Vibrations in one-dimensional hybrid Fibonacci/periodic structures

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We have studied the vibrational frequencies and atom displacements of one-dimensional systems formed by combinations of Fibonacci quasi-periodic stackings with periodic ones. The materials are described by nearest-neighbor force constants and the corresponding atom masses. These systems exhibit differences in the frequency spectrum as compared to the original simple Fibonacci generations. The most important feature is the presence of separate confinement of the atom displacements in one of the sequences forming the total composite structure for different frequency ranges.

Keywords: Multilayer systems; quasi-periodic structures, phonons.

1. Introduction

Quasi-regular structures have been intensively studied after the discovery of the quasicrystals [1–3]. These structures do not appear in nature, but can be produced in the laboratory [4–7] by molecular beam epitaxy (MBE) techniques. The interest of these systems was increased after the predictions that they would exhibit peculiar electron and phonon critical states and highly fragmented fractal energy spectra [8–15]. Many works have been devoted to study the properties of quasi-regular structures, as it can be seen in [16, 17]. These systems can be characterized by the presence of two different orders at different length scales. The periodic order of the crystalline arrangement of atoms in each layer is present at the atomic level, whereas the quasi-regular order due to the disposition of the different atomic layers following a given building sequence is the main feature at the long scale. This order is artificially produced during the growth process and is carefully controlled. Because the relevant physical scales influence different physical phenomena, it is possible, in principle, to exploit the quasi-regular order introduced in the system by tuning the corresponding length scales, thus opening new possible applications. The peculiar characteristics of these systems come from the interplay of these two different orders. Aspects of the role of this quasi-regular or aperiodic order in science and technology can be found in a recent review [18].

It is also important to find out if these materials can exhibit some additional physical characteristics or better performances than the periodic structures for specific applications. This has been found in the optical capabilities of quasi-regular systems concerning second [19] and third-harmonic generation [20], as well as the localization of light in these systems [21, 22]. Hybrid-order devices formed by periodic and Fibonacci quasi-regular blocks have been found to exhibit complementary optical responses [23]. Perfect optical transmission has been found in symmetric Fibonacci-class multilayers [24, 25]. Broad omnidirectional reflection bands have been predicted when combining Fibonacci sequences and periodic 1D photonic crystals [26].

The vibrational spectrum of quasi-regular structures presents a highly fragmented character [12, 15, 27]. By using different materials as the starting ones, we can have different realizations (ABAAB..., BABBA..., etc.), and thus, we can
have systems with primary and secondary gaps in different frequency ranges. By combining them, it could be possible to modify the frequency spectrum, and thus the vibrational properties of the resulting system as compared to those of the constituent quasi-regular systems. These are the structures to be studied here. In order to describe the properties of real quasi-regular systems it is necessary to describe these structures with enough physical realism in spite of the simplicity of the models.

We shall maintain in our study the basic simplicity employed in the majority of calculations [16], thus employing 1D linear chains while keeping all the basic physical ingredients in the model. The Fibonacci systems are the most studied ones because they can serve as 1D realizations of the quasicrystals [1–3].

The theoretical model and method of calculation are presented in Sec. 2. Section 3 deals with the results for the hybrid systems. Conclusions are presented in Sec. 4.

2. Theoretical model and method of calculation

We shall consider systems formed by combining a Fibonacci sequence, let us say ABAAB, and a periodic one ABABAB. We shall use the simplest model enabling us to get the essential physical data. Thus, we shall consider 1D linear chains with nearest neighbor interactions. In spite of its simplicity, this kind of model has been applied to the study of the properties of real materials with good results: theoretical analysis of Raman spectra of ultrathin Si-Ge superlattices [28] and finite stage Si-Ge Fibonacci superlattices [29], longitudinal phonons of alkali-metal graphite intercalation compounds [30] compared with the corresponding neutron scattering data [31]. This model can describe in a simple, but reasonably realistic way, the longitudinal phonons of a system in which two different materials A and B form the generating blocks of the different structures. The basic requirements are the force constants $k_A$, $k_B$ and the atom masses $m_A$, $m_B$, corresponding to the bulk materials A and B, respectively. The interactions between both materials will be represented by a force constant $k_I$, which we shall take as the mathematical average of both force constants $k_A$ and $k_B$, $k_I = (k_A + k_B)/2$, without loss of generality. Different choices of $k_I$ would modify numerical values in the frequency spectrum but not the overall physical picture. The minimum of requirements for the analysis of the problem is thus satisfied.

We shall specialize our model to the case of metals Al (medium A) and Ag (medium B). They have a very good lattice-parameter matching (within 0.3%) and they can be grown forming good quality interfaces [32] and superlattices [33]. The force constants for the bulk materials calculated from their elastic constants together with the atom masses are given in Table I.

<table>
<thead>
<tr>
<th>Material</th>
<th>$k$ (dyne/cm)</th>
<th>$m$ (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>$4.416 \times 10^4$</td>
<td>$4.805 \times 10^{-23}$</td>
</tr>
<tr>
<td>Ag</td>
<td>$5.032 \times 10^4$</td>
<td>$1.7912 \times 10^{-22}$</td>
</tr>
</tbody>
</table>

Our building blocks will be:

(i) a finite periodic repetition of blocks A-B formed by $N(N_A + N_B)$ atoms, where N is the number of A-B periods and $N_A$ ($N_B$) is the number of atoms of material A (B) included;

(ii) a finite Fibonacci generation grown by recursive stacking with generator blocks A and B, mapping the mathematical rule in the Fibonacci sequence.

We consider our structures as the period of a polypeptide superlattice, with $N_A=4$ and $N_B=3$, and obtain the eigenvalues by means of a direct diagonalization. The eigenvectors (atom displacements) are obtained by using the method described in Refs. 34 to 36 for block-tridiagonal matrices.

Other different boundary conditions, as the case with the extreme free atoms, give essentially the same frequency spectrum with the addition of some frequencies in the gaps corresponding to localized modes, as it could be expected.

3. Hybrid Fibonacci systems

The Fibonacci systems are produced by stacking recursively with two generator blocks A and B, mapping the mathematical rule in the Fibonacci sequence

$$S_1 = \{A\}, \quad S_2 = \{AB\}$$

$$S_3 = \{ABA\}, \cdots, \quad S_n = S_{n-1}S_{n-2}, \quad (1)$$

In Fig. 1a we present the frequency spectrum versus the order number for a periodic system formed by the repetition of the AB blocks 49 times. Figure 1b presents this information for a tenth order Fibonacci generation (composed of 220 A atoms and 102 B atoms). Figure 1c presents the same information for a hybrid structure having the former Fibonacci generation sandwiched between two blocks, each one formed by the periodic repetition of the AB blocks 49 times. Figure 1d gives the same information for a hybrid structure formed by the former periodic block sandwiched between two tenth order Fibonacci generations. One can see how the addition of the periodic block modifies the frequency spectrum of the Fibonacci generation. The fragmentation of the spectrum is kept, but the gaps at middle and intermediate frequencies are modified, in such a way that we can hope that some effects on the vibration patterns will also be affected.

Only from the spectra presented in the above figures, it is not possible to ascertain if some new features will be present in these structures. The atom displacements are important in the analysis of spectroscopic experiments [37]. To see if
some special feature of the vibrational spectrum of the hybrid structures exists, we shall look now to the atom displacements of some frequencies in different ranges of the spectrum.

Figure 2 gives information on the system formed by combining a periodic repetition of 49 $AB$ blocks sandwiched between two tenth order Fibonacci generations. In Fig. 2a we present the frequency spectrum, whereas in the other panels we present the atom displacement versus the atom number.

Figure 2b corresponds to $\omega=0.1097 \times 10^{14}$ Hz. This frequency belongs to the Fibonacci frequency spectrum and not to that corresponding to the periodic structure. It is seen now that only the atoms in the left block corresponding to the tenth Fibonacci generation exhibit non-negligible atom displacements.

Figure 2c corresponds to $\omega=0.3991 \times 10^{14}$ Hz. This frequency does not belong to the Fibonacci frequency spectrum, but to that corresponding to the periodic structure. It is seen now that only the atoms in the periodic block at the center exhibit non-negligible atom displacements and a notable regularity.

Figure 2d corresponds to $\omega=0.4192 \times 10^{14}$ Hz. This frequency belongs to the Fibonacci frequency spectrum and not to that corresponding to the periodic structure. It is seen now that only the atoms in the right block corresponding to the tenth Fibonacci generation exhibit non-negligible atom displacements.

Figure 3 presents information for the structure formed by combining a tenth Fibonacci generation sandwiched between two periodic repetitions of 49 $AB$ blocks. Figure 3a gives the frequency spectrum, and the remaining panels give the atom displacement versus the atom number.

Figure 3b corresponds to $\omega=0.1906 \times 10^{14}$ Hz. This frequency belongs to the periodic structure frequency spectrum, and we can see how the displacement is essentially confined to the left periodic block.

Figure 3c corresponds to $\omega=0.2120 \times 10^{14}$ Hz. This frequency corresponds to the Fibonacci frequency spectrum. It is seen now that only the atoms in the central block corresponding to the Fibonacci structure exhibit non-negligible atom displacements.

Figure 3d corresponds to $\omega=0.6011 \times 10^{14}$ Hz.
new possibilities due to the spectrum fragmentation not
odic superlattices having different gaps.
is also possible in hybrid structures combining different peri-
spectrum of the hybrid structure.
another patterns seen in aperiodic systems, such as the critical localization, are also present in the frequency spectrum. Other modes can exhibit different displacement patterns as those shown in Fig. 4 for the modes of the structure formed by combining a tenth Fibonacci generation sandwiched between two periodic repetitions of 49 $AB$ blocks with frequencies $\omega=0.0336 \times 10^{14}$ Hz and $\omega=0.1691 \times 10^{14}$ Hz. We can see here how these modes can propagate along the whole structure. Other patterns seen in aperiodic systems, such as the critical localization, are also present in the frequency spectrum of the hybrid structure.

The separate confinement of the displacements seen here is also possible in hybrid structures combining different periodic superlattices having different gaps.

Hybrid structures including aperiodic sequences open new possibilities due to the spectrum fragmentation not present in the hybrid structures, including only periodic systems.

4. Conclusions

We have studied the vibrational frequencies and atom displacements of structures formed by sandwiched periodic-Fibonacci-periodic, or Fibonacci-periodic-Fibonacci 1D heterostructures. In all the cases, we have seen modifications in the frequency spectrum only in the primary and secondary gaps. The most notable feature found in these structures is the existence of modes in different frequency ranges exhibiting atom vibrations confined to only one of the sequences forming the total structure, as in the case of normal cavities. This selective confinement of the atom vibrations is achieved with structures formed by two different materials only, but with the interplay of different orders at different length scales. These structures could be useful, at least in principle, in filtering and guiding systems. This effect found at the center of the Brillouin zone presents similarities with the surface, avoiding waves recently found in periodic superlattices on a substrate [38]. There are also similarities with the properties seen in the light propagation through Fibonacci quasicrystals [39, 40].

Acknowledgments

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