Evidence of Fano-Like Interference Phenomena in Locally Resonant Materials

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Sonic crystals consisting of three-dimensional arrays of units which exhibit localized resonances have been discovered recently. Here, it is shown that their two-dimensional counterparts behave in a similar manner. Particularly, it is observed that the transmittance spectra show very asymmetric peaks which are explained as a Fano-like interference phenomenon. A finite difference time domain method is employed to perform a comprehensive study of the resonance line shape as a function of the mass density of the structural units. Also, a simple analytical model is introduced to give an intuitive account of the origin of the interference phenomenon.

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A new area of research has been opened in the field of sonic crystals since the recent work of Liu *et al.* [1] who, based on the idea of localized resonant structures, demonstrated the existence of spectral gaps at extremely low frequencies (2 orders of magnitude smaller than the Bragg frequency associated to the lattice constant). At these frequencies the transmission amplitude shows very asymmetric peaks whose origin has not been discussed yet to the best of our knowledge.

Strongly asymmetric peaks were first theoretically described by Fano [2] when he studied the inelastic autoionizing resonances in atoms. The asymmetry (Fano profile) was explained as the result of the interference between the discrete resonance with the smooth continuum background in which the former is embedded. The Fano profiles deriving from this phenomenon have been observed commonly in other atomic studies [3], but it is not exclusive of atomic physics. In semiconductor physics, these asymmetric line shapes have been reported in doped materials, such as the absorption [4] and Raman scattering [5] spectra of impurities. More recently, in intrinsic bulk GaAs and in undopped superlattices [6,7] and in quantum dots [8] a similar behavior has been found.

The analogy between scattering properties of electrons and phonons suggests that this type of feature can appear in vibrational systems [9].

This Letter analyzes the transmission of elastic waves across a crystal slab made of a two-dimensional (2D) array of structural units which exhibit localized resonances. It will be shown that the resonant features in the transmission spectra can be described by the well-known Fano profile. Moreover, the parameters that define that profile have been investigated as a function of the mass density employed in the core of the units. The resulting behavior shows a close analogy with the behavior of autoionizing resonances in He-like ions as a function of the nuclear charge Z [3]. Also, it will be shown that a very simple one-dimensional (1D) model with analytical solution reproduces the transmission features and supports our assumption that the origin of the resonance profiles is a Fano-like interference.

The structural units used to build the sonic crystal consist of infinitely long cylinders made of an inner high mass core (10 mm diameter) and a coating (2 mm thick) of an elastically soft material. The units are arranged on a square lattice (15 mm of lattice parameter) and are embedded in epoxy, which acts as a hard matrix material. As coating material we have used rubber polymer [1]. These geometrical and structural parameters have been chosen because they provide the maximum complete gap at the lowest frequencies [10]. Different materials have been employed in the core of the cylinders, whose elastic data are given in Table I.

For a normal incidence of the wave front, the elastic band structure of the periodic 2D systems made with cylindrical units can be decoupled in two kinds of modes [11]: modes corresponding to pure transverse motion $u_z(x, y)$, where z defines the cylinder axis, and in-plane modes $\mathbf{u}(x, y) = u_x\hat{x} + u_y\hat{y}$, which are associated to motions in the plane perpendicular to the cylinder axis.

As a typical example Fig. 1 shows the dispersion relation for the in-plane modes of Au cylinders in two cases: Figure 1(a) represents the structure of coated cylinders described above while Fig. 1(b) corresponds to a simple binary system made of uncoated cylinders in epoxy. It is important to notice the huge difference in the frequency

TABLE I. Physical parameters of the materials employed in the core of the coated cylinders.

Material	ρ (Kg m^{-3})	c_l (m s^{-1})	c_t (m s^{-1})
Au	19 500	3360	1239
Pb	11 600	2490	1133
Steel	7800	5050	3080
Ti	4540	6070	3125
Al	2730	6800	3240
Epoxy	1180	2535	1157

scale used in each figure. The band structures have been calculated by a variational method [12]. Details of the calculations can be found elsewhere [10].

The system made of coated cylinders [see Fig. 1(a)] has a gap at extremely low frequencies; its bottom is 2 orders of magnitude lower than the one of the corresponding binary systems (with no coating). This result mimics the one found by Liu *et al.* [1] for a cubic lattice of spheres. Also, it is worth noticing frequency regions of no dispersion in the band structure (flat bands), which corresponds to localized modes, and modes (such as the ones at the Γ point)

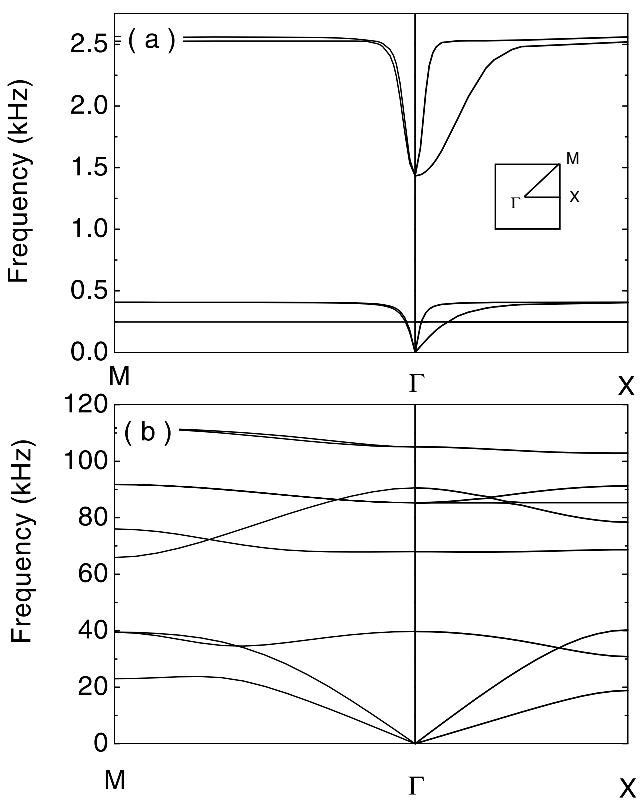

FIG. 1. (a) In-plane elastic modes, $\mathbf{u} = u_x\hat{x} + u_y\hat{y}$, of a square lattice of Au cylinder coated with rubber polymer in a epoxy background. (b) In-plane modes for a similar structure made with uncoated cylinders. The parameters used in the calculation for the coating are $\rho_{\text{poly}} = 1300$ Kg m^{-3}, $c_{l,\text{poly}} = 23$ m s^{-1}, $c_{t,\text{poly}} = 6$ m s^{-1}. The ones of the background are $\rho_{\text{epox}} = 1180$ Kg m^{-3}, $c_{l,\text{epox}} = 2535$ m s^{-1}, $c_{t,\text{epox}} = 1157$ m s^{-1}. The inset shows the 2D Brillouin Zone and its special points.

that also have zero group velocity, which also present a localized pattern. The very flat band at 0.25 kHz, which cannot be excited by an incident wave in the epoxy background, corresponds to localized modes in the polymer due to its low speeds. As discussed below, an elastic wave traveling across finite structures with localized modes interacts with them, but also part of the wave can use a nonresonant way to travel across the structure. As a consequence, an interference phenomenon between both traveling waves occurs, which results in characteristic features (resonant peaks with a very asymmetric profile) in the transmission spectra. This phenomenon was first described by Fano in atomic systems [2].

Let us consider the transmission problem through a slab of our composite. It is assumed that the layers of coated cylinders are bounded by semi-infinite media (the epoxy) on both sides. A traveling wave packet is supposed to arrive from one side and crosses the slab. The second-order time-differential equation is written in the following set of canonical, first-order equations:

$$\partial \mathbf{v}/\partial t = \nabla \cdot \boldsymbol{\sigma}/\rho(x, y), \tag{1}$$

$$\partial \mathbf{u}/\partial t = \mathbf{v}, \tag{2}$$

where $\mathbf{v}$ is the wave velocity and $\boldsymbol{\sigma}$ the stress tensor. These equations are solved by the finite-difference time-domain (FDTD) method using central differences [13–15].

Figure 2 plots the transmission spectra across different slabs of Au cylinders in a square configuration (see inset). The spectra for the structures including 3 (continuous line) and 6 ML (dashed line) of coated cylinders show resonance features absent in the structure of uncoated cylinders. These features can be assigned to localized modes in the elastic band structure of the corresponding infinite system. Thus, the transmission deep observed at 0.33 kHz corresponds to the flat band at 0.40 kHz in Fig. 1(a). On the other hand, the very asymmetric peak in the transmission centered at 1.57 kHz can be assigned to the zero group velocity modes at 1.43 kHz in the same band structure. These differences in frequency positions are mainly due to the fact that the phononic band structure is not fully defined in a finite structure. The finite slab's thickness also explains why the gap predicted by the band structure calculation is not completely formed in the transmission spectra.

In this work we concentrate on the analysis of the first resonance peak. This peak is associated with a vibrational motion of the inner core [10], such as in the systems made of coated spheres [1]. Figure 3 shows their resonance profiles for the different materials under study. On the other hand, the second resonance peak slightly depends on the inner core material, and it is mainly associated with the rubber coating.

A more physical insight of the origin of the profiles shown in Fig. 3 can be obtained using a simple 1D model. In this model we consider an infinitely long chain of masses m joined by springs of constant k simulating the continuum of frequencies for the transmission of

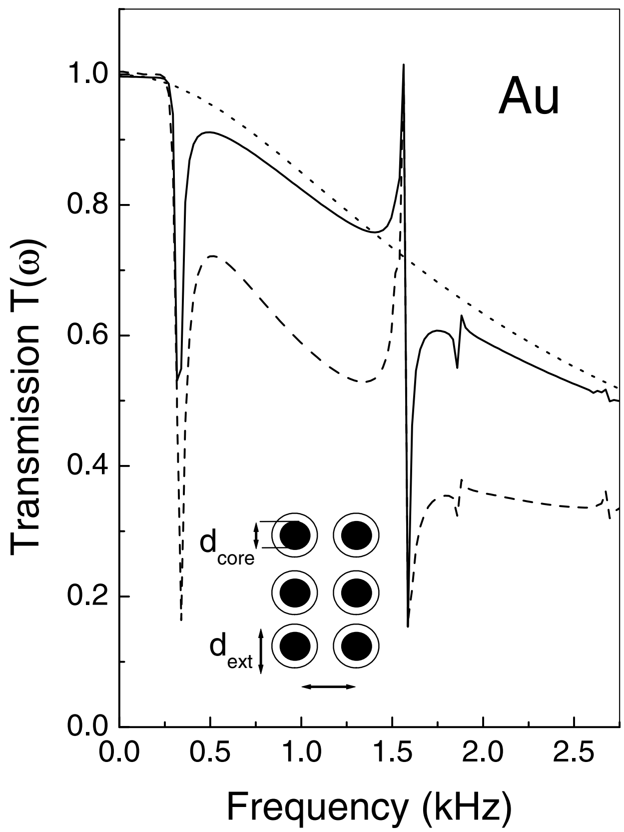

FIG. 2. The continuous (dashed) line represents the FDTD transmission amplitude across a slab of 3(6) rows of coated cylinders ($d_{ext} = 14$ mm) arranged on a square lattice ($a = 15$ mm). The cylinder inner core is gold ($d_{core} = 10$ mm). The coating and the background are the same as in Fig. 1(a). The dotted line defines the transmission for a similar structure made of uncoated cylinders.

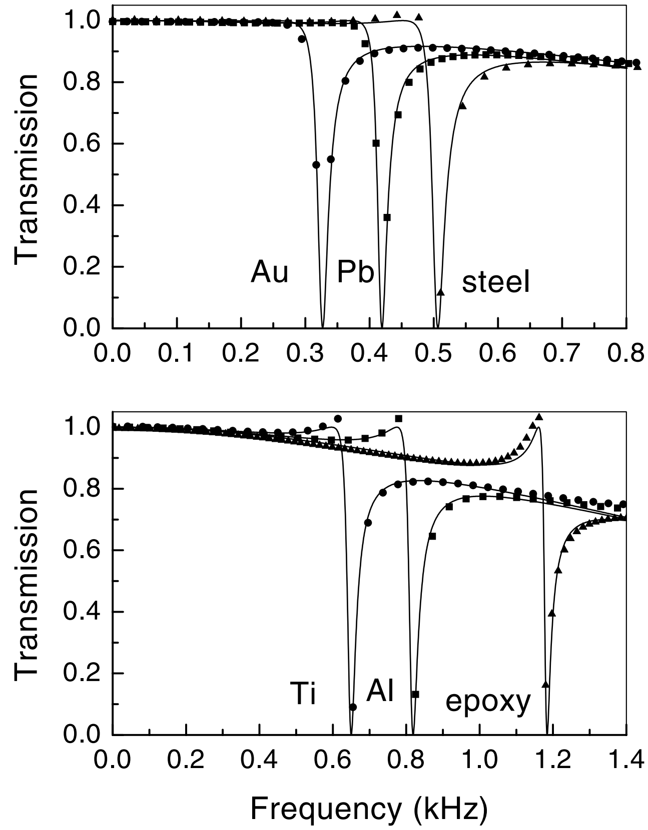

FIG. 3. Behavior of the first resonant peak observed in the transmission of in-plane elastic waves across a 3 ML slab of coated cylinders for different core materials. The symbols represent the transmission calculated by the FDTD method. The continuous lines define the fits made with the 1D model in Eqs. (6) and (7).

vibrational waves in the epoxy medium. At a certain point of the chain we introduce a different mass m_1 which is coupled to a hanging mass M by a spring of constant K. The resonant frequency $\omega_0 = \sqrt{K/M}$ represents the vibrational mode of the cylinder's core in the slab.

The transmission amplitude for a vibrational wave crossing the 1D structure described above is given by [16]

$$T(\omega) = 4k^4|G_{00}(\omega)|^2 \times \mathrm{Im}g_L \times \mathrm{Im}g_R\,, \tag{3}$$

where the left and right Green functions of the semi-infinite chain are

$$g_L = g_R = g = \frac{(\omega^2 m - 2k) + i\sqrt{\omega^2 m(4k - \omega^2 m)}}{2k^2} \tag{4}$$

and the diagonal element of the Green function of the total system is

$$G_{00}(\omega) = \frac{\omega^2 M - K}{(\omega^2 M - K)(\omega^2 m_1 - 2k^2 g - 2k) - K\omega^2 M}\,. \tag{5}$$

If one inserts Eqs. (4) and (5) into Eq. (3), the total transmission $T(\omega)$ at very low frequencies ($\omega^2 m \ll 4k$) is

$$T(\omega) = \frac{(\omega^2 - \omega_0^2)^2}{(\omega^2 - \omega_0^2)^2 + \omega^2[\sqrt{b}\,(\omega^2 - \omega_0^2) - \alpha]^2}\,, \tag{6}$$

where $b = (m_1 - m)^2/4km$, and $\alpha = K/\sqrt{4km}$.

For frequencies close to the resonance ($\omega \approx \omega_0$) it is easy to cast the above formula in an expression where the Fano profile [2] is clearly identified:

$$T(\omega) = t^0(\omega)\,\frac{(q_s + \varepsilon)^2}{1 + \varepsilon^2}\,, \tag{7}$$

where $t^0(\omega) = 1/(1 + \omega^2 b)$ gives the transmission of the background where the resonant mode is embedded, $\varepsilon = (\omega^2 - \omega_s^2)/\Gamma_s$($\omega_s$ and Γ_s being the frequency position and the width of the resonance), and the parameter q_s is proportional to the ratio of transmission amplitudes for the resonant and nonresonant channels. The sign of q_s depends on the phase shift between the two channels. These parameters are related to the parameters used in the 1D model by: $\omega_s^2 = \omega_0^2 - \Delta_s$, $\Gamma_s = \omega_0 a/(1 + \omega_0^2 b)$, and $q_s = -\Delta_s/\Gamma_s$, where $\Delta_s = \omega_0^2\sqrt{b}\,\alpha^2/(1 + \omega_0^2 b)$. They

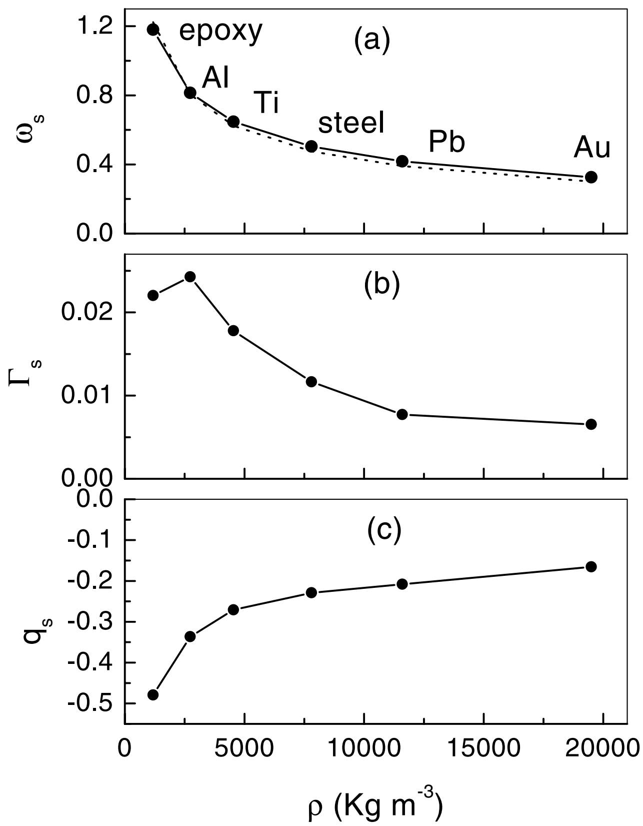

FIG. 4. Behavior of parameters ω_s (a), Γ_s (b), and q_s (c) [see Eq. (7)] used to fit the lowest resonant peak in the transmission across a 3 ML slab of coated cylinders.

can be used as a parameter set to fit the transmission calculated by the FDTD method. The solid lines in Fig. 3 show the fitted curves while the symbols represent the FDTD transmissions of the different systems under study. The fairly good fittings support both the 1D model and the parametrized Fano formula obtained from it.

In Fig. 4 the behavior of ω_s, Γ_s, and q_s is plotted as a function of the mass density. As expected, the renormalized frequency ω_s follows the law $\omega_s = \sqrt{\kappa/\rho}$. The fit to that law (the dotted line) yields and effective constant $\kappa = 1767\ \mathrm{kg\,m^{-3}\,s^{-2}}$. Figure 4 also shows the behavior of the Fano parameters when $\rho \to \infty$. Using the ρ law for ω_0, we obtain, for large ρ: $\omega_s \to 0$, $\Gamma_s \to 0$, and $q_s \to -\sqrt{b}$, which is in agreement with our findings of Figs. 4(a) and 4(b). It is interesting to compare the behavior of parameters Γ_s and q_s as a function of the density to the one of parameters Γ and q associated to photoionizing resonances in He-like ions as a function of the nuclear charge Z [3]. Both sets converge to a constant value for large Z and ρ. Nevertheless, while Γ increases when Z increases, Γ_s decreases when ρ increases. The main difference consists in the existence of more than one nonresonant channel in the atomic case. Although possible, the existence of additional nonresonant channels for the transmission in our elastic structures is not supported by our calculations. A similar analysis can be performed to the resonance feature associated with the peak at around 1.57 kHz, yielding to very good fitting with Eq. (7), and will be discussed elsewhere.

In conclusion, it has been shown that the transmission of elastic waves across structures made of coated cylinders present resonance features having a very asymmetric profile. The physical origin of these resonances has been investigated by a simple 1D mechanical model with analytical solution. It has been concluded that the existence of localized modes associated to the cylindrical units are at the origin of the interference phenomenon which results in the asymmetric profiles (Fano profiles) observed in transmission spectra. Also, their behavior have been characterized as a function of the cylinders' mass density.

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[1] Z. Liu *et al.,* Science **289**, 1734 (2000).
[2] U. Fano, Phys. Rev. **124**, 1866 (1961).
[3] I. Sánchez and F. Martín, Phys. Rev. A **49**, 5116 (1994); J. Phys. B **27**, 4105 (1994).
[4] G. Piao *et al.,* Solid State Commun. **75**, 835 (1990).
[5] F. Cerdeira *et al.,* Solid State Commun. **13**, 325 (1973); Phys. Rev. B **8**, 4734 (1973).
[6] C. Tejedor *et al.,* Phys. Rev. B **32**, 5303 (1985).
[7] V. Bellani *et al.,* Semicond. Sci. Technol. **11**, 1411 (1996).
[8] I. G. Zacharia *et al.,* Phys. Rev. B **64**, 155 311 (2001).
[9] A. Fellay *et al.,* Phys. Rev. B **55**, 1707 (1997).
[10] C. Goffaux, D. Caballero, and J. Sánchez-Dehesa (to be published).
[11] M. S. Kushwaha *et al.,* Phys. Rev. Lett. **71**, 2022 (1993).
[12] J. V. Sánchez-Pérez *et al.,* Phys. Rev. Lett. **80**, 5325 (1998).
[13] M. M. Sigalas and N. Garcia, Appl. Phys. Lett. **76**, 2307 (2000); J. Appl. Phys. **87**, 3122 (2000).
[14] J. O. Vasseur *et al.,* Phys. Rev. Lett. **86**, 3012 (2001).
[15] Ph. Lambin *et al.,* Phys. Rev. E **63**, 066605 (2001).
[16] This expression is a straightforward extension to the vibrational case of the expression known for electrons in a tight-binding model. See, for example, S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, United Kingdom, 1997).