Numerical modeling of anisotropic properties of a solid by particle dynamics method

D Ya Sukhanov, A E Kuzovova
National Research Tomsk State University, Tomsk, Russia
E-mail: sdy@mail.tsu.ru

Abstract. A method is proposed for the numerical simulation of acoustic processes in solids based on the particle dynamics approach for describing the anisotropic properties of a solid. It is proposed to consider a solid body in the form of an array of particles located in a cubic body-centered crystal lattice. To set the anisotropic properties of a solid, it is proposed to use its own proportionality force to shift coefficient for each direction. Based on the results of numerical simulation, the dependence of the longitudinal wave velocity on the direction is shown.

1. Introduction
One of the widespread methods of numerical modeling of acoustic processes in solids is the method of finite differences in the time domain [1, 2]. This method is based on discretization of differential wave equation in space and time. The particle dynamics method is widely used to describe the behavior of particles [3]. In the method of particle dynamics, the medium under consideration is represented as a set of interacting particles (material points or solids), for which the classical equations of dynamics are written. The interaction of particles is described by means of interaction potentials, the main property of which is repulsion when approaching and attraction when moving away.

The advantage of the particle dynamics method in comparison with methods based on the representation of the medium as a continuous one is that it requires significantly fewer a priori assumptions about the properties of the material. Considering the interaction of particles only through the simplest interaction potential (for example, of the Lennard-Jones type) [4, 5] and insignificant dissipation, it is possible to simulate such complex effects as plasticity, cracking, fracture, temperature change in material properties, phase transitions [6, 7]. To describe these effects in the framework of a continuous medium, a separate theory is needed for each of the effects, while in molecular dynamics modeling; these effects are obtained automatically, as a result of integrating the equations of motion.

Anisotropy during the propagation of acoustic waves in matter is characteristic of solid crystalline bodies. It is proposed to simulate the anisotropic properties of a solid in a particle model by specifying different dependences of the interaction forces on shear for each direction. In this work, only the longitudinal forces of interaction between particles are considered, however, the model does not exclude the possibility of taking into account the shear forces.
2. Method description

In this paper, it is proposed to use the particle dynamics method to model the anisotropic properties of a solid, representing a solid in the form of a set of interacting particles located in a cubic body-centered crystal lattice. In such a crystal lattice, each particle has 14 nearest neighbors: 6 at a distance $d$ and 8 at a distance $d\sqrt{3}/2$ (Figure 1).

![Figure 1. Body-centered cubic crystal lattice cell.](image)

Each particle in the crystal lattice has its own mass $m = \rho d^3 / 2$ depending on the density of the substance under consideration $\rho$, the step of placing particles in the crystal lattice $d$ ($d^3$ – the volume of the cube, divided by 2 due to the presence of particles in the center of each cube, which leads to a doubling of the total number of particles).

The elastic properties of a substance are determined by the dependence of the force of interaction between particles on the distance. We consider linear dependence of force on shift in approximation of small deformations. For each particle, its acceleration is calculated according to Newton's law as the ratio of the applied force to the particle mass. The speed and coordinate of the particle are calculated by numerical integration of its acceleration over time. A change in the coordinate of a particle entails a change in the force applied to it due to interaction with neighboring particles. This interaction provides the possibility of propagation of acoustic waves in the system under consideration.

Particle mass and interaction force determine the type of material. The force of interaction depends on the distance between particles, but the main influence is exerted by the dependence of the force of interaction near the equilibrium point.

We describe the force interaction between particles by the function $F(x)$ where $x$ - is the distance between particles. On distance $d$ or $d\sqrt{3}/2$ particles from each other are in a state of stable equilibrium and are not affected by forces from their neighbors.

The dependence of the force of attraction between particles on the distance is proposed to be characterized by the following formula:

$$F(x) = k_n(x - R)$$  \hspace{1cm} (1)

where $R$ – is the equilibrium distance between particles ($R = d$ or $R = d\sqrt{3}/2$), $x$ – actual distance between particles, $k_n = c_n^2m / R^2$ – proportionality coefficient between force and distance in linear approximation in N/m, $n$ – is the number of neighboring particles symmetric pair, $c_n$ – the speed of sound in the medium for specific direction. The value of the coefficient $k$ follows from the
reduction of the one-dimensional model of interacting particles to the wave equation. In formula (1), the value of the coefficient \( k \) is specified for each pair of interacting particles. We consider that two opposing particles had the same force coefficient \( k_n \) to ensure pulse preservation law. If \( k_n \) is different in different directions than it should allow to simulate anisotropic waves propagation in the media. On the Figure 2 is shown the placement of 14-n neighboring particles with coefficients \( k_n \) that corresponds to each of them.

![Figure 2. Placement of particles and the corresponding coefficients of interaction with the central particle.](image)

3. Numerical modeling
In the model under consideration, each particle has 14 neighboring particles. Since the interaction coefficient \( k_n \) is the same for opposing particles, there are only 7 independent values of the \( k_n \) coefficients. The anisotropy of a rigid body is taken into account by setting different proportionality coefficients for different directions.

In order to test the possibility of modeling wave processes in an anisotropic medium, the modeling of the structure was carried out, which is a body-centered lattice, consisting of 161040 particles. Distance between particles (grid step) \( R =50 \) mkm time step \( dt = 2.5 \) ns. A spherical wave of short-pulse source was generated from the middle of the simulated volume. For computation of \( k_1 \) we considered \( c =6000 \) m/s, \( \rho = 2500 \) kg/m\(^3\).

An isotropic source in the form of a symmetric shift of particles from the center was considered as an introduced source. The shift of particles decreased with distance according to the Gaussian function with a half-width of 2 mm. At the initial moment of time, a shift is introduced, and then the process of numerical simulation of particle dynamics is started. Introducing an initial offset is equivalent to applying a short pulse.

If we take into account that 6 neighboring particles are located at a distance \( d \), and 8 particles are at a distance \( d\sqrt{3}/2 \), then the equality of all coefficients will not ensure complete isotropy of the medium. For isotropy, it is necessary to provide a ratio between the coefficients \( k_{1-3} \) and \( k_{4-7} \) as \( 2/3 \). Numerical simulation was carried out for the case when all coefficients are the same (Figure 3a) for simulation time 4 mks. It can be seen that the wave is propagated with different speed in different directions that indicates on anisotropy.
At the same time, we modeled the case when there is no interaction between particles along the coordinate axes $k_{1-3} = 0$. The simulation results for 7.5 mks are shown in Figure 3b. In this case, the amplitude of the longitudinal wave depends on the direction, which also indicates anisotropy.

Figure 3. Distribution of particles velocity after short pulse isotropic source introduced. The red color represents X component of particle velocity; the green color – Y component; the green color – Z component; (a – the case of the media with $k_1 = k_2 = k_3 = k_4 = k_5 = k_6 = k_7$; b – the case of the media with $k_1 = k_2 = k_3 = k_4 = k_5 = k_6 = k_7 \neq 0$)

Figure 4 shows the spatial distribution of particle velocity after 3750 ns of simulated time for two different types of anisotropic media. It can be seen that the field of an initially isotropic source was transformed into a wave propagating at different speeds in different directions. This indicates the anisotropic nature of the simulated medium.

With an increase in the interaction coefficient $k_n$, the speed of propagation of waves in the corresponding direction increases. We mainly consider longitudinal waves in a particle system. But transverse waves also arise due to interactions $k_{4-7}$, the speed of transverse waves is significantly less than the speed of longitudinal ones.

It should be noted that the model of particle dynamics is not limited to the body-centered crystal lattice we have considered with longitudinal interaction forces. It is possible to introduce transverse forces of interaction; consideration of more neighboring particles; change in the crystal lattice. An increase in the number of model parameters allows considering a wider class of acoustic effects. The advantage of the particle dynamics method is the possibility of embedding it in the simulation of the macroscopic motion of solids, the simplicity of describing the interaction of several bodies, various states of aggregation within the framework of one model.
**Figure 4.** Distribution of particles velocity after short pulse isotropic source introduced. The red color represents X component of particle velocity; the green color – Y component; the green color – Z component; (a – the case of the media with $k_1 = k_3 = k_4 = k_5 = k_6 = k_7$ and $k_2 = k_1/2$; b – the case of the media with $k_1 = k_3 = k_4 = k_5 = k_6 = k_7$ and $k_2 = 2k_1$.)

### 4. Conclusion

A method is proposed for the numerical simulation of the propagation of acoustic waves in anisotropic media based on the dynamics of interacting particles. A body-centered crystal lattice is considered. A linear dependence of the force of interaction between neighboring particles on the shift from the equilibrium position is assumed. Each particle has 14 neighbors. Due to the need to fulfill the law of conservation of momentum, it is necessary that the interaction for opposing particles be described in the same way, so there are 7 coefficients left to describe the anisotropy of the medium. Numerical modeling has shown the possibility of modeling waves in the structure under consideration.

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