Classical wave propagation in periodic structures: Cermet versus network topology

E. N. Economou* and M. M. Sigalas†
Research Center of Crete–FORTH, P.O. Box 1527, 71110 Heraklion, Crete, Greece
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We have investigated classical waves propagating in periodic binary composites. For electromagnetic waves the network topology, in which the low-velocity material forms a continuous network, is more favorable for the appearance of gaps. In contrast, for scalar and elastic waves the cermet topology, in which the low-velocity material consists of isolated inclusions surrounded by the high-velocity host material, is more favorable.

I. INTRODUCTION

In the last few years the problem of classical wave (CW) propagation in composite random or periodic media has received increased interest,[1,2] initially because of its connection to the problem of localization. It soon became apparent that future useful devices may be based on some aspects of CW propagation,[1] in particular on the possible existence of frequency gaps. Subsequently, a lot of theoretical and experimental work concerning this question has been done.[3–11] The theoretical methods have been proved very accurate and they can actually be used to design materials with the desired properties.[5,6]

The composite materials in question consist of two components of different propagation velocities. It should be pointed out that in the case of a single inclusion embedded in an infinite host material, stronger scattering is produced if the inclusion is a low-velocity material than vice versa. Thus, in all cases we shall refer to the low-velocity component of the composite as the scattering material (or component), while the high-velocity component shall be referred to as the host material. One can distinguish two cases regarding the topology of the scattering component: the cermet topology,[12] where the scattering material consists of isolated inclusions, each of which is completely surrounded by the host material, and the network topology, where the scattering material is connected and forms a continuous network running throughout the whole composite.

Previous theoretical studies have indicated that for elastic (EL), acoustic (AC), or scalar (SC) waves, the cermet topology is, in general, more favorable for the development of gaps. In contrast, for electromagnetic (EM) waves, the network topology seems to be the more favorable. In the present paper we analyze some results from previous studies, we present some new results for two-dimensional (2D) cases and we briefly discuss possible explanations of these observations. In 2D, the components of the vector waves, such as EM and EL waves, could be decoupled, so we can more easily study the effect of each wave component in the appearance of the gaps.

There are two criteria for deciding which topology is more favorable for the appearance of gaps. The first one is to check the ratio of the size of the gap over the midgap frequency ($\delta\omega/\omega_g$) vs the filling ratio f, of the scattering material or the ratio r, of the velocity of the host to the velocity of the scattering component. The most favorable structures are those with the greater values of $\delta\omega/\omega_g$; the latter is usually computed for high-r values (where saturation is taking place) and at the optimum value of f. The second way is to consider the critical velocity ratio r_c, for which the first gap just opens up vs the filling ratio f, of the scattering component; in general, these curves have a minimum for $f=f_m$, at which $r_c=r_c^m$; the structures with the smallest r_c^m are the most favorable.

II. CLASSICAL WAVE EQUATIONS AND NUMERICAL METHODS FOR THEIR SOLUTION

In the present paper, as well as in the previous relevant work,[3–9] the following classical waves were studied.

(i) Acoustic (scalar) waves (in fluids):

$$-\omega^2 p=\lambda\nabla\left[\frac{\nabla p}{\rho}\right], \tag{2.1}$$

where p is the pressure, ρ is the density, and λ is the Lamé coefficient (which, for an isotropic fluid is the same as the bulk modulus). In the case where ρ is everywhere, the same Eq. (2.1) reduces to the ordinary scalar wave equation,

$$-\omega^2 p=\frac{\lambda}{\rho}\nabla^2 p\ . \tag{2.2}$$

(ii) Electromagnetic waves in an isotropic (but not homogeneous) medium:

$$\nabla\times(\varepsilon^{-1}\nabla\times\mathbf{H})=\frac{\omega^2}{c^2}\mathbf{H}\ , \tag{2.3}$$

where $\mathbf{H}$ is the magnetic field, $\mathbf{E}=(ic/\omega\varepsilon)\nabla\times\mathbf{H}$ is the electric field, ε is the dielectric function, and c is the velocity of light in the vacuum.

(iii) Elastic waves in solids:

$$-\omega^2 u_i=\frac{1}{\rho}\left\{\frac{\partial}{\partial x_i}\left[\lambda\frac{\partial u_1}{\partial x_1}\right]+\frac{\partial}{\partial x_1}\left[\mu\left[\frac{\partial u_i}{\partial x_1}+\frac{\partial u_1}{\partial x_i}\right]\right]\right\}, \tag{2.4}$$

where u_i ($i=1,2,3$) are the Cartesian components of the displacement vector, ρ is the density, λ and μ are the Lamé coefficients, x_i $(i=1,2,3)$ are the Cartesian components of the position vector, and summation over repeated indices is implied. In the elastic case, the bulk modulus B equals $\lambda+\frac{2}{3}\mu$.

The parameters ρ, λ, μ, and ε in the scattering component (low-velocity material) are indicated by a subscript s and that of a host (high-velocity material) by a subscript h. The wave velocities in each component for cases (i)–(iii) are given by $\sqrt{\lambda/\rho}$, $c/\sqrt{\varepsilon}$, and $\sqrt{(\lambda+2\mu)/\rho}$ (longitudinal) or $\sqrt{\mu/\rho}$ (transverse), respectively.

Due to the periodicity of the coefficients ρ, λ, μ, and ε, the solutions can always be chosen to satisfy the Floquet-Bloch theorem,

$$f(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}\varphi_{\mathbf{k}}(\mathbf{r}) , \tag{2.5}$$

where f is the solution (in the scalar case) or any component of the solution (in the vector cases) of Eqs. (2.1)–(2.4); $\varphi_{\mathbf{k}}(\mathbf{r})$ has the same periodicity as the coefficients of the corresponding CW equation; and the wavevector $\mathbf{k}$ is restricted to the first Brillouin zone. According to the so-called plane-wave method, the periodic functions ρ, λ, μ, ε, and φ_k are expanded in a Fourier series. Thus, the wave equation is transformed to an (infinite) matrix equation for the coefficients of the Fourier series of $\varphi_{\mathbf{k}}(\mathbf{r})$. By keeping in the expansion a finite number M of Fourier components, an approximate $M\times M$ [case (i)], or $2M\times 2M$ [case (ii)], or $3M\times 3M$ [case (iii)] matrix equation is obtained. M is increased until a satisfactory convergence (or the order of 1% or less) is obtained. Usually, a value of M around 350 is adequate to achieve a 1% accuracy. In Secs. III and IV we present results obtained through the plane-wave method just described.

III. WAVES IN THREE-DIMENSIONAL SYSTEMS

A. Scalar and acoustic waves

We consider here the fcc structure which is the most favorable for the appearance of gaps, although similar conclusions are reached if we consider other structures such as bcc, diamond, simple cubic (sc), simple hexagonal (sh), and hexagonal-closed-packed (hcp). For $r\geq 4$ and for the cermet topology (with spherical inclusions and $f=0.10$) the maximum $\delta\omega/\omega_g$ is 0.35. Again, for $r\geq 4$ but for the network topology (where the scattering material occupies the space left between overlapping spheres) with $f=0.05$, the maximum $\delta\omega/\omega_g$ equals 0.30. The corresponding figures for r_c^m are: 1.73 for the cermet topology (obtained when $f_m\approx 0.10$) and 2.24 for the network topology (obtained when $f_m\approx 0.05$).[7,8] The above results strongly suggest that the cermet topology is more favorable than the network topology for the appearance of gaps in the propagation of scalar waves.

For acoustic waves there is an additional parameter, the density ratio $y=\rho_s/\rho_h$ (s refers to the scattering and h to the host component); for the cermet topology, by decreasing y below unity, the gaps become wider and the bands narrower. In any case, this extra parameter does not seem to modify our conclusion regarding the superiority of the cermet topology.

B. Elastic waves

We consider here extreme solids (in the sense that the ratio of the shear elastic constant μ to the bulk modulus B has the maximum empirical value, $\mu/B=1.5$, corresponding to a minimum ratio of longitudinal to transverse velocity equal to $\sqrt{2}$), although similar conclusions have been reached by considering more realistic values of the ratio μ/B. It is worthwhile to mention that in the case of solids (with μ/B of the order of unity), in contrast to what happens to fluids, by increasing the ratio $y\equiv\rho_s/\rho_h$ above unity we favor the formation of spectral gaps.[8,9] We report here results based on the fcc structure; similar conclusions can be reached by considering other structures including the diamond which seems to produce slightly wider gaps.[8] For the cermet topology (with spherical inclusions, $y=1$ and $f_m\approx 0.3$) the minimum threshold value of the velocity ratio is $r_c^m=4.2$ (the corresponding value for the diamond lattice is about 4). For the network topology (consisting of the space left between slightly overlapping spheres) and for $y=1$, $r_c\approx 7.5$ for $f_m\approx 0.25$. Thus, for the elastic cases examined here, the cermet topology seems again to be more favorable for the creation of spectral gaps.

C. Electromagnetic waves

In this case, in contrast to SC and EL waves, gaps do not seem to appear but for a few lattice structures; in particular, the lowest lying "would be" gap for EM waves propagating in fcc, bcc, sh, hcp structures[3,6] does not quite open up, although a region appears where the density of states is almost zero, the so-called pseudogap,[5] however, a rather wide gap appears in the diamond lattice.[5] It has been found that in the quasicermet topology (with spherical inclusions just touching each other, i.e., $f_m\approx 0.34$), the maximum $\delta\omega/\omega_g$ is 0.21. In the opposite case of the network topology (where the scattering material occupies the space left between overlapping spheres) the maximum $\delta\omega/\omega_g$ is 0.29 for $f_m=0.19$ and r_c as low as 3.6; $\delta\omega/\omega_g\approx 0.46$ at saturation[5] for $r\geq 8$ and $f_m\approx 0.19$. Several other—easier to construct—structures with an appreciable gap have been proposed,[6,13] all these structures have the network topology.

The main conclusion from the previous discussion is that for EM waves, in contrast to what happens with SC and EL waves, the network topology seems to be more favorable for gap creation than the cermet topology.

IV. WAVES IN TWO-DIMENSIONAL SYSTEMS

In this section we report new results for systems consisting of identical parallel (to the z axis) infinite cylinders periodically placed within a material matrix; when the propagation is perpendicular to the z axis the problem becomes a 2D one. The filling ratio of the cylinders is denoted by x; when the cylinders are the low-velocity (scattering) component, $x=f$, and we have the cermet topology [as long as x is below a critical value x_c (e.g.,

$x_c = 0.785$ for circular cylinders in a square lattice)]. If the cylinders are the high-velocity material, the scattering component is the matrix, $f = 1 - x$, and we have the network topology (as long as $x < x_c$, or, equivalently, $f > 1 - x_c$).

A. Scalar waves

In Fig. 1 we plot the threshold value r_c, for the first and second gap vs the filling ratio x, of the cylinders (in the present case the cylinders have square cross section and are placed in such a way that their axes of symmetry coincide with the corresponding axes of the unit cell). For cylinders of the low-velocity material (i.e., for the cermet topology) the first (second) lowest gap appears for r_c^m about 1.73 (2.2) for cylinders with $f_m = x_m \sim 0.25$ (0.30); in the opposite case where the cylinders are the high-velocity material (i.e., for the network topology) the threshold value r_c^m is 1.92 or 2.8 at $f_m = 1 - x_m = 0.42$ or $f_m = 1 - x_m = 0.3$ for the second and the first gap, respectively. The results are nearly the same for cylinders with circular cross section. We have also considered a 2D hexagonal lattice; for cylinders of the low-velocity material (i.e., for the cermet topology) the first gap appears for r_c^m as low as 1.31, in contrast to the opposite case (network topology) in which the first gap does not appear at all, due to a degeneracy at the $(\frac{4}{3}, 0)$ point.

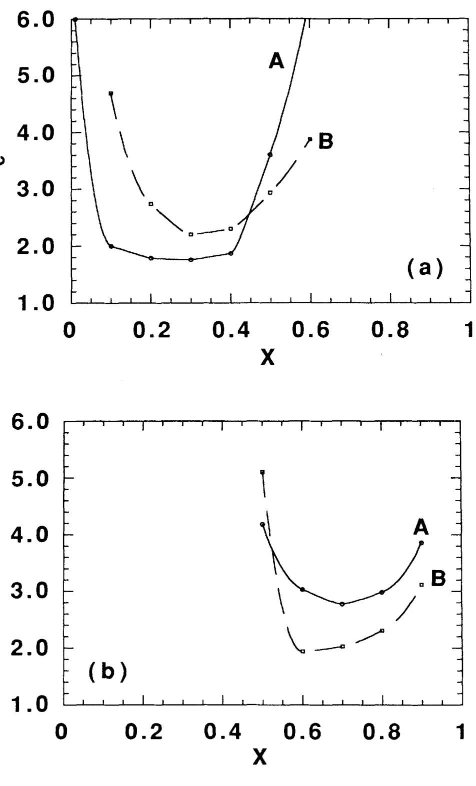

FIG. 1. The threshold value of the velocity ratio, r_c, vs the filling ratio of the cylinders x, for the first (A) and second (B) gap and for SC waves propagating in 2D square lattice consisting of cylinders with square cross section and with axes of symmetry coinciding with the corresponding axes of the unit cell. The cylinders are either the low- (panel a, cermet topology) or the high- (panel b, network topology) velocity material; the scattering material filling ratio f, equals x (case a) or $1-x$ (case b).

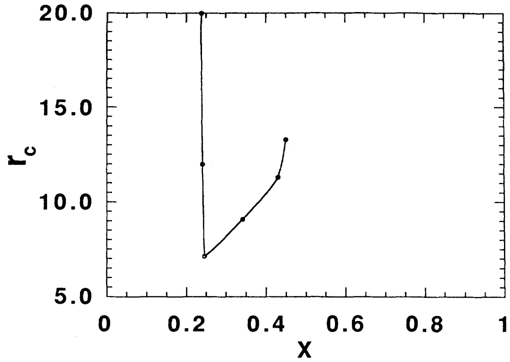

FIG. 2. r_c vs x for EL waves in square lattice with cylinders of circular cross section; the cylinders are the low-velocity material (cermet topology case) ($c_1/c_t = \sqrt{2}$ everywhere, $y \equiv \rho_s/\rho_h = 4$).

B. Elastic waves

It is more difficult to find EL wave gaps in 2D systems rather than in 3D systems,[8] in particular, for density ratio $y = 1$ it is impossible to find gaps even for r as high as 25. Figure 2 shows the value of r_c for the first gap of EL

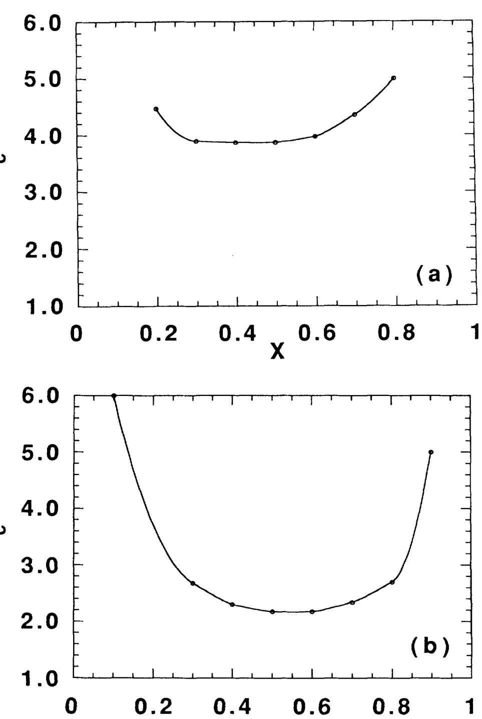

FIG. 3. r_c vs x for p-polarized EM wave in square lattice with cylinders of square cross section and with axes of symmetry coinciding with the corresponding axes of the unit cell; the cylinders are either the low- (panel a, cermet topology) or the high- (panel b, network topology) velocity material; the scattering material filling ratio f equals x (case a) or $1-x$ (case b).

waves propagating in a square lattice consisting of cylinders (with circular cross section) which are the low-velocity material; (i.e., the cermet topology case); the density ratio is $y=4$. There is a sharp minimum for $f_m=x_m \sim 0.25$ and $r_c^m=7.2$. When the cylinders are the high-velocity materials (i.e., the network topology) it is again impossible to find gaps even for r as high as 25.

C. Electromagnetic waves

For waves propagating perpendicularly to the z axis the s (**E** field parallel to the cylinder axis) and p (**E** field perpendicular to the cylinder axis) polarized waves can be described by two decoupled wave equations. The equation for the s-polarized wave is

$$\nabla^2 E+\frac{\omega^2}{c^2}\varepsilon E=0 , \tag{4.1}$$

where $E \equiv E_Z$; $\varepsilon=\varepsilon(r)$ is the dielectric constant, ω is the frequency, and c is the speed of light in the vacuum. Equation (4.1) is identical with the SC wave equation which we have already considered in a previous subsection. The equation for the p-polarized wave has the form

$$\nabla \cdot \left[\frac{\nabla H}{\varepsilon} \right] + \frac{\omega^2}{c^2} H=0 , \tag{4.2}$$

where $H=H_Z$. In Fig. 3 we plot r_c vs x for p-polarized waves, square lattice, and cylinders with square cross section placed with their axes of symmetry coinciding with the corresponding axes of the unit cell; for cylinders of the low-velocity material (i.e., the cermet topology case) $r_c^m \approx 3.9$ at $f_m=x_m \approx 0.40$; in the opposite case where the cylinders are the high-velocity material (i.e., the network topology case) $r_c^m \approx 2.1$ (at $f_m=1-x_m \approx 0.45$) which is about half the previous value. For cylinders with circular cross section, $r_c^m \sim 3.6$ (2.4) for the cermet (network) topology at filling ratios nearly the same as for cylinders with square cross section. We have also considered a 2D hexagonal structure consisting of cylinders with circular cross section; the corresponding r_c^m is 2.9 and 1.4 for the cermet and the network topology, respectively, at the same filling ratios as in the square lattice.

In conclusion, the network topology, in which the low-velocity material forms a continuous, connected network is much more favorable for gap formation in all cases we have examined; this seems to be a rather universal feature for EM waves independently of the geometric shapes and lattice structures. The size of the gap depends, of course, on these parameters with circular cylinders arranged in a hexagonal lattice being the most favorable configuration.

TABLE I. The minimum threshold velocity ratio r_c^m, for some representative cases.

Type of wave	Topology	Lattice structure	Geometry of the scattering material	Filling ratio of scattering material	Minimum threshold velocity ratio r_c^m
SC	C	fcc	Isolated spheres	0.10	1.7
SC	N	fcc	Between overlapping spheres	0.05	2.2
EL	C	fcc	Isolated spheres	0.30	4.2
EL	N	fcc	Between overlapping spheres	0.25	7.5
EM	quasi-C or quasi-N	Diamond	Touching spheres	0.34	2
EM	N	Diamond	Between overlapping spheres	0.19	2
SC	C	2D square	Isolated tetragonal cylinders	0.25	1.7
SC	N	2D square	Between isolated tetragonal cylinders	0.30	2.8
EL	C	2D square	Isolated circular cylindersr	0.25	7.2
EL	N	2D square	Between isolated circular cylinders	No gap	No gap
EM p-polarized	C	2D square	Isolated tetragonal cylinders	0.50	3.9
EM p-polarized	N	2D square	Between isolated tetragonal cylinders	0.50	2.1

V. CONCLUSIONS

The minimum threshold values r_c^m of the velocity ratio for which the first gap just opens up are shown in Table I for some representative cases. For scalar (SC) and elastic (EL) waves propagating in both 3D and 2D structures, a universal feature seems to emerge in spite of all the differences: the cermet topology (where the low-velocity component consists of isolated inclusions, each one surrounded by the high-velocity host material) is more favorable for spectral gap formation than the network topology (where the low-velocity material is connected to form a continuous network running throughout the material).

In contrast, for the electromagnetic (EM) waves, the network topology is clearly more favorable; this is more obvious in the case of p-polarized EM waves propagating in 2D structures (see Table I); for the 3D case, it appears that there is no difference between a pure network case and a quasinetwork (or quasicermet) case as far as the value of r_c^m is concerned. However, even in this not so clear comparison, the pure network case produces maximum values of $\delta\omega/\omega_g$ twice as big as the quasinetwork case, thus providing further supporting evidence for our conjecture. It is tempting to associate the different behavior of the EM waves to the greater polarizability of the network topology. Indeed, the polarizability is an increasing function of the linear dimension of a connected body. In the network topology, the linear dimension of the scattering material is infinite and, consequently, the polarizability and the scattering amplitude is maximized. However, given the fact that gaps appear at wavelengths comparable to the size of the unit cell and that the polarizability is not expected to continue to increase with the linear dimension for sizes exceeding the wavelength, it appears that the previous argument is not so convincing. Another path towards an explanation of the observed differences between the SC and EL waves on the one hand and the EM waves on the other may possibly start out from the scattering amplitude by a single sphere (or circle in 2D). For SC and EL waves the lowest lying resonance is due to the isotropic scattering (s-wave scattering). In the periodic composite, this resonance is reinforced by multiple scattering from neighboring spheres and may lead to the formation of the gap. Since the scattering is mainly isotropic, the close packed arrangement (associated with cermet topology) seems to be more favorable for enhancing the multiple scattering than the network topology which, by its very nature, is more directional. On the other hand, for EM waves (due to their pure transverse nature) there is no isotropic scattering from a sphere and the lowest lying resonances are of p character (corresponding to spherical harmonics of $l=1$). The directionality of this single-scattering amplitude may possibly be better exploited by a network topology leading to wider gaps.

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*Also at the Department of Physics, University of Crete.
†Present address: Ames Laboratory, ISU, Ames, Iowa 50011-3020.

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