Acoustic Band Structure of Periodic Elastic Composites

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We present the first full band-structure calculations for periodic, elastic composites. For transverse polarization of the vibrations we obtain a "phononic" band gap which extends throughout the Brillouin zone. A complete acoustic gap or a low density of states should have important consequences for the suppression of zero-point motion and for the localization of phonons, and may lead to improvements in transducers and in the creation of a vibrationless environment.

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This Letter concerns a periodic composite—a repetitive structure made up of two materials with different elastic properties. We shall present the eigenfrequencies as a function of the Bloch wave vector, $\omega(\mathbf{k})$, that is the band structure of the composite. This is the first full calculation of an "acoustic" or "phononic" band structure.

Our inspiration is drawn from exciting developments dealing with macroscopic, periodic constructions of two transparent dielectrics, and the corresponding "optical" or "photonic" band structures. Such "crystals" have been machined out of low-loss dielectric materials; they contain up to $\sim$8000 "atoms," and the lattice parameter is $a \sim 13$ mm [1,2]. Consequently the experiments involve the microwave region, $\omega/2\pi \sim 15$ GHz. It is expected that these photonic crystals will be eventually scaled down, utilizing the technique of reactive ion etching [3]. For $a \lesssim 1$ μm the optical region would be attained, opening the way to diverse applications associated with semiconductor physics and technology [4]. It is appropriate to note that colloidal crystals composed of charged polystyrene spheres can have $a < 0.2$ μm [5]. Indeed, studies of *visible* light scattering from such crystals date back 30 years [6].

On the theoretical side, the photonic band structure was calculated for face-centered-cubic crystals having different compositions of the unit cell [2,7,8]. Of special importance is the obtainment of a *complete* band gap, in which no eigenfrequency is permitted for any value of $\mathbf{k}$ and for any polarization of the wave. This does *not* happen to be the case for a simple face-centered-cubic structure [7]. However, for more complex unit cells (such as the diamond structure), full "photonic gaps" were found [2,8], provided that the dielectric constant ratio of the two constituents is sufficiently large (a condition that is not realized for colloidal crystals). Periodic arrays of dielectric cylinders in a background medium were also studied. The corresponding two-dimensional band structure was determined both theoretically and experimentally [9,10]. For a brief review of photonic band structure see Ref. [11].

There are three motivations for this work and they are largely associated with complete acoustic or phononic band gaps. First, in analogy to the photonic case, in the frequency range of a complete phononic gap vibrations, sound, and phonons would be forbidden. Thus a vibrator or a small (real) crystal introduced into a periodic composite as a defect would be unable to emit or generate phonons within the band gap. Indeed, for periodic dielectrics, the inhibition of spontaneous emission of *photons* has been predicted [4] and observed [5,12]. In the case of a hydrogen atom, the inability to decay freely leads to photon bound states and to dressed atoms [13]. The inhibition of spontaneous emission is directly related to the suppression of zero-point (vacuum) fluctuations, for phonons as well as for photons.

Our second motivation is the possibility of applications. A complete acoustic gap could be engineered to provide a vibrationless environment for high-precision mechanical systems in a chosen range of frequencies. In addition, periodic arrays of piezoelectric and pyroelectric composites have had long-standing applications as transducers for transmitting and receiving signals in water [14]. These are used in sonar and depth-finding systems (at frequencies of tens of kHz and above) [15] and have been also designed for medical ultrasonic imaging (0.5–20 MHz) [14,16]. However, the corresponding computations of band structure were very limited in scope [17,18]. Obviously, the availability of full band-structure calculations for elastic composites could lead to improvements in the design of transducers.

The third and last motivation is related to the suggestion that the Anderson localization transition may be observed for electromagnetic waves propagating in strongly scattering dielectric structures [19]. The localization of classical waves in random media is a topic of considerable interest [20]. In fact, photon localization of microwaves has been observed for a three-dimensional *disordered* system of dielectric and metallic balls [21]. This was associated with a minimum of the diffusion constant—rather than its vanishing—in a narrow window of frequencies and filling fractions of the metallic spheres. Also, very recently localization of bending waves in a steel plate, decorated with Lucite blocks, has been detected experimentally [22]. As in the photonic case [21], the localiza-

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TABLE I. Band-structure-related properties of three periodic systems.

Property	"Electronic" crystal	"Photonic" crystal	"Phononic" crystal
Materials	Crystalline (natural or grown)	Constructed of two dielectric materials	Constructed of two elastic materials
Parameters	Universal constants, atomic numbers	Dielectric constants of constituents	Mass densities, sound speeds c_l, c_t of constituents
Lattice constant	1–5 Å (microscopic)	0.1 μm–1 cm (mesoscopic or macroscopic)	Mesoscopic or macroscopic
Waves	de Broglie (electrons) ψ	Electromagnetic or light (photons) $\mathbf{E},\mathbf{B}$	Vibrational or sound (phonons) $\mathbf{u}$
Polarization	Spin $\uparrow,\downarrow$	Transverse: $\nabla\cdot\mathbf{D}=0$ $(\nabla\cdot\mathbf{E}\neq 0)$	Coupled trans.-longit. $(\nabla\cdot\mathbf{u}\neq 0, \nabla\times\mathbf{u}\neq 0)$
Differential equation	$-\frac{\hbar^2}{2m}\nabla^2\psi+V(\mathbf{r})\psi=i\hbar\frac{\partial\psi}{\partial t}$	$\nabla^2\mathbf{E}-\nabla(\nabla\cdot\mathbf{E})=\frac{\epsilon(\mathbf{r})}{c^2}\frac{\partial^2\mathbf{E}}{\partial t^2}$	See Refs. [27,28]
Free particle limit	$W=\frac{\hbar^2k^2}{2m}$ (electrons)	$\omega=\frac{c}{\sqrt{\epsilon}}k$ (photons)	$\omega=c_{t,l}k$ (phonons)
Band gap	Increases with crystal potential; no electron states	Increases with $\lvert\epsilon_a-\epsilon_b\rvert$; no photons, no light	Increases with $\lvert\rho_a-\rho_b\rvert$, etc. no vibration, no sound
Spectral region	Radio wave, microwave, optical, x ray	Microwave, optical	$\omega\lesssim 1$ GHz

tion was caused by resonant scattering. Localization could also be the consequence of a delicate interplay between order and disorder [23]. A defect in an otherwise periodic composite produces strong localization [24], as also happens in the familiar case of an impurity in a semiconductor. It is entirely plausible that the study of complete gaps in classical-wave band structures will elucidate the conditions for strong localization of these waves [23,25]. By now many such calculations are available for light waves, taking into account the vectorial character of the fields [2,7,10]. In the case of elastic waves band-structure calculations are scarce [17,18,22] and are restricted to a single direction of the wave vector. We expect that the present work will bring to bear the issue of phonon localization [20,26].

Periodic structures—ordinary crystals, dielectric composites, and elastic composites—with identical Bravais lattices give rise to essentially the same Bragg diffractions. There are, however, numerous differences, and in Table I the peculiarities of phononic crystals (elastic composites) are contrasted with those of electronic (ordinary) and photonic crystals.

Various theoretical aspects of elastic waves in inhomogeneous media have been studied by a number of scientists [17,18,27]. Unlike electromagnetic waves, which are transverse ($\nabla\cdot\mathbf{D}=0$), sound waves in solids can be longitudinal, as well as transverse. In a homogeneous medium the longitudinal and transverse waves are independent, and the corresponding material displacements $\mathbf{u}_l$ and $\mathbf{u}_t$ satisfy separate wave equations with wave velocities c_l and c_t. On the other hand, in an inhomogeneous medium the displacement $\mathbf{u}$ is in general *not* separable into components $\mathbf{u}_l$ and $\mathbf{u}_t$ such that $\nabla\times\mathbf{u}_l=0$ and $\nabla\cdot\mathbf{u}_t=0$. Thus the calculation of acoustic band structures is a much more difficult undertaking than that of optical band structures. To illustrate the ideas involved we shall consider a particularly simple situation.

Our system is composed of an array of straight, infinite cylinders made of an isotropic solid "a" and embedded in an elastic background "b," which is also isotropic. There is translational invariance in the direction z parallel to the cylinders and the system has (two-dimensional) periodicity in the transverse plane. In the corresponding electromagnetic case wave propagation was limited to this plane [9,10]. Following this restriction the wave vector $\mathbf{k}$ is the two-dimensional Bloch vector. Then it turns out that there are two independent modes of vibration [28]. One is a mixed-polarization mode with the displacement $\mathbf{u}$ perpendicular to the cylinders; the oscillations are neither longitudinal nor transverse. For the other mode the vibrations are parallel to the cylinders; hence $\mathbf{u}\cdot\mathbf{k}=0$, so this mode is strictly transverse. In this Letter we calculate the band structure only for the transverse polarization, that is $\mathbf{u}=u\hat{\mathbf{z}}$. The justification is that this seems to be the only case in which the wave equation for inhomogeneous solids greatly simplifies. Of course this wave equation is nothing but the equation of motion for an element of mass of density ρ. We find that [28]

$$\rho\frac{\partial^2 u}{\partial t^2}=\nabla_t\cdot(\rho c_t^2\nabla_t u)\,, \tag{1}$$

where c_t is the transverse speed of sound and ∇_t is the two-dimensional nabla. (For a homogeneous medium ρ and c_t are position independent; the ρ cancels out and one is left with the usual wave equation.) In the optical case the only material function involved is the speed of light at a point $\mathbf{r}$; in Eq. (1) we must consider two such functions, $c_t(\mathbf{r})$ and $\rho(\mathbf{r})$. Making use of the periodicity of our system we expand $\rho(\mathbf{r})$ and $\rho c_t^2\equiv\tau(\mathbf{r})$ in two-dimensional Fourier series. The Fourier transforms of these functions are denoted $\rho(\mathbf{G})$ and $\tau(\mathbf{G})$, where $\mathbf{G}$ is the two-

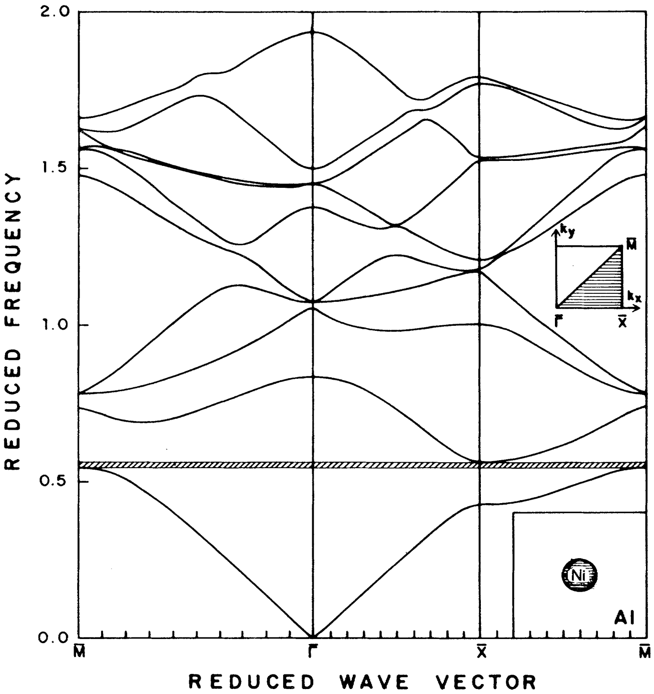

FIG. 1. Band structure for a periodic array of nickel alloy cylinders in an aluminum alloy background. We plot the normalized frequency vs the normalized, two-dimensional Bloch vector. The insets show the unit cell and the corresponding Brillouin zone. The parameters used are $\rho=8.936$ (2.697) g/cm^3 and $c_{44}\equiv\rho c_t^2=7.54$ $(2.79)\times10^{11}$ dyn/cm^2 for Ni (Al) [29], and $f=0.1$. There is a phononic band gap (shaded) extending throughout the Brillouin zone for vibrations parallel to the cylinders.

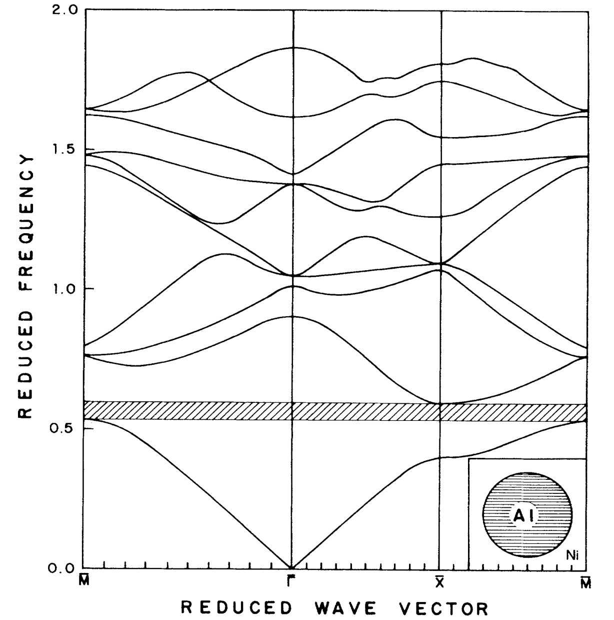

FIG. 2. As in Fig. 1 for aluminum alloy cylinders in a nickel alloy background. Here $f=0.75$.

dimensional reciprocal-lattice vector. For the displacement u we use the Bloch theorem,

$$u(\mathbf{r},t)=e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\sum_{\mathbf{G}}u_{\mathbf{k}}(\mathbf{G})e^{i\mathbf{G}\cdot\mathbf{r}}\,. \tag{2}$$

Substitution in Eq. (1) yields

$$\sum_{\mathbf{G}'}[\tau(\mathbf{G}-\mathbf{G}')(\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G}')-\omega^2\rho(\mathbf{G}-\mathbf{G}')]u_{\mathbf{k}}(\mathbf{G}')=0\,. \tag{3}$$

The cylinder (background) material has a density ρ_a (ρ_b) and it occupies a fraction f of the area of the unit cell. It is easy to show that

$$\rho(\mathbf{G})=\begin{cases}\rho_a f+\rho_b(1-f)\equiv\bar{\rho}, & \mathbf{G}=0\,,\\ (\rho_a-\rho_b)F(\mathbf{G})\equiv\Delta\rho F(\mathbf{G}), & \mathbf{G}\neq0\,,\end{cases} \tag{4}$$

$$F(\mathbf{G})=A_c^{-1}\int_a d^2r\exp(-i\mathbf{G}\cdot\mathbf{r})\,. \tag{5}$$

A_c is the area of the unit cell, and the integration is over the cross-sectional area of a cylinder. An analogous formula holds for $\tau(\mathbf{G})$ in terms of $\bar{\tau}=\overline{\rho c_t^2}$ and $\Delta\tau=\rho_a c_a^2-\rho_b c_b^2$. Then we can rewrite Eq. (3) employing the average parameters $\bar{\rho}$ and $\bar{\tau}$, the "contrast" parameters $\Delta\rho$ and $\Delta\tau$, and the structure factor $F(\mathbf{G})$:

$$[\bar{\tau}|\mathbf{k}+\mathbf{G}|^2-\bar{\rho}\omega^2]u_{\mathbf{k}}(\mathbf{G})+\sum_{\mathbf{G}'\neq\mathbf{G}}[\Delta\tau(\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G}')-\Delta\rho\omega^2]F(\mathbf{G}-\mathbf{G}')u_{\mathbf{k}}(\mathbf{G}')=0\,. \tag{6}$$

If $\mathbf{G}$ is permitted to take all the possible values, this is a set of linear, homogeneous equations for the eigenvectors $u_{\mathbf{k}}(\mathbf{G})$ and the eigenfrequencies $\omega(\mathbf{k})$. By letting $\mathbf{k}$ scan the area of the irreducible region of the Brillouin zone, the band structure is obtained.

We choose the rods to have circular cross sections of radius r_0. Then integrating in Eq. (5) we get $F(\mathbf{G})=2fJ_1(Gr_0)/Gr_0$, where J_1 is the Bessel function of the first kind of order 1 [9]. It is assumed that the array of cylinders forms a square lattice of lattice constant a; thus $\mathbf{G}=(2\pi/a)(n_x\hat{\mathbf{x}}+n_y\hat{\mathbf{y}})$, where n_x and n_y were permitted to take the integer values between -10 and $+10$ (441 plane waves). This resulted in a very good convergence. The first ten phononic bands were computed for nickel alloy rods in an aluminum alloy matrix, Fig. 1, and vice versa in Fig. 2. The plots are rendered in terms of the normalized frequency $\omega a/2\pi c_0$ versus the normalized Bloch wave vector $ka/2\pi$. Note that, in the vicinity of the $\bar{\Gamma}$ point, the slope is not much different from 1. This corresponds to a speed of sound, in the long-wavelength limit, of $\sim(\overline{\rho c_t^2}/\bar{\rho})^{1/2}$. The dimensionless parameters which must be specified are ρ_a/ρ_b, τ_a/τ_b, and a/r_0 or $f(=\pi r_0^2/a^2)$.

In both figures there is a vibrational band gap between the first two bands. In order to establish this phononic gap we have scanned the interior of the irreducible triangle $\bar{\Gamma}\bar{X}\bar{M}$ of the Brillouin zone (see inset of Fig. 1), as well as its pheriphery. Because the gaps shown extend throughout the Brillouin zone, wave propagation in the transverse plane is forbidden for vibrations parallel to the cylinders. In a future publication we shall examine the dependences of these band gaps on the parameters of the composite [28].

We have not calculated the band structures for the mixed longitudinal-transverse mode with **u** perpendicular to the cylinders. Therefore the gaps found are not "complete" or independent of polarization. The study of the mixed mode is of considerable interest, as are band-structure calculations—for other composites with two- and three-dimensional periodicities. The special situation investigated here involves three parameters; however, in general there would enter two more, namely, the ratio of the *longitudinal* sound velocities and the ratio of the longitudinal to transverse velocities in either medium. This contrasts with only two dimensionless parameters for dielectric composites. Clearly, elastic composites offer a richer—and more complicated—behavior. Because of the coupling in general of transverse and longitudinal vibrations, and because $c_t \neq c_l$, it may take rather large contrasts to realize a *full* phononic gap. The prospect of achieving a complete gap would much improve for a periodic system of liquids and/or gases, because these support only longitudinal sound propagation. The search for a complete phononic gap should be an undertaking of comparable importance to the pursuit of full photonic gaps. In the frequency region of a complete acoustic gap vibrations, sound, and phonons are absent, thus profoundly affecting diverse fundamental properties. Moreover, such a gap is intimately associated with the prospect of Anderson localization of phonons. Also, the ideas presented here could pave the way toward applications such as transducers and a vibration-free environment. Finally we wish to stress that, to a large extent, this interest in band structure of periodic elastic composites is still valid in the presence of a low density of state— rather than a full gap.

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Note added.—A recent paper [30] reports a narrow, however, complete gap for Au cylinders in Be host.

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