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► **To cite this version:**

R. Hornreich, M. Kugler, S. Shtrikman, C. Sommers. Phonon Band Gaps. Journal de Physique I, 1997, 7 (3), pp.509-519. 10.1051/jp1:1997172 . jpa-00247340

HAL Id: jpa-00247340

<https://hal.science/jpa-00247340>

Submitted on 4 Feb 2008

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Phonon Band Gaps

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(Received 14 October 1996, received in final form 25 November 1996, accepted 26 November 1996)

PACS.63.20.-e – Phonons in crystal lattices

PACS.63.20.Dj – Phonon states and bands, normal modes, and phonon dispersion

PACS.63.20.Pw – Localized modes

Abstract. — We present structures, based on rods, that exhibit phonon band gaps. Structures based on rods made out of segments of different materials have very large gaps or multiple gaps. For homogeneous cylinders smaller gaps exist. Possible applications are discussed.

1. Introduction

Recent evidence has shown the existence of periodic materials exhibiting photonic gaps [1–4,16], namely frequency ranges where electromagnetic waves can not propagate in any direction. These gaps have been shown in the above references to lead to several interesting applications. They have also led to the investigation of phonon bands in periodic structures [6–8].

The existence of phonon band gaps is not *a priori* guaranteed, since the details of the band structure depend on the nature of the wave equation under study.

One of the important differences between the cases studied here concerns the polarization of the wave. Sound waves are described by a vector field which can be both longitudinal and transverse. These equations differ from those for scalar waves [9] and transverse electromagnetic waves as described by Maxwell's equations [5]. Sound waves thus have three branches in each band, combinations of two transverse and one longitudinal mode, rather than one branch for the scalar and two for the transverse electromagnetic waves. One branch may thus fill the gaps left open by the other branches.

Kushwaha *et al.* [5,6] establish the existence of phonon gaps for sound propagating in two dimensions in a structure that consists of cylinders perpendicular to the direction of propagation. These cylinders are embedded in a different substance. While this study may have some technological implications, it is easier to find such gaps in two dimensions than in three dimensions. The structure studied in this reference does not possess gaps for sound propagating in three dimensions.

(*) This article is in memory of our dear friend and colleague Richard Hornreich with whom we started this work. He did not live to finish what he started and we dedicate this paper in his honor.

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Economou *et al.* [7] as well as Kafesaki *et al.* [8] have obtained structures that exhibit full band gaps in three dimensions. These structures consist of metallic spheres or cubes embedded in plastic. The reason these authors give for the existence of their band gaps is analogous to the tight binding approximation for electron bands. The spheres act as resonators which are weakly coupled by the background material. This gives rise to very flat non-crossing bands producing gaps over the entire Brillouin zone. They also note that if this mechanism prevails it is much more difficult to find a structure based on rods that would produce gaps and indeed they find none. The reason for this is that sound propagation along the rods tends to delocalize the resonances thus closing the gaps.

Based on our previous work [4] we consider rods made up of segments of different materials. This inhibits the propagation along the rods at certain frequencies and produces gaps. In fact we obtain even larger gaps than in previous studies, as well as multiple wide gap structures.

In addition we show that gaps exist even in cases where the localized resonance mechanism does not apply. Structures with homogeneous rods can also give rise to gaps in disagreement with the resonance mechanism.

In Section 2 we discuss the physics of sound and electromagnetic wave propagation in periodic media in analogy with electron band theory. We draw upon analogies with the two extreme situations in electron theory: tight binding on one hand and nearly free electrons on the other. The picture that emerges helps in understanding the physics of band gaps.

To calculate the allowed frequencies, we follow the standard procedure and solve the wave equations in a periodic structure by expanding it in a Fourier series. The necessary formalism is presented in Section 3. One of the difficulties in using this method is controlling the error introduced by cutting off high Fourier components in the expansion. We estimate these errors by studying a periodic crystal made of material with vanishing shear modulus, essentially a periodic liquid. For such materials the long wave length limit of sound velocity can be calculated directly. Comparing this calculation to the one obtained by using the Fourier method allows us to estimate the errors introduced by the cutoff in k .

In Section 4 we discuss the structures based on segmented rods, these are rods that are made of sections of different materials. To hinder sound propagation along the rod we chose alternating sections made of materials with a large acoustic impedance mismatch, such as heavy metal and light plastic. Such rods can then be inserted in a gas or liquid forming a periodic structure. The large impedance mismatch between the rods and the background gas tends to increase the size and number of the gaps.

In Section 5 we study rods made from a single material. To obtain band gaps we were forced to break the high symmetry usually considered, and use an orthorhombic Pmmm [10] structure as well as materials with unrealistic elastic properties. This section also presents the convergence test resulting from the low frequency sound velocity. While the structures discussed in this section can not be manufactured, we feel that they are important in clarifying the mechanism that leads to band gaps.

In Section 6 we conclude by discussing possible physical applications of materials that exhibit sound band gaps. These include sound filters, mirrors, materials where the direction of propagation depends on the frequency and possible applications to surface acoustic wave devices.

2. A Physical Description

Different waves can propagate in periodic media. One may consider scalar waves, electron waves that are described by the Schroedinger equation in a periodic electromagnetic field, electromagnetic waves and sound waves. The existence of bands follows directly from

the periodicity of the medium and is thus a common feature for all types of waves. The detailed properties of the bands do however depend on the nature of the equations. The number of components describing the propagating field plays a crucial role in determining the gap structure and warrants further discussion.

The task of searching for periodic structures that exhibit band gaps is more difficult the larger the number of components. One reason for this is technical, for a field with n components one has to diagonalize an $(nN \times nN)$ matrix where N is the number of Fourier components included in the calculation. This implies that memory requirements increase as n^2 and time requirements increase as n^3 . The second difficulty is essential, when dealing with an n component field each band has n branches. For phonons there are three branches, each a combination of longitudinal and transverse waves. Gaps that are left open by one branch may be closed by other branches and finding a structure with band gaps becomes more difficult.

Of the many wave solutions in periodic media the best studied one is that describing electron bands in solids. We may thus borrow some of the intuition developed in that field. In this paper we consider only linear elastic waves. In analogy, nonlinearities due to electron-electron and electron-phonon interactions are neglected in our discussion.

When dealing with electrons nobody is surprised that insulators exist, and these imply the existence of band gaps. Why then was it surprising when photonic band gaps were discovered? The answer lies in using a different intuitive picture for photon and phonon bands than the one used for electrons.

Two extreme regimes of electron bands are easy to understand physically. The tight binding situation on one hand, and the nearly free electrons on the other. In tight binding each atom separately has bound states. Bound states from different atoms are weakly coupled when the atoms are brought together. This results in narrow bands separated by wide gaps. Under these conditions it is not at all surprising that the wide gaps that exist for each value of momentum k can overlap and produce complete band gaps. On the other hand in the nearly free picture, the potential that splits the bands is weak. The bands closely resemble free electron propagation with only narrow k -dependent gaps separating the bands at the edges. This makes it unlikely that gaps exist for all k in more than one dimension.

The structures used in studying photon and phonon band gaps are composed of transparent materials. Since waves are free to propagate in each material separately one naturally tended to think in terms of a nearly free propagation picture and not in terms of a tight binding picture, and the existence of band gaps was surprising. The insight gained in [8] is that spheres of a heavy metal have their own sound resonances, and that the coupling between such spheres through a light plastic material is indeed relatively weak, so that a tight binding picture is appropriate. The above authors support their argument by showing that one can explain the locations of gaps by this mechanism. They also note that when the heavy spheres touch band gaps disappear, because the coupling between spheres is no longer weak.

Applying the intuition based on tight binding to structures made out of rods, one may understand that sound can always propagate along the rods, therefore no localized resonances exist and band gaps are unlikely [8]. Indeed structures that contain rods and lead to complete band gaps were not found [8]. To overcome this difficulty we have introduced segmented rods [4]. These are rods made out of segments of different materials. By appropriately combining heavy metal segments alternating with light plastic segments we have effectively created weakly coupled sound resonators and propagation of sound along the rod is inhibited at some frequencies. In addition to being easier to produce, the rod geometry allows for the insertion of the rod into gases or liquids. These less dense materials that have a vanishing shear modulus weaken the coupling between the heavy metal resonators, and produce larger gaps and multiple gaps depending on the exact parameters used.

The tight binding intuition discussed above helps us to understand some structures that produce band gaps. It is, however, not the only possible mechanism that can result in complete band gaps. To show this we discuss a structure based on homogeneous rods that exhibits complete band gaps. Obviously the tight binding intuition does not apply in this case. Indeed finding band gaps in such structures is more difficult and we had to use unrealistic parameters in this case. The mechanism that produces gaps in this case is more complicated than tight binding.

One more subject to be discussed is the choice of materials. Since we want to minimize the energy flow from one material to the next, it would be good to have a large acoustic impedance mismatch. Acoustic impedances are given by:

$$\begin{aligned} Z_l &= \sqrt{\rho\kappa} \\ Z_t &= \sqrt{\rho\mu} \end{aligned} \quad (1)$$

for longitudinal and transverse waves respectively. This is why we have chosen tungsten and polyethylene as the two materials in the graphs we exhibit.

3. Formalism

In order to calculate the phonon band structure we study the solutions of elastic waves in periodic media. As described by Landau and Lifshitz [11] we write the equations of motion for an elastic medium as:

$$\rho\ddot{u}_i = \partial\sigma_{ik}/\partial x_k = \sigma_{ik,k} \quad (2)$$

where u_i is the displacement, and $\sigma_{ik,k}$ is the internal stress tensor. A comma denotes a derivative and repeated indices are summed over.

The stress strain relations can be written as

$$\sigma_{ik} = \kappa u_{ll}\delta_{ik} + 2\mu(u_{ik} - \frac{1}{3}u_{ll}\delta_{ik}) \quad (3)$$

where $u_{ik} \equiv \frac{1}{2}[u_{i,k} + u_{k,i}]$. Thus

$$\sigma_{ik,k} = (\kappa u_{ll})_{,i} + 2 \left[\mu(u_{ik} - \frac{1}{3}u_{ll}\delta_{ik}) \right]_{,k} \quad (4)$$

Based on the analysis of Turbe [12] we expand the solutions of the elastic equations of motion in a periodic medium in terms of Bloch functions. The displacement vector u_i can then be written as $u_i = u_i(\mathbf{k})e^{i\omega t}$. Expanding relevant quantities such as the displacement and the density in a Fourier series as a function of reciprocal lattice vectors \mathbf{G} gives

$$u_i = \sum_{\mathbf{G}} u_i^{\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \quad (5)$$

where we have omitted the dependence of $u_i^{\mathbf{G}}$ on \mathbf{k} and

$$\rho(\mathbf{r}) = \sum_{\mathbf{G}} \rho_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \quad (6)$$

with similar expressions for κ and μ . Thus

$$u_{ll} = \frac{i}{2} \sum_{\mathbf{G}'} \left[u_i^{\mathbf{G}'}(\mathbf{k} + \mathbf{G}')_l + u_i^{\mathbf{G}'}(\mathbf{k} + \mathbf{G}')_i \right] e^{i(\mathbf{k}+\mathbf{G}')\cdot\mathbf{r}} \quad (7)$$

Substituting equations (4), (5) and (6) into equation (2) gives rise to the general equations of motion

$$\omega^2 \sum_{G''} \rho_{G-G''} u_i^{G''} = \sum_{G'} \left\{ (\kappa_{G-G'} - \frac{2}{3} \mu_{G-G'}) u_i^{G'} (\mathbf{k} + \mathbf{G}')_l (\mathbf{k} + \mathbf{G})_l + \mu_{G-G'} \left[u_i^{G'} (\mathbf{k} + \mathbf{G}')_l (\mathbf{k} + \mathbf{G})_l + u_i^{G'} (\mathbf{k} + \mathbf{G}')_z (\mathbf{k} + \mathbf{G})_l \right] \right\}. \quad (8)$$

As a test for convergence we also consider a simplified system with vanishing shear modulus, $\mu = 0$. This then gives for equation (7)

$$\omega^2 \sum_{G''} \rho_{G-G''} u_i^{G''} = \sum_{G'} \kappa_{G-G'} u_i^{G'} (\mathbf{k} + \mathbf{G}')_l (\mathbf{k} + \mathbf{G})_l. \quad (9)$$

In general for each value of \mathbf{k} , there exist three polarization modes, one longitudinal and two transverse. By setting $\mu = 0$ the transverse modes have $\omega = 0$ and decouple, only the longitudinal modes are of interest. In k space the identification of longitudinal modes is nontrivial. One can, in principal, solve equation (8), and obtain for each k three eigenvalues of ω . The longitudinal modes are identified by having non-zero frequency. This still implies solving a $3N \times 3N$ eigenvalue problem, where N is the number of plane waves. To further simplify this calculation, we consider a constant density where the longitudinal mode can be identified analytically. Setting $\rho_G = \rho_0 \delta_{G,0}$ gives

$$\omega^2 \rho_0 u_i^G = \sum_{G'} \kappa_{G-G'} u_i^{G'} (\mathbf{k} + \mathbf{G}')_l (\mathbf{k} + \mathbf{G})_l. \quad (10)$$

If we then multiply both sides of equation (9) by $(\mathbf{k} + \mathbf{G})_z / |\mathbf{k} + \mathbf{G}|$ and define the longitudinal mode along $(\mathbf{k} + \mathbf{G})$ as

$$v^G = u_i^G \frac{(\mathbf{k} + \mathbf{G})_z}{|\mathbf{k} + \mathbf{G}|} \quad (11)$$

we have

$$\omega^2 \rho_0 v^G = \sum_{G'} \kappa_{G-G'} |(\mathbf{k} + \mathbf{G}')| \cdot |(\mathbf{k} + \mathbf{G})| v^{G'} \quad (12)$$

This definition of v^G makes equation (12) an $N \times N$ Hermitian eigenvalue problem. Equation (12) is used in this paper to study the effects of the cutoff in k .

4. Segmented Rod Structures

The first structure we discuss is based on segmented rods. We use circular rods of radius r . In a cubic unit cell of size a , sections of length l of one material are separated by sections of length $a - l$ made out of a second material. Without loss of generality we may put $l < a/2$.

These rods are arranged to resemble a bcc structure. We take all the rods in the z direction. Centers of the rods are located in the $\{x, y\}$ plane at the positions $\{0, 0\}$ $\{a, 0\}$ $\{0, a\}$ $\{a, a\}$ and $\{a/2, a/2\}$. The cylinders are arranged so that the first four have the centres of the short sections on the $z = 0$ plane while the fifth one has the centre of the short section on the $z = a/2$ plane, as shown in Figure 1. Thus the centres of the short segment are located on a bcc lattice.

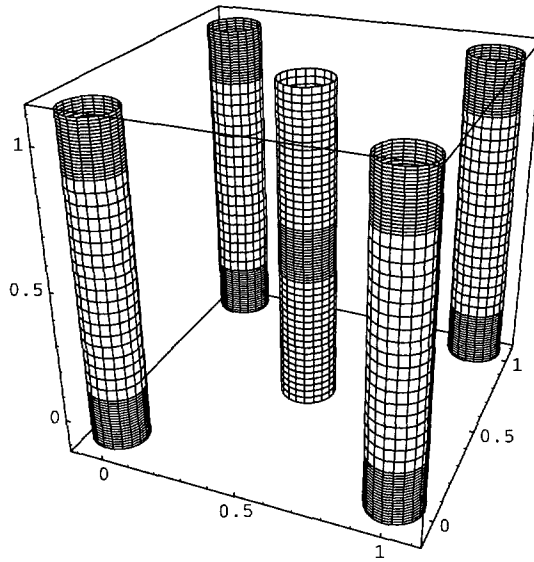


Fig. 1. — Unit cell for segmented rods.

Once we have picked the materials out of which we make the rods only two parameters may be varied: the radius r and the length of the short segment l . The band structure will depend only on these parameters.

We have used up to 887 k values to test convergence. In practice about 400 k values were sufficient to obtain an accuracy of several percent. The high symmetry of this structure gives rise to a relatively rapid convergence. In the cases with lower symmetry that we discuss in the next section the convergence problem is much more severe.

To illustrate typical bands and gaps that can be obtained using this structure we present results for two sets of parameters. The short segments of the rods are made out of tungsten and the long segments are polyethylene. The space between cylinders is filled with air.

Figure 2 shows several wide gaps. In Figure 3 we have increased the radius of the cylinder. We chose a different way to present the results by showing the density of states as a function of frequency. One gap is present in this plot, it is easily recognized by the vanishing of the density of states in the gap.

The above figures clearly show that staggered rods in the configuration that we used are efficient in producing sound gaps.

5. Homogeneous Rods

The difficulty in producing band gaps with uniform rods, was discussed in Section 2. Indeed a straightforward generalization of Figure 1 to continuous rods does not yield band gaps. Geometries that were successful in producing gaps for electromagnetic waves [4] also failed to produce phonon gaps. We also tried the symmetries based on a rod arrangement as described in the paper by Ho *et al.* [2]. This geometry, which produced several large photon band gaps, did not give rise to gaps in the phonon case.

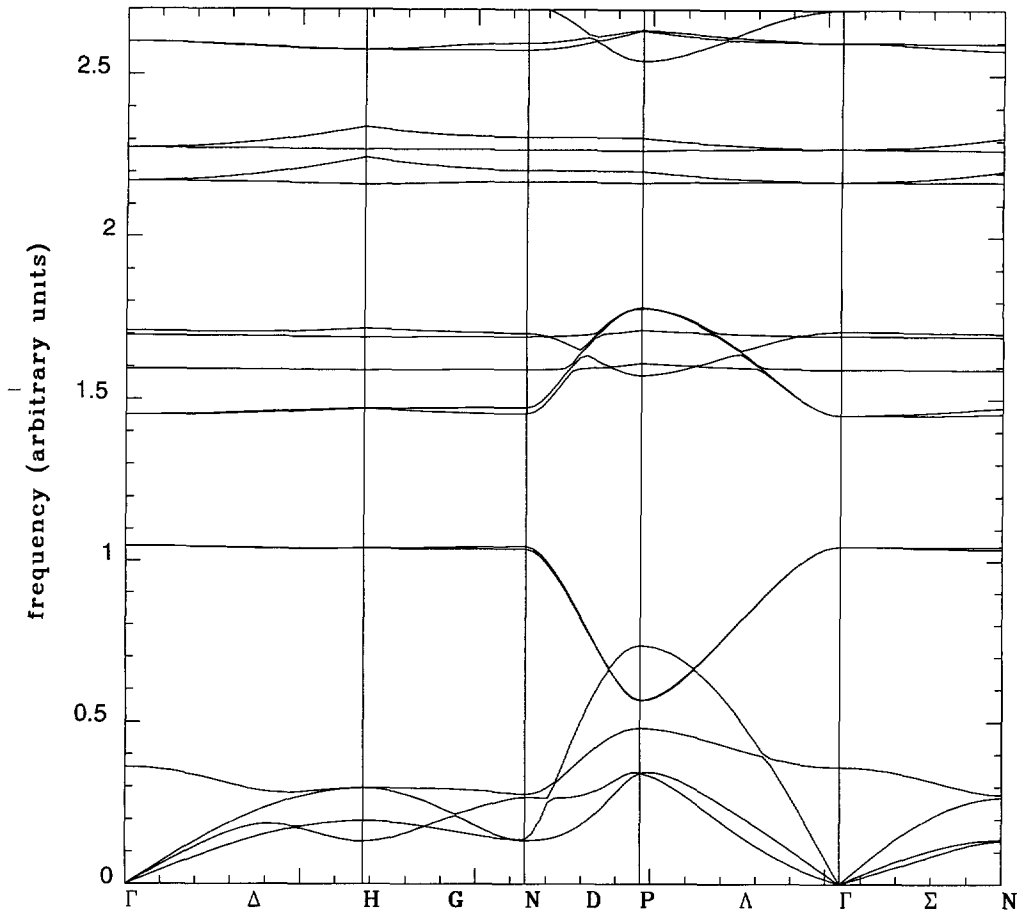


Fig. 2. — Band structure for segmented tungsten-polyethylene rods. The parameters are $r = 0.18$, $l = 0.2$.

The geometry that did give rise to a small gap was a system of cylinders arranged as follows.

A unit cell of dimensions $a \times a \times c$ contained cylinders of radius r with

- 1) cylinders in the z direction centered at $\{x, y\} = \{0, 0\}, \{0, a\}, \{a, 0\}, \{a, a\}$;
- 2) cylinders in the y direction centered at $\{x, z\} = \{0, 0\}, \{0, c\}, \{a, 0\}, \{a, c\}$;
- 3) one cylinder in the x direction centered at $\{y, z\} = \{a/2, c/2\}$.

Figure 4 shows the unit cell in detail.

In order to produce gaps we had to use several extra features:

- 1) break the cubic symmetry by putting $a \neq c$;
- 2) introduce different elastic moduli and densities for cylinders in different directions;
- 3) use unrealistic values for elastic moduli and densities.

The symmetry of our crystal was thus reduced to a Pmmm [10] symmetry. The gaps that were obtained were still quite narrow.

The calculation using cylinders of constant bulk modulus converged rather slowly. This is due to the low symmetry of the structure we discuss. The slow convergence when combined with the narrow size of the gap that requires high accuracy, gave rise to computing difficulties. Even with 2 700 plane waves no reliable results could be obtained.

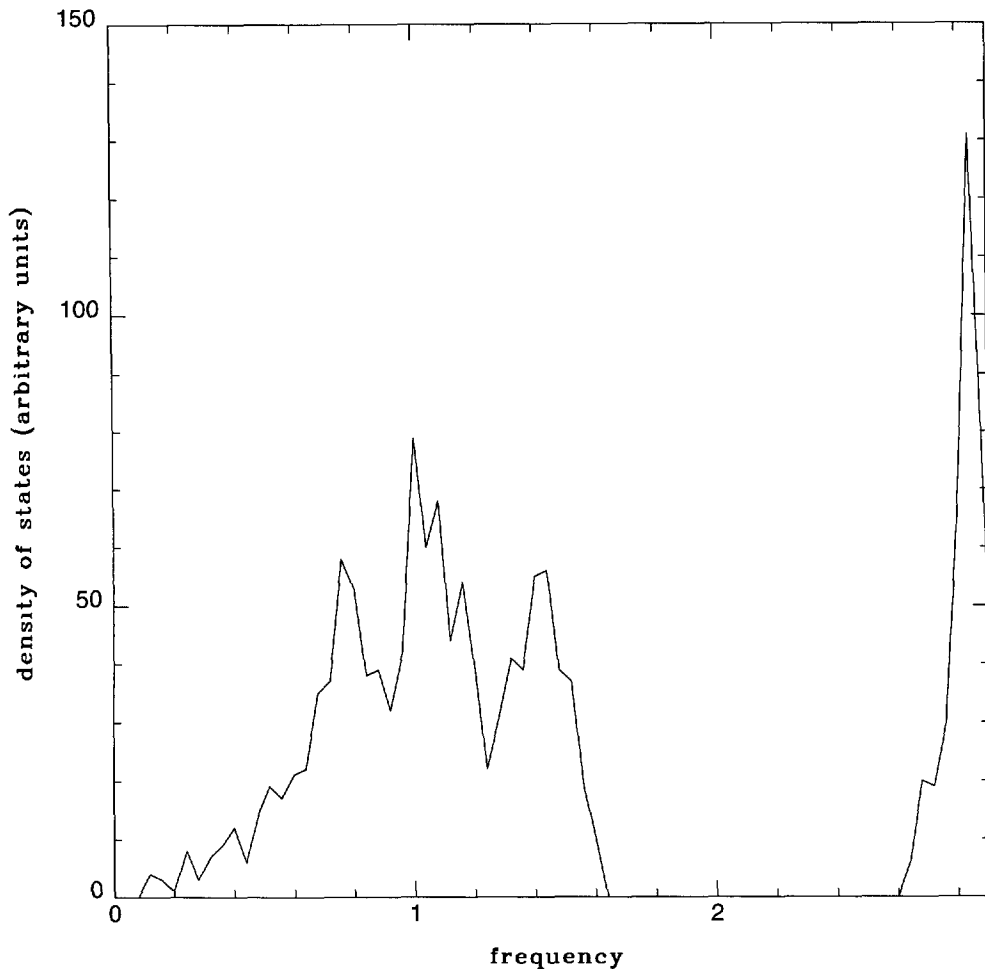


Fig. 3. — Density of states for segmented tungsten-polyethylene rods. The parameters are $r = 0.26$, $l = 0.2$.

Since we were not trying to construct a realistic material but rather to make a physical point that band gaps can be produced in structures with homogeneous rods we improved convergence by using a Gaussian distribution for the bulk modulus [13] in each cylinder

$$\kappa(x, y) = \kappa_0 e^{-\frac{x^2 + y^2}{2r^2}} \quad (13)$$

with similar distributions for the shear modulus and the density.

Such a distribution gives rise to good convergence and is sufficient to demonstrate the existence of phonon band gaps. In practice on the order of 900 planes waves were sufficient to produce three figure accuracy in the bands we studied.

As a test for convergence we calculated the zero frequency limit of the sound velocity. For a general non-homogeneous medium with vanishing shear modulus and constant density,

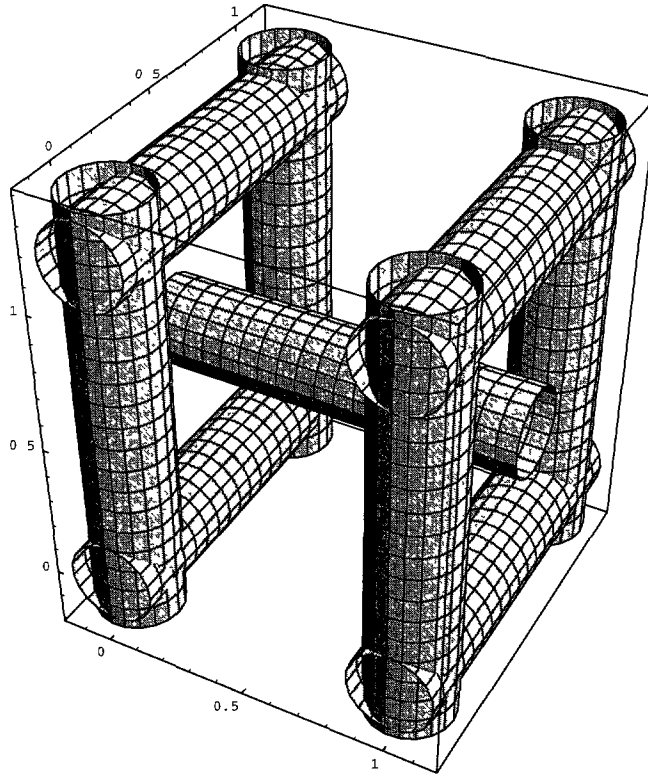


Fig. 4. — Unit cell for homogeneous rods. $c = 1.2$, $a = 1$.

the zero frequency sound velocity is isotropic and is given by $V_0 = \sqrt{\kappa_{\text{eff}}/\rho}$, where

$$\frac{1}{\kappa_{\text{eff}}} = \int \frac{d^3x}{\kappa(x)}. \tag{14}$$

Using 953 plane waves we obtained a V_0 that was isotropic to within 10^{-4} and agreed with equation (14) to within 5×10^{-3}

The $\mu = 0$ case discussed so far and its low energy limit were useful as a check on the numerical accuracy and the convergence of the plane wave expansion. We consider the accuracy obtained above as sufficient. This enables us to proceed and study the full problem including shear for continuous rods. To study this case we solve equation (8).

Figure 5 shows the results obtained for a crystal with structure as in Figure 4 including both shear and bulk moduli. We observe that gaps can be obtained.

6. Possible Applications

We have shown that structures based on rods can produce complete gaps in three-dimensional systems. With staggered rods, very large and/or multiple gaps can exist, depending on the values of the parameters that are used. It is much harder to produce complete band gaps for continuous rods. The evidence we produced had to rely on unrealistic values of the elastic parameters. The continuous rods example served to show that gaps exist also in cases where

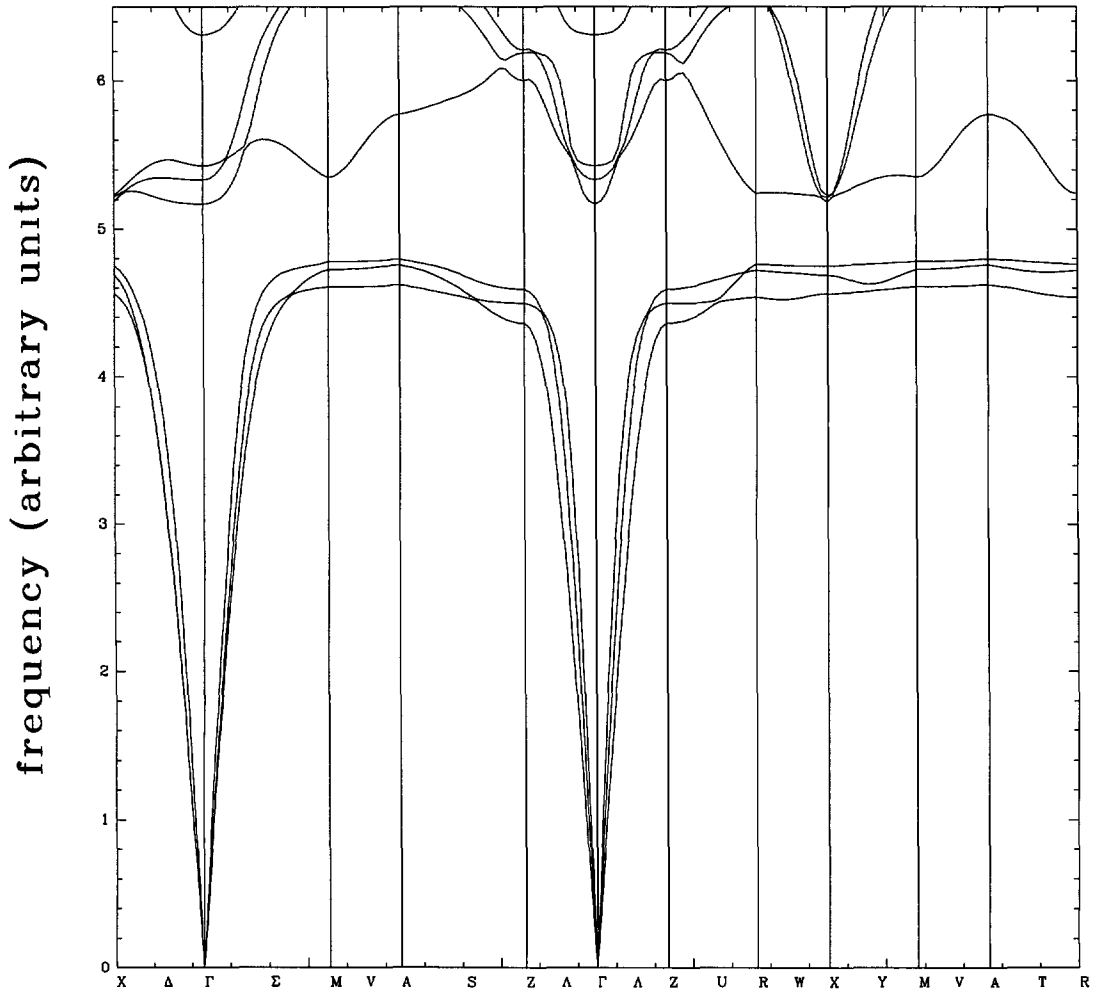


Fig. 5. — Band structure for continuous rods. The bulk moduli for the three types of cylinders are: 40, 40, 1. The shear moduli are: 1, 1, 40. The densities are: 400, 400, 1. $r = 0.18$. $c = 1.2$, $a = 1$. Units are arbitrary.

the tight binding analogy does not hold. The exact gap mechanism in this case is more complicated.

The study of composites where phonon gaps exist is not a mere exercise in wave propagation. Phonon band gaps can lead to several applications. The most obvious application is that of sound filters and mirrors. Sound with a frequency inside the gap does not propagate in the material and is thus reflected from the surface. For frequencies inside the gap we have therefore both insulators and ideal mirrors.

A less obvious application concerns frequencies just at the edges of the gaps. It is usually the case that the lowest propagating frequency above the gap is allowed for one value of \mathbf{k} . Sound at that frequency can propagate therefore only in the direction given by that \mathbf{k} and the crystal acts as a wave guide. A similar situation may exist at the highest allowed frequency below the gap, usually for a different value of \mathbf{k} . The crystal can thus act as a beam splitter

and a frequency dependent wave guide, directing different frequencies in different directions. Directional sound propagation in systems with band gaps is due to a different mechanism than in the case where the directionality is due to anisotropy of the elastic constants [14]. In particular the latter systems do not give rise to frequency dependent directionality.

Other applications may exist in the field of surface acoustic waves. Surface acoustic wave (SAW) devices are useful because the short wave length of sound allows for more compact devices than electromagnetic waves of the same frequency. SAW devices make use of the fact that surface waves and bulk waves have different dispersion relations. Thus by creating a signal with well defined frequency and wave length we may constrain it to propagate on the surface of a solid. Still, when surface waves encounter an obstacle on the surface they may scatter into the bulk and part of the energy may be lost. When the system is such that certain frequencies are inside a band gap and can not propagate in the bulk signals at these frequencies are restricted to propagate on the surface. There is no need to control both wave length and frequency, and energy in the signal can not be lost into the bulk. No detailed study of surface modes in systems with phonon gaps has been made so far, the studies that exist are only for the case of photons [15]. Additional applications may result when periodic disturbances are placed on the surface of SAW devices so that the surface band gaps can act as new means for signal processing. As outlined above, filters, mirrors and wave guide that depend on frequency may be obtained. These problems are now under study and the results will be reported elsewhere.

Acknowledgments

This work was partially supported by the MINERVA Foundation, Munich, Germany. C.S. acknowledges the financial support of the Einstein Center for Theoretical Physics of the Weizmann Institute of Science, as well as the computational support given by the CNRS computing center (IDRIS) at Orsay.

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