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Dispersion properties of the phononic crystal consisting of ellipse-shaped particles

I.S. Pavlov^{a,b,*}, A.A. Vasiliev^c, A.V. Porubov^{d,e,f}^a Mechanical Engineering Research Institute of the Russian Academy of Sciences, 85, Belinsky str., 603024, Nizhny Novgorod, Russia^b Nizhny Novgorod Lobachevsky State University, 23, Gagarin av., 603950, Nizhny Novgorod, Russia^c Department of Mathematical Modelling, Tver State University, Sadoviy per. 35, 170002 Tver, Russia^d Institute of Problems in Mechanical Engineering, Bolshoy 61, V.O., Saint-Petersburg 199178, Russia^e St. Petersburg State University, 7-9, Universitetskaya nab., V.O., Saint-Petersburg 199034, Russia^f St. Petersburg State Polytechnical University, Polytechnicheskaya st., 29, Saint Petersburg 195251, Russia

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ABSTRACT

A two-dimensional model is considered in the form of a phononic crystal having a rectangular lattice with elastically interacting ellipse-shaped particles possessing two translational and one rotational degrees of freedom. The linear differential-difference equations are obtained by the method of structural modeling to describe propagation of longitudinal, transverse and rotational waves in the medium. It is found analytically how the coefficients of the equations depend on the sizes of the particle and on the parameters of interactions between them. The dispersion properties of the model are analyzed. Existence of a backward wave is established. The threshold frequencies of acoustic and rotational waves in some crystalline materials with cubic symmetry are estimated.

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1. Introduction

In recent years, **metamaterials** or composite materials with unique physical and mechanical properties due to their microstructure, have become more widely applied [1]. The models of these materials are composed not of the material points, but of the bodies of small size having internal degrees of freedom (fullerenes, molecular clusters, nanotubes, granules, grains, domains, and etc.). In particular, the *photonic* and *phononic* crystals are the good examples of metamaterials [2–4].

The term “photonic crystals” appeared in the early 1990s for media having a periodic system of dielectric inhomogeneities giving rise to emergence of zones opaque both for light and electromagnetic waves [5]. From a general viewpoint, a photonic crystal is a superlattice or a medium, in which an additional field has been artificially created, and its period is of some orders greater than the basic lattice period. The behavior of photons is radically different from their behavior in the ordinary crystal lattice if the optical superlattice period is comparable with the length of the electromagnetic wave. They do not transmit the light with a wavelength comparable with the lattice period of the photonic crystal and determine the effect

* Corresponding author at: Mechanical Engineering Research Institute of the Russian Academy of Sciences, 85, Belinsky str., 603024, Nizhny Novgorod, Russia.

E-mail addresses: ispavlov@mail.ru (I.S. Pavlov), alvasiliev@yandex.ru (A.A. Vasiliev), alexey.porubov@gmail.com (A.V. Porubov).

of the light localization. Photonic lattices are in the gap between the atomic crystal lattices and the macroscopic artificial periodic structures.

Subsequently, natural or artificial periodic structures became known as “phononic” crystals (acoustic superlattices) by analogy if they consist of non-pointwise particles, in which the length of the acoustic waves is comparable with the lattice period [2,6–8]. The velocity of propagation of elastic waves in solids is about 10^5 times less than the light wave velocity. Therefore all effects inherent to photonic crystals should take place in acoustics but for significantly lower frequencies. High interest in materials of this type is caused by the unique properties of the materials that enable one to apply them in many fields, primarily, in nanoelectronics. The ordering of the geometric structure is typical for the periodic (crystalline) media. It is a decisive factor leading to anisotropy of the properties of crystals and to the predominance of the collective motions of the wave type in the crystal lattice [9]. Some features of thermal conductivity behavior associated with passing of acoustic phonons, were detected at low temperatures in such phononic crystals as synthetic opals [6,10].

Recently, a “photon-phononic crystal” was created from the silicon nanorods in California Institute of Technology. This crystal is capable to localize the light and mechanical vibrations simultaneously. The authors called it the “optomechanical crystal” [11,12]. According to [11,12], optomechanical crystals can be useful in quantum computers, as they are able to “encode” the light information into mechanical vibrations and back, but at other frequencies. Also they may be used for creation of ultrasensitive biological and chemical sensors, as well as in experiments on detection of quantum effects at the macro-level.

The dependence of physical and mechanical properties of such materials on their microstructure is the most important subject for studies for the last two decades due to the development of nanotechnology, when the control of the material structure has become possible at the level of individual molecules and even atoms. However, it is rather difficult to carry out such investigations without models adequately describing physical and mechanical properties of metamaterials.

Mathematical models of advanced materials should take into account the presence of several medium scales (structural levels), their self-consistent interaction and the ability to transfer an energy from one level to another [13,14]. The method of structural modeling is appropriate for elaboration of such models [15–19] since it provides deep multi-level (multi-scale) penetration into the material. The material is represented by a regular or a quasi-regular lattice of the finite-size particles. Elaboration of a structural model starts from selection of some minimal volume – a structural cell (analog of a periodicity cell in a crystal) in a material that is capable of characterizing the basic features of the macroscopic behavior [20]. As a rule, the structural cell represents a particle, whose behavior is characterized by an interaction with the environment and is described by the kinematic variables. The granules, grains, domains, fullerenes, nanotubes, clusters of nanoparticles may play the role of the cells. In contrast to the point objects, the structural cells possess both translational and rotational degrees of freedom, and the kinematic features of the model become richer [21]. For example, taking into account the microrotations with respect to the mass centers of the particles leads to an appearance of a microrotation waves in microstructured media.

The force interaction between the particles of the medium is described by the model potentials used in the molecular mechanics and in the solid state physics. The presence of finite-size elements in a lattice enables one to introduce rather simply central and couple interactions between the particles [22]. Then the kinetic and potential energies are derived in the discrete form.

As distinct from the phenomenological models of generalized continua [23,24], the structural models directly contain the parameters of the microstructure of a medium (the lattice period, the size and shape of the particles in the lattice, as well as the parameters of the force and couple interactions). The last ones define effective elastic constants of various orders. The relations between the structure of the lattice and the macroparameters of a medium open up the possibility of purposeful design of materials with desired properties [25].

Transformation from a discrete model to a continuum one is suitable when the long-wavelength processes are studied [26,27]. In this case, a comparison of the elaborated model with the well-known continuum theories becomes possible. For the short-wavelength processes, it is necessary either to remain within a discrete model, or to pass to a generalized continuum model, for example, in the framework of the multi-field approach [28] or on the base of Pade approximations [29,30]. At present, the properties of acoustic waves of different types, both bulk and surface, are studied in two- and three-dimensional artificial composite materials [8,10].

In this paper, a new discrete lattice model for microstructured material is developed that consists of anisotropic ellipse-shaped particles. Use of the method of structural modeling allows us to find out new effects due to the elliptical form of the particles. In particular, a backward wave will be shown to exist in the medium for some values of the microstructure parameters. An influence of the microstructure of the crystal on its dispersion properties is also studied, and theoretical estimates of the threshold frequencies of the acoustic and optical phonons are obtained for some crystals with cubic symmetry. The main goal of this work is creation of a theoretical basis for modeling of artificial periodic structures consisting of particles of non-zero size comparable with the wavelengths of the considered phenomena. The structures possess predetermined dispersion properties.

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