Published in final edited form as:

Phys Rev E Stat Nonlin Soft Matter Phys. 2012 June ; 85(6 Pt 1): 061923.

Effective medium theory of elastic waves in random networks of rods

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Abstract

We formulate an effective medium (mean field) theory of a material consisting of randomly distributed nodes connected by straight slender rods, hinged at the nodes. Defining novel wavelength-dependent effective elastic moduli, we calculate both the static moduli and the dispersion relations of ultrasonic longitudinal and transverse elastic waves. At finite wave vector k the waves are dispersive, with phase and group velocities decreasing with increasing wave vector. These results are directly applicable to networks with empty pore space. They also describe the solid matrix in two-component (Biot) theories of fluid-filled porous media. We suggest the possibility of low density materials with higher ratios of stiffness and strength to density than those of foams, aerogels or trabecular bone.

I. INTRODUCTION

Many materials of biomedical or technological interest [1] contain a network of slender elastic rods with hinged connections at irregularly or randomly distributed nodes. In some cases the material may consist only of the network, while in others, such as trabecular bone, the space between the rods may be filled with fluid. Calculation of the elastic and acoustic properties of such a random network requires a statistical model. There have been extensive studies of fluid-filled networks ([2–7]) but these have generally concentrated on the interaction between the matrix and the pore fluid, while treating the matrix as a simple homogenous material.

The mechanical properties of networks of elastic rods are sensitive functions of their geometry. For example, simple cubic lattices have bulk moduli that scale as the volumetric filling factor ϕ of the rods but have zero stiffness to shear along the lattice planes, while in FCC and BCC lattices all moduli scale $\propto \phi$. The moduli of open-celled foams scale $\propto \phi^2$ while those of closed-cell foams scale $\propto \phi^3$ [1]. In general, if a deformation requires extension or compression of rods the corresponding modulus scales $\propto \phi$, but if it is resisted only by rod flexure or by the resistance of the nodes to changes in the rod angles the moduli

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scale as a higher power of κ^{-7} . Foams are soft because they can deform by bending their thin members without extension, changing angles at nodes or cell junctions with little resistance.

Here we develop an elementary effective medium model of the elastic properties of a statistically isotropic matrix consisting of thin elastic rods joined by hinges at randomly distributed nodes. This is surely an oversimplified description of a real material, as any analytic model of a random material must be, but may provide a useful guide to and parametrization of its properties. Statistical modeling is necessary because the full three-dimensional structure of a solid consisting of irregularly located and connected nodes is unlikely to be known quantitatively and likely varies from realization to realization. In a biomaterial like cancellous bone it may vary from individual to individual, and within a single bone in a single individual. Even in statistically homogeneous foams it depends on details of their preparation.

By connecting nodes of mean coordination number $C = D$, where D is the dimensionality, with straight rods that terminate on the nodes, we construct a model in which (except for pathological cases like a simple cubic lattice) strain implies changes in the distances between nodes that are first order in the strain, and hence extensions of the rods of that order. The resulting structure is stiffer than open or closed cell foams such as expanded polymers, aerogels, hydrogels, sponges and spongy (trabecular or cancellous) bone in which rods or cell edges join at points along their lengths [1]. In our model stiffness is derived from the resistance of the rods to extension, rather than to bending; the former is much greater for slender rods. In contrast to structures near the isostaticity limit [8–10], the nodes are overconstrained. The great stiffness of structures like those we model may have practical utility.

Within this model we calculate the dispersion of longitudinal and transverse elastic waves at finite wave vectors, where heterogeneity is significant. In this non-dissipative and non-local model dispersion is a consequence and measure of the inhomogeneous spatial structure (nonlocality invalidates one of the assumptions of the Kramers-Kronig relations). The dispersion relations, functions of a single scalar variable (the magnitude of the wave-vector), are a compact description of a complex three-dimensional structure.

II. THE MODEL

The model consists of nodes randomly, but statistically uniformly, distributed in space with a mean density n . In contrast to the related problems of the description of vibrations in a solid in which massive atoms are connected by massless elastic rods or springs [11], or a granular material in which grains are pressed into frictional contact [12], in our model the nodes are massless and serve only as geometric constraints on the rods connecting them. Each node is connected to an average of C (the coordination number) nearest neighbor nodes by uniform and identical (except for length) elastic rods that are hinged at the nodes. We expect the discrete random structure to approach the continuum (effective medium) model as $C \rightarrow \infty$. We present results for $C = 4$ and $C = 12$ to show the dependence of the model on C . Even $C = 4$ is well above the matrix's isostaticity threshold [8–10], and is sufficient to assure its stiffness against shear.

The distribution of distances ℓ_i to the i -th nearest neighbor of a node is obtained from an Erlang distribution (Gamma distribution for integer index) for the volume V_i enclosed by a sphere of radius ℓ_i containing its i nearest neighbors:

$$P_V(V_i) = \frac{V_i^{i-1} n^i \exp(-nV_i)}{\Gamma(i)}. \quad (1)$$

The probability distribution of ℓ_i is

$$P_\ell(\ell_i) = 4\pi \ell_i^2 P_V(V_i), \quad (2)$$

where $\ell_i = (3 V_i / 4\pi)^{1/3}$.

Fig. 1 shows one realization of a network of rods in a unit cube connecting randomly distributed nodes. The nodes have a mean density $n = 250$ and mean coordination number $C = 12$.

In a microscopic realization of randomly distributed nodes, such as that shown in Fig. 1, it is not possible to enforce the condition that all nodes have the same coordination number; if node j' is the C -th nearest neighbor of node j , to which it is connected, node j may (for example) be the $C + 1$ -st nearest neighbor of node j' . Such complications are ignored, by definition, in an effective medium theory, in which C may be regarded as a *mean* coordination number.

We consider the dispersion relations of elastic waves in this medium of thin straight massive elastic rods connecting massless nodes, with the rods completely hinged (free to change direction and to rotate about their axes) at the nodes. The effective medium model describes the motion of the nodes by a sinusoidal plane wave. The latter approximation is valid in the limit $kn^{-1/3} \rightarrow 0$, but breaks down for short waves with $kn^{-1/3} \gtrsim \pi$, for which scattering and localized modes are also important [13, 14]. In the limit of small amplitude (an assumption made throughout) compressive loads are below the rods' Euler buckling thresholds.

The fundamental equations for a small amplitude plane longitudinal wave propagating in the x direction in an infinite medium are

$$\frac{\partial v_x}{\partial t} = - \frac{1}{\rho_0} \frac{\partial \sigma_{xx}}{\partial x} \quad (3)$$

$$\frac{\partial u_{xx}}{\partial t} = - \frac{\partial v_x}{\partial x}, \quad (4)$$

where σ_{xx} is the xx component of the stress tensor, $u_{xx} \ll 1$ is the xx component of the strain tensor describing the elastic wave, v_x is the x component of material velocity and ρ_0 is the mean density (including void space) of the matrix. In an effective medium model we consider σ_{xx} , u_{xx} and v_x to be continuous functions of space, as they would be in a continuous medium. The wave variables v_x/c_0 and $\sigma_{xx}/\mathcal{B}(k)$ are of the same order of smallness as u_{xx} , where c_0 is the thin fiber longitudinal sound speed of the rods and $\mathcal{B}(k)$ is the effective longitudinal modulus (defined below) of the matrix.

These equations are closed with a constitutive relation

$$\sigma_{xx} = \mathcal{B}_\ell(k) u_{xx}, \quad (5)$$

where the effective longitudinal modulus $\mathcal{B}(k)$ is independent of space in an effective medium theory, but depends on the mechanical properties of the rods and is a nontrivial function of their spatial structure and of the wave vector k (a scalar in an isotropic

effective medium). By taking $\mathcal{B}_\ell(k)$ to be real the model is lossless by assumption. A dissipative model could be defined by taking $\mathcal{B}_\ell(k)$ to be complex or, equivalently, by adding a term $\mathcal{B}'_\ell(k)\dot{u}_{xx}$ to Eq. 5.

The modulus is defined by the relation

$$\varepsilon_{el} = \frac{1}{2} \mathcal{B}_\ell(k) u_{xx}^2, \quad (6)$$

where the elastic energy density ε_{el} is obtained by calculating the elastic energy added to the rods by the strain field $u_{xx}(x, t)$.

The resulting wave equation

$$\frac{\partial^2 v_x}{\partial t^2} - \frac{\mathcal{B}_\ell(k)}{\rho_0} \frac{\partial^2 v_x}{\partial x^2} = 0 \quad (7)$$

has solutions

$$v_x = v_{x0} \exp i(kx \pm \omega t), \quad (8)$$

with the dispersion relation

$$v_{ph} = \frac{\omega}{k} = \sqrt{\frac{\mathcal{B}_\ell(k)}{\rho_0}}. \quad (9)$$

For infinitesimal displacements of a hinged straight rod's endpoints it remains straight and below its buckling limit, so that its elastic energy is that of stretching. For slender rods, bending and torsional energy may be ignored even if the nodes are not hinged. Taking a cross-section A , Young's modulus E and equilibrium length ℓ stretched by an amount (not positive-definite) $\Delta\ell$ satisfying $|\Delta\ell| \ll \Delta\ell$, the elastic energy is

$$\varepsilon_{rod} = \frac{(\Delta\ell)^2 AE}{2\ell}. \quad (10)$$

We describe a longitudinal elastic wave of amplitude a propagating in an infinite medium in the x direction with wave vector $k\hat{x}$ by a displacement field

$$u_x(x) = a \sin(kx + \varsigma), \quad (11)$$

corresponding to a strain field

$$u_{xx} = ak \cos(kx + \varsigma). \quad (12)$$

The difference in x -displacements of the ends of a rod, one end of which defines $x = 0$ and the other is at $x = \ell \cos \theta + \delta u_x$, where θ is the angle between the unstrained rod and the x axis, is

$$\delta u_x = a[\sin(k\ell \cos \theta + \varsigma) - \sin \varsigma]; \quad (13)$$

$\delta u_y = \delta u_z = 0$. The choice of one end of the rod as defining $x = 0$ is equivalent to a choice of phase ς ; either may be chosen freely if, in the computation of total elastic energy and modulus, an average is taken over the other.

The rod undergoes a change in length (to first order in a)

$$\Delta\ell = \sqrt{\ell^2 \sin^2\theta + (\ell \cos\theta - \delta u_x)^2} - \ell \quad (14)$$

$$\approx \cos\theta \delta u_x \quad (15)$$

$$\approx a \cos\theta [\sin(k\ell \cos\theta + \varsigma) - \sin\varsigma]. \quad (16)$$

Its elastic energy is

$$\varepsilon_{rod} = \frac{AE}{2\ell} \cos^2\theta \delta u_x^2 = \frac{AE}{2\ell} a^2 \cos^2\theta [\sin(k\ell \cos\theta + \varsigma) - \sin\varsigma]^2. \quad (17)$$

The mean elastic energy per volume is

$$\varepsilon_{el} = n \frac{C}{2} \frac{AEa^2}{2} \left\langle \frac{\cos^2\theta}{l} [\sin(k\ell \cos\theta + \varsigma) - \sin\varsigma]^2 \right\rangle_{\varsigma, \theta, l} \equiv \frac{1}{2} \mathcal{B}_\ell(k) \langle u_{xx}^2 \rangle, \quad (18)$$

where the factor of $n \frac{C}{2}$ allows for the presence of two rods per node of coordination number C .

For the sinusoidal wave (12)

$$\langle u_{xx}^2 \rangle = \frac{1}{2} a^2 k^2 \quad (19)$$

and

$$\mathcal{B}_\ell(k) = nC \frac{AE}{k^2} \left\langle \frac{\cos^2\theta}{l} [\sin(k\ell \cos\theta + \varsigma) - \sin\varsigma]^2 \right\rangle_{\varsigma, \theta, l}. \quad (20)$$

The dispersion relation (9) becomes

$$\omega = \sqrt{\frac{2E}{\langle \ell \rangle_{\rho m}} \left\langle \frac{\cos^2\theta}{l} [\sin(k\ell \cos\theta + \varsigma) - \sin\varsigma]^2 \right\rangle_{\varsigma, \theta, l}}, \quad (21)$$

where $\rho_0 = n \frac{C}{2} A \langle \ell \rangle \rho_m$ and ρ_m is the material density of the rods. The coordination number enters only through the average over ℓ which is weakly dependent on C at finite $kn^{-1/3}$.

The long wavelength limit is:

$$\lim_{k \rightarrow 0} \mathcal{B}_\ell(k) \rightarrow \frac{\mathcal{F}}{5} E, \quad (22)$$

independent of C , where the volumetric filling factor

$$\mathcal{F} \equiv \frac{\rho_0}{\rho_m} = \frac{1}{2} n C A \langle \ell \rangle. \quad (23)$$

The dispersion relation in this limit is

$$\frac{\omega}{k} \rightarrow \sqrt{\frac{E}{5\rho_m}} = \frac{v_{rod}}{\sqrt{5}}, \quad (24)$$

where $v_{rod} \equiv \sqrt{E/\rho_m}$ is the phase and group velocity of the longitudinal wave in an individual rod in the (non-dispersive) thin-rod limit.

The derivation has assumed $\mathcal{A} \ll 1$, a condition implicit in the description of the matrix as a network of long slender straight rods with $\ell \gg A^{1/2}$. If this condition is not met, then the assumption that the rods do not intersect between the pre-determined nodes is invalid.

III. TRANSVERSE DISPERSION RELATION

The dispersion relation of transverse waves is found from an analogous calculation. Defining y as the polarization direction, we replace u_x by u_y , v_x by v_y , u_{xx} by u_{xy} and σ_{xx} by σ_{xy} . In Eqs. 14, 17, 18, 20 and 21, outside the brackets $\sin \theta$ is replaced by $\cos \theta$ and $\cos \theta$ by $\sin \theta \cos \phi$, where ϕ is the azimuthal angle of the rod, taking $\phi = 0$ in the x - y plane.

Averaging over ϕ introduces additional factors of $\frac{1}{2}$. The results Eqs. 22, 24 for the static limit become

$$\lim_{k \rightarrow 0} \mathcal{B}_t(k) \rightarrow \frac{1}{15} \mathcal{F} E \quad (25)$$

$$\frac{\omega}{k} \rightarrow \sqrt{\frac{E}{15\rho_m}} = \sqrt{\frac{1}{15}} v_{rod}. \quad (26)$$

IV. RESULTS

The dispersion relations for the longitudinal and transverse modes are shown in Fig. 2 for $C = 4$ and $C = 12$. The frequency dependences of the corresponding phase and group wave velocities v_{ph} and v_{gr} are shown in Fig. 3.

From the preceding results for the longitudinal and transverse wave speeds the static ($\omega, k \rightarrow 0$) Young's modulus E_{matrix} and Poisson's ratio ν_{matrix} of the bulk matrix may be obtained [15]:

$$E_{matrix} = \frac{1}{6} \mathcal{F} E \quad (27)$$

$$\nu_{matrix} = \frac{1}{4}. \quad (28)$$

The model predicts the ratio $v_{tr}/v_{long} = 1/\sqrt{3}$ of long wavelength ($\lambda \gg n^{-1/3}$) wave speeds, independent of the properties of the rods.

For comparison, we present results for the elastic constants of cubic lattices of rods and for the propagation speeds along the crystal axes of long-wavelength waves in Table I.

The acoustic properties of fluid-filled porous media, such as aquifers, petroleum reservoirs and cancellous (trabecular) bone, are described by models originally developed by Biot [2–7]. These are also effective medium models that describe the wave modes of the fluid filled medium as if it were homogeneous and continuous, and do not attempt to include the dispersion at finite k , other than that which is a consequence (by the Kramers-Kronig relations [16–18]) of dissipation. The properties of the empty matrix, such as those we have modeled, are required to calculate the properties of the Biot modes.

We have found elastic moduli (Eq. 27 and Table I) that are proportional to the density or filling factor. Our model shows how stiff low density structures can be, if designed or evolved to maximize stiffness. Our model describes a random structure; similar stiffness has been found for ordered structures [19]. This is in contrast to aerogels [20, 21, 25] that typically show $E \propto \rho_0^m$ with $2 \lesssim m \lesssim 4$. These values are characteristic of closed-cell foams for which $m = 3$ [1], although one study of aerogels [22] found $m \approx 1.5$. The structures of aerogels are complex and sensitive to their preparation [21–25].

A study of water-filled trabecular bone [26] found results that can be fitted by a value for the matrix of $m \approx 3.7$. These properties are very different from those of our model, and mechanical stiffness cannot have driven the evolution of trabecular bone. The remarkably low modulus of the trabecular matrix explains the observation [27] that at low matrix filling factor the fluid properties largely determine the elastic wave speed and attenuation in trabecular bone. This may explain why Biot models of fluid-filled trabecular bone have required phenomenological fitting of their parameters [28–32].

In our effective medium model dispersion is a consequence of microstructure and is present even without dissipation. The apparent contradiction with the Kramers-Kronig relations as adopted in [16–18] is resolved, as it is in textbook point mass and spring models of phonons in crystals [11], by noting that the effective medium model, like the phonon models, is nonlocal: the force on a mass is determined by the instantaneous positions of other masses. This violates the Kramers-Kronig assumption of locality, that response at one point is determined only by the history of fields at that point [33]. The mechanical compliance, analogous to the dielectric permittivity, is here a function of both ω and k . Our model makes first-principles quantitative predictions of the dispersion and elastic wave speeds of vacuum-filled matrices that may be tested experimentally.

Acknowledgments

We thank P. V. Bayly, L. M. Canel-Katz, A. E. Carlsson, G. M. Genin, M. Holland, B. Johnson, M. Milne, N. D. Mermin, A. Nelson, D. R. Nelson and Z. Nussinov for unpublished results and discussions. This work was supported in part by NIH grant R01AR057433, by grant P30AR057235 from the National Institute of Arthritis and Musculoskeletal and Skin Diseases to the Washington University Core Center for Musculoskeletal Biology and Medicine and by the American Chemical Society Petroleum Research Fund #51987-ND9.

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FIG. 1.

Rods connecting randomly distributed nodes. One realization of randomly distributed nodes with mean density 250 within a unit cube is shown. The closest nodal neighbors are connected by rods, for a mean coordination number $C=12$; some of these are outside the cube. The network is characterized by a length $\pi^{-1/3} = 0.159$ and is not fractal. The complexity of spatial structure, including voids and tongues of multiply connected nodes, is evident, but difficult to quantify except by its mechanical properties.

FIG. 2.

Dispersion relations $\omega(k)$ of longitudinal and transverse waves. $v_{rod} \equiv \sqrt{E/\rho_m}$ is the slender rod longitudinal wave propagation speed of the individual rods making up the matrix. The effective medium theory is expected to break down for $kn^{-1/3} \gtrsim \pi$ where scattering is strong. At finite $kn^{-1/3}$ these dispersion relations depend on the coordination number, as shown for $C=4, 12$. Dispersion is greater for larger C because of the presence of longer rods with larger values of $k\ell$ for $C=4$, $\langle \ell \rangle n^{1/3} = 0.778$ while for $C=12$, $\langle \ell \rangle^{1/3} = 1.085$.

FIG. 3.

Phase and group velocities of longitudinal and transverse waves as functions of frequency. C is indicated in subscripts. The effective medium theory is expected to break down for $\omega/(n^{1/3}v_{rod}) \gtrsim 1$. At finite $kn^{-1/3}$ these velocities depend on the coordination number.

TABLE I

Elastic constants (from Eq. 18) and wave speeds for propagation along crystal axes for cubic lattices of rods.

	Face Centered Cubic	Body Centered Cubic	Simple Cubic
C_{11}	$\frac{1}{6}\mathcal{F}E$	$\frac{1}{9}\mathcal{F}E$	$\frac{1}{3}\mathcal{F}E$
C_{12}	$\frac{1}{12}\mathcal{F}E$	$\frac{1}{9}\mathcal{F}E$	0
C_{44}	$\frac{1}{12}\mathcal{F}E$	$\frac{1}{9}\mathcal{F}E$	0
v_{long}	$\frac{1}{\sqrt{6}}v_{rod}$	$\frac{1}{3}v_{rod}$	$\frac{1}{\sqrt{3}}v_{rod}$
v_{tr}	$\frac{1}{\sqrt{12}}v_{rod}$	$\frac{1}{3}v_{rod}$	0