The Structure Modeling of Material Composed of the Orthotropic Crystals*

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Abstract. In this paper the model of a elastic composite medium which consists of a matrix containing a set of orthotropic crystals with the random orientation of the anisotropy axes is presented. The axes orientation is described by the Gauss distribution. The numerical investigation is proposed for rectangular plate, when the normal strains are given in the one side. Other sides are free of strain. The finite - difference technique is used for model discretization.

Keywords: orthotropic crystals, elasticity moduli, shear moduli, isotropy, anisotropy, difference scheme.

1 Introduction

Modeling of short wave propagation process is of key importance for solution of very different problems [1, 2]. The measurement methods based on wave phenomena present an important and challenging field of wave modeling applications. Identification and recognition of defects in continuous structures, detection of impurity particles or coagulation centers in liquids, recognition of geometric shapes of objects by measuring reflections of waves, etc., can be mentioned as examples. The term “short wave” is actually the matter of a scale, however, it is

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usually understood that the length of the short wave is hundreds or thousands times less than the dimensions of the structure in which the propagation of the wave is analyzed. The inherent distortions of propagating short wave in discrete meshes usually are avoided by using very dense meshes that requires huge computational resources. The main difficulties arising in ultrasonic measurement process simulation are caused by: a) computational models of very large dimensionality, b) very large number of time integration steps, c) adequacy of continua-based models, to reality. We consider the ultrasonic wave propagation problem taking into account the structure of composites. More precisely, we examine a linearly elastic composite medium which consists of a matrix containing a set of orthotropic crystals with random by orientated anisotropy axes. To determine the effective elastic moduli we replace the composite medium by the homogeneous elastic structure. Results of the numerical investigation of the ultrasonic waves propagation and their interaction with a free boundary in 2-D case will be discussed.

2 Mathematical model

There were analyzed materials with granular structure. Materials grains during their technological processing are approximately oriented by special law. Let say that there is known distribution density of the crystal main directions. Let investigate plane case, which means that crystals are oriented in the plane (Fig. 1). The crystal orientation in the plane case is described by the vectors $l_3^\nabla = l_3$, $l_1^\nabla = \cos\theta \cdot l_1 + \sin\theta \cdot l_2,\ l_2^\nabla = -\sin\theta \cdot l_1 + \cos\theta \cdot l_2$, where l_1, l_2, l_3 being the orthonormed vectors.

In the case of the small deformation, the rheological equation of a single crystal is described by the double scalar product of elasticity and deformation moduli tensors $P^\nabla = c : \varepsilon$ (see [3]), here P^∇, c, ε are strain, elasticity and deformation moduli tensors, and symbol: means double scalar product of tensors c and ε. In the general case the rheological equation is nonlinear [3].

Suppose that elasticity moduli tensors of all the crystals are the same. Then the rheological equation is $P^\nabla = P_{ij}^\nabla l_i^\nabla l_j^\nabla$, $\varepsilon = \varepsilon_{ij} l_i l_j$, $c = c_{ijks} l_i^\nabla l_j^\nabla l_k^\nabla l_s^\nabla$, $\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$, here $u = u_i l_i$ is the point displacement vector during deformation. The equality $P^\nabla = c : \varepsilon$ can be changed by $P^\nabla = c_{ijks} l_i^\nabla l_j^\nabla \alpha_{sp}\alpha_{kq}\varepsilon_{pq}$. Define tensor $P = \int_{-\theta_1}^{\theta_1} f(\theta) P^\nabla(\theta) d\theta$, $\int_{-\theta_1}^{\theta_1} f(\theta) d\theta = 1$; here $f(\theta)$ is direction

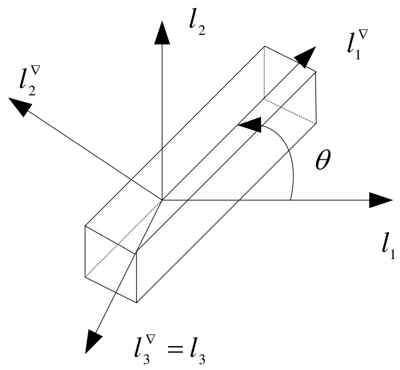

Fig. 1. The crystal orientation in the plane case.

density of the vector l_1^∇.

Then $P = l_n l_m \int_{-\theta_1}^{\theta_1} f(\theta)\alpha_{in}\alpha_{jm}\alpha_{sp}\alpha_{kq}d\theta \cdot c_{ijks}\varepsilon_{pq} = P_{nm}l_n l_m$. In the case of plane deformation we have $\varepsilon_{11} = \frac{\partial u_1}{\partial x_1},\ \varepsilon_{22} = \frac{\partial u_2}{\partial x_2}$, $2\varepsilon_{12} = \gamma_{12} = \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}$, $\varepsilon_{13} = \varepsilon_{31} = \varepsilon_{23} = \varepsilon_{32} = \varepsilon_{33} = 0,\ u_3 = 0$ and

$$\begin{aligned}
P_{nm} &= A_{11nm}\varepsilon_{11} + A_{22nm}\varepsilon_{22} + 2A_{12nm}\varepsilon_{12},\\
A_{11nm} &= \int_{-\theta_1}^{\theta_1} f(\theta)\alpha_{in}\alpha_{jm}\alpha_{s1}\alpha_{k1}d\theta \cdot c_{ijks},\\
A_{22nm} &= \int_{-\theta_1}^{\theta_1} f(\theta)\alpha_{in}\alpha_{jm}\alpha_{s2}\alpha_{k2}d\theta \cdot c_{ijks},\\
2A_{12nm} &= \int_{-\theta_1}^{\theta_1} f(\theta)\alpha_{in}\alpha_{jm}(\alpha_{s1}\alpha_{k2} + \alpha_{s2}\alpha_{k1})d\theta \cdot c_{ijks}.
\end{aligned}$$

Components of tensor P can be written as follows:

$$\begin{aligned}
&P_{11} = A_{1111}\varepsilon_{11} + A_{2211}\varepsilon_{22},\\
&P_{22} = A_{1122}\varepsilon_{11} + A_{2222}\varepsilon_{22},\\
&P_{21} = P_{12} = 2A_{1212}\varepsilon_{12} = A_{1212}\gamma_{12},\\
&P_{13} = P_{31} = P_{23} = P_{32} = P_{33} = 0, \quad A_{2211} = A_{1122}.
\end{aligned}$$

Equations of the linear elasticity theory read:

$$\begin{cases} \rho\dfrac{\partial^2 u_1}{\partial t^2} = \rho F_1 + A_{1111}\dfrac{\partial^2 u_1}{\partial x_1^2} + A_{1212}\dfrac{\partial^2 u_1}{\partial x_2^2} + (A_{2211} + A_{1212})\dfrac{\partial^2 u_2}{\partial x_1 \partial x_2}, \\ \rho\dfrac{\partial^2 u_2}{\partial t^2} = \rho F_2 + (A_{1212} + A_{1122})\dfrac{\partial^2 u_1}{\partial x_1 \partial x_2} + A_{1212}\dfrac{\partial^2 u_2}{\partial x_1^2} + A_{2222}\dfrac{\partial^2 u_2}{\partial x_2^2}. \end{cases} \tag{1}$$

Here F_1, F_2 are the components of earth acceleration, t – time and x_1, x_2 – point coordinates.

Let us investigate plane case, when the stab is to part of side right or sharp angle (Fig. 2).

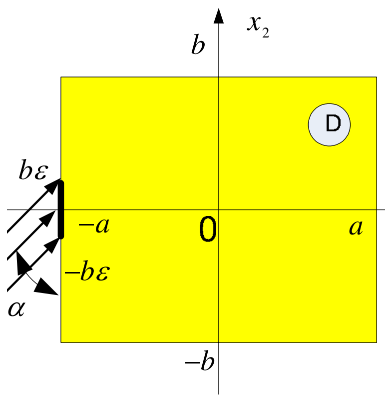

Fig. 2. Rectangular plate.

We do not take into account earth acceleration, id est, $F_1 = F_2 = 0$. Hence, equation (1) can be written in the dimensionless form:

$$\begin{cases} \dfrac{\partial^2 u_1}{\partial t^2} = \xi \cdot \left(A_{1111}\dfrac{\partial^2 u_1}{\partial x_1^2} + A_{1212}\dfrac{\partial^2 u_1}{\partial x_2^2} + (A_{2211} + A_{1212})\dfrac{\partial^2 u_2}{\partial x_1 \partial x_2} \right), \\ \dfrac{\partial^2 u_2}{\partial t^2} = \xi \cdot \left((A_{1212} + A_{1122})\dfrac{\partial^2 u_1}{\partial x_1 \partial x_2} + A_{1212}\dfrac{\partial^2 u_2}{\partial x_1^2} + A_{2222}\dfrac{\partial^2 u_2}{\partial x_2^2} \right), \end{cases}$$

here $\xi = \frac{T^2}{\rho \cdot L^2} \cdot 10^{14}$.

We investigated the ultrasonic waves propagation in rectangular plate and their interaction with a free boundary. Waves were generated by determining the normal strain, which was given in the small area of one side. We used the following boundary and initial conditions:

$$\left(A_{1111}\frac{\partial u_1}{\partial x_1}+A_{2211}\frac{\partial u_2}{\partial x_2}\right)\bigg|_{x_1=-a}=-\sin wt\cdot f(x_2)\cdot\sin\alpha,$$

$$\left(A_{1111}\frac{\partial u_1}{\partial x_1}+A_{2211}\frac{\partial u_2}{\partial x_2}\right)\bigg|_{x_1=a}=0,$$

$$x_2\in[-b\varepsilon,b\varepsilon],$$

where $f(x_2)=10^3\big((b\cdot\varepsilon)^2-x_2^2\big)$,

$$\left(A_{1111}\frac{\partial u_1}{\partial x_1}+A_{2211}\frac{\partial u_2}{\partial x_2}\right)\bigg|_{x_1=-a}=0,$$

$$\left(A_{1111}\frac{\partial u_1}{\partial x_1}+A_{2211}\frac{\partial u_2}{\partial x_2}\right)\bigg|_{x_1=a}=0,$$

$$x_2\in[-b,-b\varepsilon],\ x_2\in[b\varepsilon,b],$$

$$\left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)\bigg|_{x_1=-a}=0,$$

$$\left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)\bigg|_{x_1=a}=0,$$

$$x_2\in[-b,-b\varepsilon],\ x_2\in[b\varepsilon,b],$$

$$\left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)\bigg|_{x_1=-a}=-\sin wt\cdot f(x_2)\cdot\cos\alpha,$$

$$\left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)\bigg|_{x_1=a}=0,$$

$$x_2\in[-b\varepsilon,b\varepsilon],$$

$$\left(A_{2211}\frac{\partial u_1}{\partial x_1}+A_{2211}\frac{\partial u_2}{\partial x_2}\right)\bigg|_{x_2=-b}=0,$$

$$\left(A_{2211}\frac{\partial u_1}{\partial x_1}+A_{2222}\frac{\partial u_2}{\partial x_2}\right)\bigg|_{x_2=ab}=0,$$

$$x_1\in[-a,a],$$

$$\left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)\bigg|_{x_1=-b}=0,$$
$$\left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)\bigg|_{x_1=b}=0,$$
$$x_1\in[-a,a],$$

where $t>0$,

$$u_1(0,x_1,x_2)=0,\quad \frac{\partial u_1}{\partial t}(0,x_1,x_2)=0,\quad (x_1,x_2)\in\bar{D},$$
$$u_2(0,x_1,x_2)=0,\quad \frac{\partial u_2}{\partial t}(0,x_1,x_2)=0,\quad (x_1,x_2)\in\bar{D}.$$

3 Numerical solution

Analytical solutions of most problems exist only in the simplest cases. Most scientific and engineering problems comprised the complex geometrical and loading configurations that make the analytical solution impossible. In order to obtain a solution, a numerical technique must be employed. We used the finite-difference technique [4]. Let us introduce the following uniform grid:

$$u_1(t_n,x_{1i},x_{2j})=u_1(n,i,j)=\bar{u}_{ij}^n,\quad u_2(t_n,x_{1i},x_{2j})=u_2(n,i,j)=\bar{\bar{u}}_{ij}^n,$$
$$0\le i\le N_1,\quad 0\le j\le N_2,\quad 0\le n\le M,$$
$$x_{1i}=x_{10}+ih_1,\quad 0\le i\le N_1,\quad x_{10}=-a,\quad x_{1N_1}=a,$$
$$x_{2j}=x_{20}+jh_2,\quad 0\le i\le N_2,\quad x_{20}=-b,\quad x_{2N_2}=b,$$
$$t_n=n\tau,\quad 0\le n\le M.$$

We used an explicit scheme to obtain difference equations:

$$A_1=\xi A_{1111},\ A_2=\xi A_{1212},\ A_3=\xi(A_{2211}+A_{1212}),\ A_4=\xi A_{2222},$$
$$\frac{\bar{u}_{ij}^{n+1}-2\bar{u}_{ij}^n+\bar{u}_{ij}^{n-1}}{\tau^2}$$
$$=A_1\frac{\bar{u}_{i+1,j}^n-2\bar{u}_{ij}^n+\bar{u}_{i-1,j}^n}{h_1^2}+A_2\frac{\bar{u}_{i,j+1}^n-2\bar{u}_{ij}^n+\bar{u}_{i,j-1}^n}{h_2^2}$$
$$+A_3\frac{\bar{\bar{u}}_{i+1,j+1}^n-\bar{\bar{u}}_{i-1,j+1}^n-\bar{\bar{u}}_{i+1,j-1}^n+\bar{\bar{u}}_{i-1,j-1}^n}{4h_1h_2},$$

$$
\begin{aligned}
&\frac{\bar{\bar{u}}_{ij}^{n+1} - 2\bar{\bar{u}}_{ij}^{n} + \bar{\bar{u}}_{ij}^{n-1}}{\tau^2} \\
&\qquad = A_3 \frac{\bar{u}_{i+1,j+1}^{n} - \bar{u}_{i-1,j+1}^{n} - \bar{u}_{i+1,j-1}^{n} + \bar{u}_{i-1,j-1}^{n}}{4h_1h_2} \\
&\qquad\quad + A_2 \frac{\bar{\bar{u}}_{i+1,j}^{n} - 2\bar{\bar{u}}_{ij}^{n} + \bar{\bar{u}}_{i-1,j}^{n}}{h_1^2} + A_4 \frac{\bar{\bar{u}}_{i,j+1}^{n} - 2\bar{\bar{u}}_{i,j}^{n} + \bar{\bar{u}}_{i,j-1}^{n}}{h_2^2},
\end{aligned}
$$

here $1 \le i \le N_1 - 1,\ 1 \le j \le N_2 - 1,\ 1 \le n \le M - 1.$

Set: $\bar{\tau} = \frac{1}{\tau^2},\ \bar{h}_1 = \frac{A_1}{h_1^2},\ \bar{h}_2 = \frac{A_2}{h_2^2},\ \bar{h}_{12} = \frac{A_3}{4h_1h_2},\ \bar{\bar{h}}_2 = \frac{A_2}{h_1^2},\ \bar{\bar{h}}_4 = \frac{A_4}{h_2^2}.$

Then the system of difference equations reads:

$$
\begin{cases}
\bar{u}_{ij}^{n+1} = \dfrac{\bar{h}_1}{\bar{\tau}}\left(\bar{u}_{i+1,j}^{n} + \bar{u}_{i-1,j}^{n}\right) + \dfrac{\bar{h}_2}{\bar{\tau}}\left(\bar{\bar{u}}_{i,j+1}^{n} + \bar{\bar{u}}_{i,j-1}^{n}\right) \\
\qquad\quad + \dfrac{\bar{h}_{12}}{\bar{\tau}}\left(\bar{\bar{u}}_{i+1,j+1}^{n} - \bar{\bar{u}}_{i-1,j+1}^{n} - \bar{\bar{u}}_{i+1,j-1}^{n} + \bar{\bar{u}}_{i-1,j-1}^{n}\right) \\
\qquad\quad + \dfrac{2(\bar{\tau} - \bar{h}_1 - \bar{h}_2)}{\bar{\tau}}\bar{u}_{ij}^{n} - \bar{u}_{ij}^{n-1}, \\
\bar{\bar{u}}_{ij}^{n+1} = \dfrac{\bar{h}_{12}}{\bar{\tau}}\left(\bar{u}_{i+1,j+1}^{n} - \bar{u}_{i-1,j+1}^{n} - \bar{u}_{i+1,j-1}^{n} + \bar{u}_{i-1,j-1}^{n}\right) \\
\qquad\quad + \dfrac{\bar{\bar{h}}_2}{\bar{\tau}}\left(\bar{\bar{u}}_{i+1,j}^{n} + \bar{\bar{u}}_{i-1,j}^{n}\right) + \dfrac{\bar{h}_4}{\bar{\tau}}\left(\bar{\bar{u}}_{i,j+1}^{n} + \bar{\bar{u}}_{i,j-1}^{n}\right) \\
\qquad\quad + \dfrac{2\left(\bar{\tau} - \bar{h}_4 - \bar{\bar{h}}_2\right)}{\bar{\tau}}\bar{\bar{u}}_{ij}^{n} - \bar{\bar{u}}_{ij}^{n-1},
\end{cases}
$$

here $1 \le i \le N_1 - 1,\ 1 \le j \le N_2 - 1,\ 1 \le n \le M - 1.$

In the similar way we got approximation of the boundary and initial conditions. As the result we got:

$$
\begin{aligned}
&A_{1111}\frac{\bar{u}_{1j}^{n+1} - \bar{u}_{0j}^{n+1}}{h_1} + A_{2211}\frac{\bar{\bar{u}}_{0j+1}^{n+1} - \bar{\bar{u}}_{0j}^{n+1}}{h_2} = -\sin wn\tau \cdot f_j \cdot \sin\alpha, \\
&A_{1111}\frac{\bar{u}_{N_1j}^{n+1} - \bar{u}_{N_1-1,j}^{n+1}}{h_1} + A_{2211}\frac{\bar{\bar{u}}_{N_1,j+1}^{n+1} - \bar{\bar{u}}_{N_1j}^{n+1}}{h_2} = 0, \\
&\frac{\bar{u}_{0,j+1}^{n+1} - \bar{u}_{0j}^{n+1}}{h_2} + \frac{\bar{\bar{u}}_{1j}^{n+1} - \bar{\bar{u}}_{0j}^{n+1}}{h_1} = -\sin wn\tau \cdot f_j \cdot \cos\alpha, \\
&\frac{\bar{u}_{N_1,j+1}^{n+1} - \bar{u}_{N_1j}^{n+1}}{h_2} + \frac{\bar{\bar{u}}_{N_1j}^{n+1} - \bar{\bar{u}}_{N_1-1,j}^{n+1}}{h_1} = 0,
\end{aligned}
$$

when $1 \le j \le N_2 - 1,\ 1 \le n \le M - 1.$

$$A_{2211}\frac{\bar{u}_{i+1,0}^{n+1} - \bar{u}_{i0}^{n+1}}{h_1} + A_{2222}\frac{\bar{\bar{u}}_{i1}^{n+1} - \bar{\bar{u}}_{i0}^{n+1}}{h_2} = 0,$$
$$A_{2211}\frac{\bar{u}_{i+1,N_2}^{n+1} - \bar{u}_{iN_2}^{n+1}}{h_1} + A_{2222}\frac{\bar{\bar{u}}_{iN_2}^{n+1} - \bar{\bar{u}}_{i,N_2-1}^{n+1}}{h_2} = 0,$$
$$\frac{\bar{u}_{i1}^{n+1} - \bar{u}_{i0}^{n+1}}{h_2} + \frac{\bar{\bar{u}}_{i+1,0}^{n+1} - \bar{\bar{u}}_{i,0}^{n+1}}{h_1} = 0,$$
$$\frac{\bar{u}_{iN_2}^{n+1} - \bar{u}_{i,N_2-1}^{n+1}}{h_2} + \frac{\bar{\bar{u}}_{i+1,N_2}^{n+1} - \bar{\bar{u}}_{i,N_2}^{n+1}}{h_1} = 0,$$

when $1 \le j \le N_1 - 1,\ 1 \le n \le M - 1,$

$$\bar{u}_{ij}^0 = 0, \quad \bar{\bar{u}}_{ij}^0 = 0,$$
$$\frac{\bar{u}_{ij}^{n+1} - \bar{u}_{ij}^n}{\tau} = 0, \quad \text{when} \quad n = 0, \quad \text{we get} \quad \bar{u}_{ij}^1 = \bar{u}_{ij}^0,$$
$$\frac{\bar{\bar{u}}_{ij}^{n+1} - \bar{\bar{u}}_{ij}^n}{\tau} = 0, \quad \text{when} \quad n = 0, \quad \text{we get} \quad \bar{\bar{u}}_{ij}^1 = \bar{\bar{u}}_{ij}^0,$$

when $1 \le j \le N_1,\ 0 \le j \le N_2.$

4 Results of calculations and discussion

We examined isotropy and anisotropy cases. In the first case, when $E_1 = E_2 = 2.3$ we got the following wave movement (Fig. 3).

By stab into the rectangular plate left side the wave dynamics is similar to that of experiments. The wave spread with cylindrical wave elements was observed. When the wave reached the free right side of the plate and began coming back we noticed the wave fissure.

The same analysis was made for the anisotropy case (there were chosen different values of the elasticity moduli) with stab of $\frac{\pi}{4}$. In this case the wave dynamics changes, that is the wave fissure is observed before the wave reaches the right side of the plate (Fig. 4).

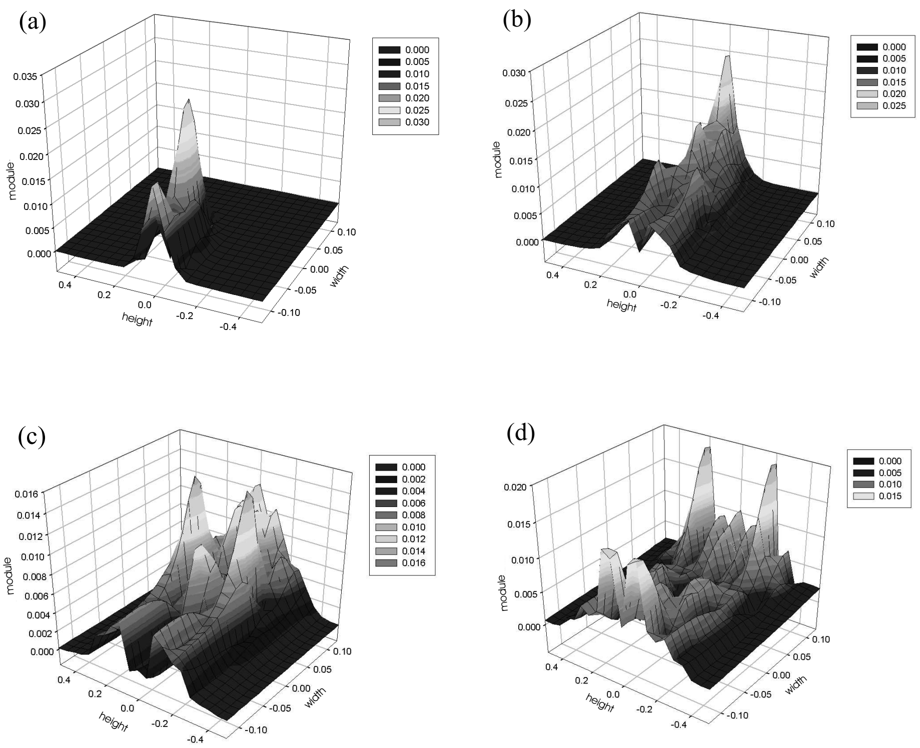

Fig. 3. Wave movement to the free right side of the pate and coming back: (a) wave reached the middle of the plate; (b) wave reached the right side of the plate; (c) the wave coming back; (d) wave reached left side of the plate.

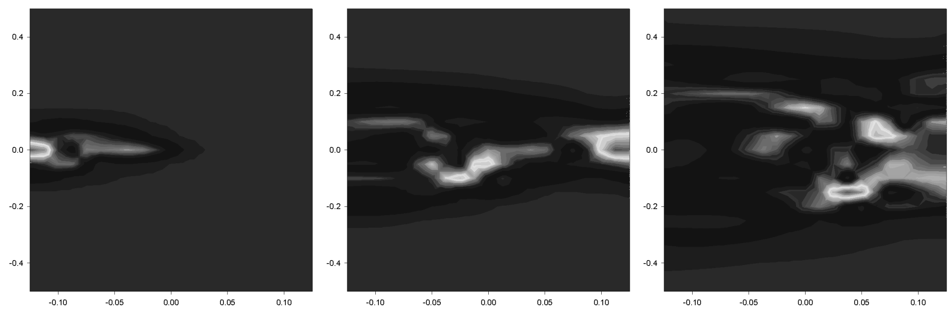

Fig. 4. Dynamics of the wave in the anisotropy case with stab by the sharp angle.

5 Conclusions

1. In the isotropy and anisotropy cases when the stab is right the results of computer modeling are similar to those of the real experiments.

2. The mathematical model with the stab by a sharp angle needs more detail investigation.

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