{33}$$

where $\varepsilon_{11} = \varepsilon_1$, $\varepsilon_{22} = \varepsilon_2$, $\varepsilon_{33} = \varepsilon_3, 2\varepsilon_{23} = \varepsilon_4, 2\varepsilon_{13} = \varepsilon_5, 2\varepsilon_{12} = \varepsilon_6$ are arbitrary nonzero real numbers. And from (33) and the second condition in (7) we have

$$\mathcal{V}^*\bar{C}\mathcal{V} = \sum_{\alpha,\beta=1}^{6} C_{\alpha,\beta}\varepsilon_\alpha\varepsilon_\beta + 2\sum_{\alpha=1}^{6}\sum_{i,j=1}^{3} R_{\alpha,ij}\varepsilon_\alpha w_{ij} + \sum_{i,j,k,l=1}^{3} K_{ij,kl} w_{ij} w_{kl} > 0,$$

where $\mathcal{V} = (\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5, \varepsilon_6, w_{11}, w_{22}, w_{33}, w_{23}, w_{31}, w_{12}, w_{32}, w_{13}, w_{21}) \in R^{15}$ are arbitrary nonzero vectors.

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