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# Phonon transmission via nanojunctions in BCC waveguides

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## Abstract

Coherent and ballistic phonon transport via nanojunctions between bcc lattices is presented. The model system A/B/A consists of a finite number of bcc atomic layers of an element B sandwiched between two bcc semi-infinite crystals of another element A. The matching method theoretical approach is used to study the dynamical properties of the bcc sandwich system. A calculation is presented for the coherent reflection and transmission scattering probabilities of the system phonons, as elements of a Landauer type scattering matrix. The scattering and transmission spectra via the nanojunctions are analyzed as a function of the incident frequency per propagating mode of the perfect bcc waveguides and as a function of the thickness of the sandwiched film and of a parameter that describes the nanojunction zones. The possible experimental measurements of this ballistic transmission in comparison with theoretical results should be a useful probe for the determination of alloying force constants across the interface between two such elements. Our results show that the nanojunction is an effective phonon splitter and suggest that its characteristics may be controlled by varying its nanometric parameters. Knowledge of these characteristics enables the authors to study all the vibrational properties of such a system.

**Key Words:** Nanojunction, coherent transport, sandwich system, elastic waves

**PACS:** 63.20.-e; 68.35.Ja; 68.35.Dv

## 1. Introduction

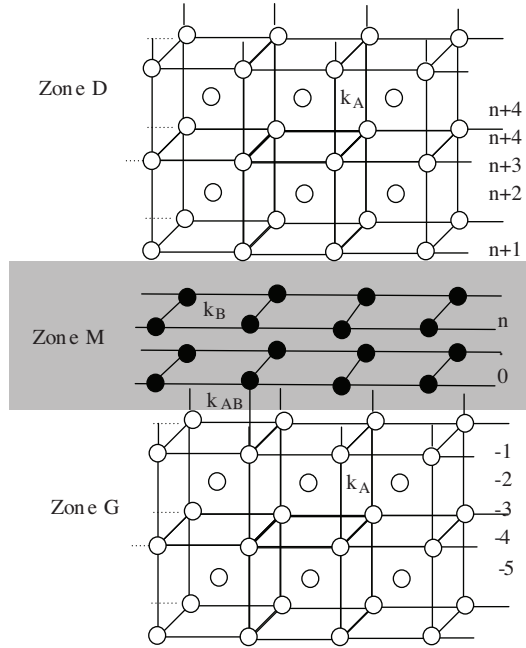
The theoretical and experimental understanding of the phonons and the dynamical properties of surfaces [1], with and without adsorbed atomic monolayer, are presently at a level comparable to that of the phonons of bulk in crystals. On the other hand, results of work on phonons in the adsorbed thin layers, interface and the

sandwich systems have yet to make their debut [2–3]. Recently in the largest laboratories of the world, several works [4–8] have been launched, with more attention accorded to sandwich systems.

A sandwich system is constituted from three different sub-systems: an ultra thin film and two semi-infinite materials. The thin film is placed between surfaces of both semi-infinite systems. This leads to the formation of two nanojunctions in the sandwiched system, due to both engendered interfaces.

Current techniques make possible the fabrication of nanojunctions which consist of only few atomic layers sandwiched between the semi-infinite crystals. Such nanojunctions are of increasing importance in many technical applications, [9–11]. The use of such nanojunctions in high technology requires a necessary basic knowledge for the adequate control of their properties. It is hence of interest to develop numerical calculations for appropriate models for these interfaces; and thus important focus is now being placed on theoretical techniques [2, 3, 12, 13] that address the problem of phonon transport across interfaces defined at the nanoscale and atomic level.

The purpose of this work is to present a calculation for the phonon ballistic transmission via a nanojunction of the A/B/A type, where B is an ultra thin film sandwiched between two bcc semi-infinite A crystals. In particular, we apply the theoretical calculations to the case where the thin film B is composed respectively by one, three and five atomic layers. A typical geometry is shown in Figure 1. We indicate that the dynamical properties of composite materials with surfaces or interfaces in the case of simple cubic system were also studied previously [14].



**Figure 1.** Schematic representations of a sandwiched B thin film between two perfect bcc semi-infinite A lattices. In the perfect lattice A, the atoms have the mass  $m_A$  and are connected to each other by elastic force  $k_A$ . In B lattice, each atom has the mass  $m_B$  and is connected by elastic force  $k_B$ . Atoms on opposite sides of the nanojunction are connected by elastic force  $k_{AB}$ . The layers  $m = 0, \dots, n$  constitute the slab zone.

In Section I, a description of the model is given and equations of motion are derived in a convenient form. Our study uses the harmonic approximation [15] and the equations of motion consider interaction between the nearest neighbors. In Section II, we present the expressions of the coherent and ballistic transmission and reflection coefficients as a function of the incident frequency, followed by a brief outline of the numerical algorithm used to evaluate these quantities. In Section III, we give the principal numerical results, their interpretations for the cases examined. Conclusions of this work is given in Section IV.

## 2. Basic elements of the model

We formulate the problem of phonon transmission across a two bcc solid-solid interfaces (labeled sandwich system) by considering two identical semi-infinite lattices A attached to a “scattering region.” The two semi-infinite perfect crystals are envisaged as waveguides for incident and scattered phonons. The scattering region (defect domain) consists of a finite number of bcc layers of lattice B integrated as a nanostructure coupling the independent two semi-infinite bcc A waveguides. A typical geometry is shown in Figure 1. The sandwiched film corresponds to the grey area. It gives two effective nanojunction domains.

The elastic constants on the perfect lattices, which represent the inter-atomic interactions in the harmonic approximation, are considered as  $k_A$  and  $k_B$  for nearest neighbor, respectively, on the A and B lattices. The elastic constants between neighbor sites, at the nanojunction domain, may differ from perfect values, and is hence labeled  $k_{AB}$ . The atomic masses, of A and B lattices, are denoted, respectively, by  $m_A$  and  $m_B$ . It is convenient next to define the following ratios:  $\mu = m_B/m_A$ ,  $r_d = k_{AB}/k_A$  and  $r_B = k_B/k_A$ . For simplicity we consider identical interatomic distance  $a$  between all adjacent atomic sites in different Cartesian directions on the interface domain and on the perfect bcc waveguide, neglecting any relaxation effects. The spacing between nearest neighbors is  $(\sqrt{3}/2)a$ . We take the axes  $x$  and  $y$  to be parallel to the plane of the lattices A and B, and the  $z$ -axis normal to the plane of the surfaces.

The dynamics of the perfect bcc system are described by the equations of motion of atomic sites  $l$ , which in the harmonic approximation may be expressed as

$$\omega^2 m(l) u_\alpha(l) = - \sum_{l' \neq l} \sum_{\beta} k(l, l') d_\alpha d_\beta / d^2 [u_\beta(l) - u_\beta(l')] \quad (1)$$

for  $(\alpha, \beta) \in \{x, y, z\}$ , and  $m(l)$  is the atomic mass at  $l$ .

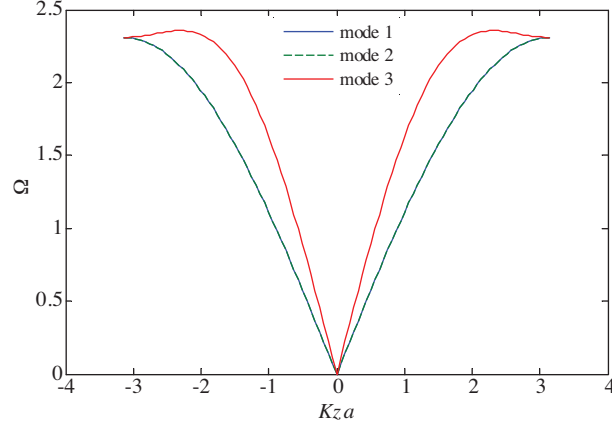
The radius vector  $\mathbf{d}$  between the atomic sites  $l$  and  $l'$  has Cartesian components  $d_\alpha$ . The elastic force constant between two sites is  $k(l, l')$ . The  $u_\alpha(l)$  is the corresponding vibration displacement vector for site  $l$ .

For sites  $l$  and  $l'$  distant from the inhomogeneous boundary to the left and right of the nanojunctions in Figure 1, the equations of motion may be cast in the matrix form

$$[\Omega^2 I - D(e^{i\varphi_x}, e^{i\varphi_y}, e^{i\varphi_z})] |u\rangle = 0 \quad (2)$$

where  $[\Omega^2 I - D(e^{i\varphi_x}, e^{i\varphi_y}, e^{i\varphi_z})]$  is a  $3 \times 3$  matrix, and  $|u\rangle$  is the corresponding vector for a column of the perfect bcc waveguide,  $I$  denotes a unit matrix. The quantities  $e^{i\varphi_x}$ ,  $e^{i\varphi_y}$ , and  $e^{i\varphi_z}$ , are the Bloch phase factors along the principal axes. Here,  $\varphi_\alpha = q_\alpha \mathbf{a}$  is the normalized wave vector, and runs over the interval  $[-\pi, +\pi]$  in the first BZ.  $\Omega = \omega / \omega_0$  is a dimensionless frequency. Note that the characteristic frequency  $\omega_0$  is not the same for the perfect A and B lattices;  $\omega_0 = \sqrt{k_A/m_A}$  for A, and  $\omega_0 = \sqrt{k_B/m_B}$  for B.

By diagonalizing the matrix of equation (2), one obtains the phonon dispersion branches for the perfect waveguides. The branches along the  $z$ -direction are presented in Figure 2, for a choice of incident angle  $\varphi_y = \varphi_x = 0$ , in terms of the normalized frequency for each of the A and B systems in the present approximation.



**Figure 2.** Typical dispersion curves of the perfect bcc crystallographic waveguide, presented over  $k_z a = [-\pi, +\pi]$  the first Brillouin zone, for incidence angle  $\varphi_x = \varphi_y = 0$ .

To illustrate the model, the propagating modes for the bcc perfect waveguides are shown in Figure 2 for a choice of incident angle  $\varphi_x = \varphi_y = 0$ , as a function of the normalized wavevector  $\varphi_z = k_z a$ , where  $\varphi_z$  runs in the interval  $[-\pi, +\pi]$  over the first Brillouin zone (BZ).

In this direction: ( $\varphi_x = 0$  and  $\varphi_y = 0$ ), there are three acoustical modes characterized by the limiting behavior  $\Omega_1$ ,  $\Omega_2$  and  $\Omega_3$  of their phonon branches, tending to zero frequency when the wavevector tends to zero. We note that two modes are degenerate in the interval frequency  $\Omega \in [0, 2.32]$ .

### 3. Nanostructure boundary dynamics and scattering

Analysis of the dynamics of the inhomogeneous atomic nanostructure generates an infinite set of coupled equations on both sides of the atomic nanojunction. In order to render the problem tractable we need to decouple the dynamics of a representative and irreducible set of sites at the inhomogeneous boundary of the interface domain from the rest of the system. This irreducible set is located in the scattering zone M of Figure 1.

For an incoming propagating wave in eigenmode with index  $i = 1, 2, 3$ , incident from the bottom in Figure 1 at a frequency  $\Omega$ , the resulting scattered waves due to the presence of the nanojunction domain are composed of reflected and transmitted parts. They are both solutions of equation (2) at the same frequency.

For atoms inside the perfect waveguide A to the bottom of the scattering region, the Cartesian components  $u_\alpha$  of the displacement field may be expressed as the sum of an incident propagating wave and a superposition of the reflected eigenmodes of the perfect waveguide A at the same frequency. It may be written, using the matching approach [16–18], as

$$u_\alpha = u_i \eta_i^m + \sum_j \eta_j^{-m} R_{ij} u_j, \text{ with } m < 0, \quad (3)$$

whereas for a site in the region to the top of the boundary (zone D), this is given as

$$u_\alpha = \sum_j \eta_j^m T_{ij} u_j \text{ with } m > n. \quad (4)$$

The coefficients  $R_{ij}$  denote the reflection amplitudes into eigenmodes  $j = 1, 2, 3$  of the perfect bcc waveguide for the incident propagating wave  $i$ , and the quantities  $T_{ij}$  are the corresponding transmission coefficients for  $i = 1, 2, 3$  eigenmodes. The vectors  $u_i$  and  $u_j$  are the associated eigenvectors of the dynamic matrix for the bcc perfect waveguide, at the frequency  $\Omega$  and at the given incident angle.

Consider a Hilbert space for the scattering and denote by  $[|R\rangle, |T\rangle]$  the basis vector for the reflection and transmission coefficients in this space, and by  $|U\rangle$  that for the displacements of a set of irreducible sites in the scattering domain. The equations of motion for the nanostructure, coupled to the rest of the systems, may be written in terms of vector  $[|U\rangle, |R\rangle, |T\rangle]$ . Using the appropriate transformations connecting the displacement fields in equations (3), (4), we obtain a square linear inhomogeneous system of the equations of the form

$$[\Omega^2 I - D(e^{i\varphi x}, e^{i\varphi y}, e^{i\varphi z}, \mu, r_B, r_d)] [|U\rangle, |R\rangle, |T\rangle] = -|IH\rangle \quad (5)$$

where  $-|IH\rangle$  is the vector containing the inhomogeneous terms that describe the incident propagating wave when mapped appropriately onto the basis vectors. The solution to equation (5) gives, for any incident phonon in eigenmode  $i$ , the vector  $|U\rangle$  as well as the reflection and transmission amplitudes.

The solution to equation (5) yields the displacement  $|U\rangle$  of the irreducible set of atomic sites for the bcc sandwiched film, as well as the components  $R_{ij}$  and  $T_{ij}$ . The scattering behavior is usually described in terms of the scattering matrix, which elements are given by the relative reflection and transmission probabilities  $r_{ij}$  and  $t_{ij}$  at the scattering frequency  $\Omega$ . These are given by the relation

$$r_{ij} = (V_{gi}/V_{gi})|R_{ij}|^2 \text{ and } t_{ij} = (V_{gj}/V_{gi})|T_{ij}|^2. \quad (6)$$

To ensure unitarity of the scattering matrix, the scattered waves have to be normalized with respect to their group velocity.  $V_{gi}$  is the group velocity of the eigenmodes, set equal to zero for evanescent modes. We can further define total reflection and transmission probabilities for a given eigenmode at scattering frequency  $\Omega$  by summing over all the contributions

$$r_{i,\varphi x,\varphi y}(\Omega) = \sum_j r_{ij}(\Omega) \text{ and } t_{i,\varphi x,\varphi y}(\Omega) = \sum_j t_{ij}(\Omega) \quad (7)$$

In order to describe the overall transmission of the sandwich system A/B/A at a given frequency  $\Omega$  and at the given incident angle, it is useful to define the total transmission of the system (or the domain defect transmittance)  $t(\Omega)$ , by summing over all input and output channels:

$$t(\Omega) = \sum_i \sum_j t_{ij}(\Omega). \quad (8)$$

The transmission probabilities per eigenmode  $i$  and the average phonon transmittance are important quantities to calculate since each corresponds to an experimentally measurable observable. They play an essential role in the calculation, for example, of the net heat current across a given junction between semi-infinite domains held at different temperatures [19].

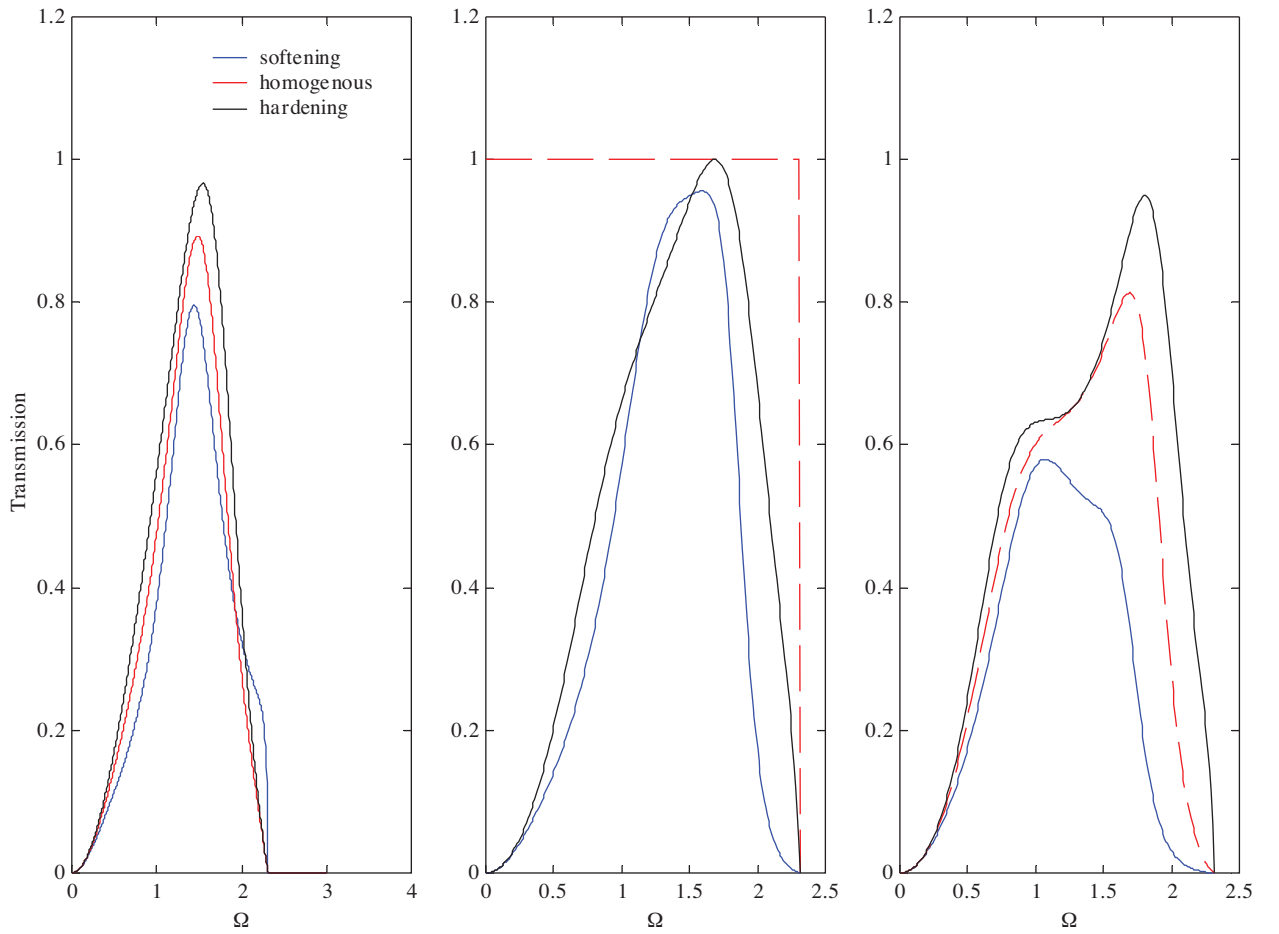
## 4. Numerical results and discussion

Phonon transmission via the nanojunction zones in the A/B/A system is studied with reference to elastic waves incident from the bottom to the top of the scattering region (see Figure 1). The numerical applications of our scattering model are presented for three configurations of the nanostructure B sandwiched between the A lattices. These configurations are determined by the number of the layers of the thinner film B; the first corresponds to the B

lattice having one atomic layer, the second for three atomic layers and finally, the B film is composed by five atomic layers. In each configuration, the phonon transmission is carried out for three possibilities of the atomic mass of the B lattice in comparison of the atomic mass of the A lattice. They are named, respectively, light ( $\mu = 0.5$ ), homogenous ( $\mu = 1.0$ ) and heavy defect masses ( $\mu = 1.5$ ).

Furthermore, for each possibility of the atomic masses of the B lattice, we examine the phonon transmission under three different boundary conditions as regards the local elastic interaction on the sandwiched film and the nanojunction domain. The force elastic constant  $k_B$  in lattice B takes, respectively, the values 0.5, 1.0 and 1.5. In the other hand, at the interface domain, the elastic interaction  $k_{AB}$  is  $(k_A + k_B)/2$  in all cases.

The first situation corresponds to a softening of the B elastic constants in comparison to the bulk of the lattice A, the second case is the situation where the elastic constants are the same, and the third case corresponds to a hardening of its elastic constants.

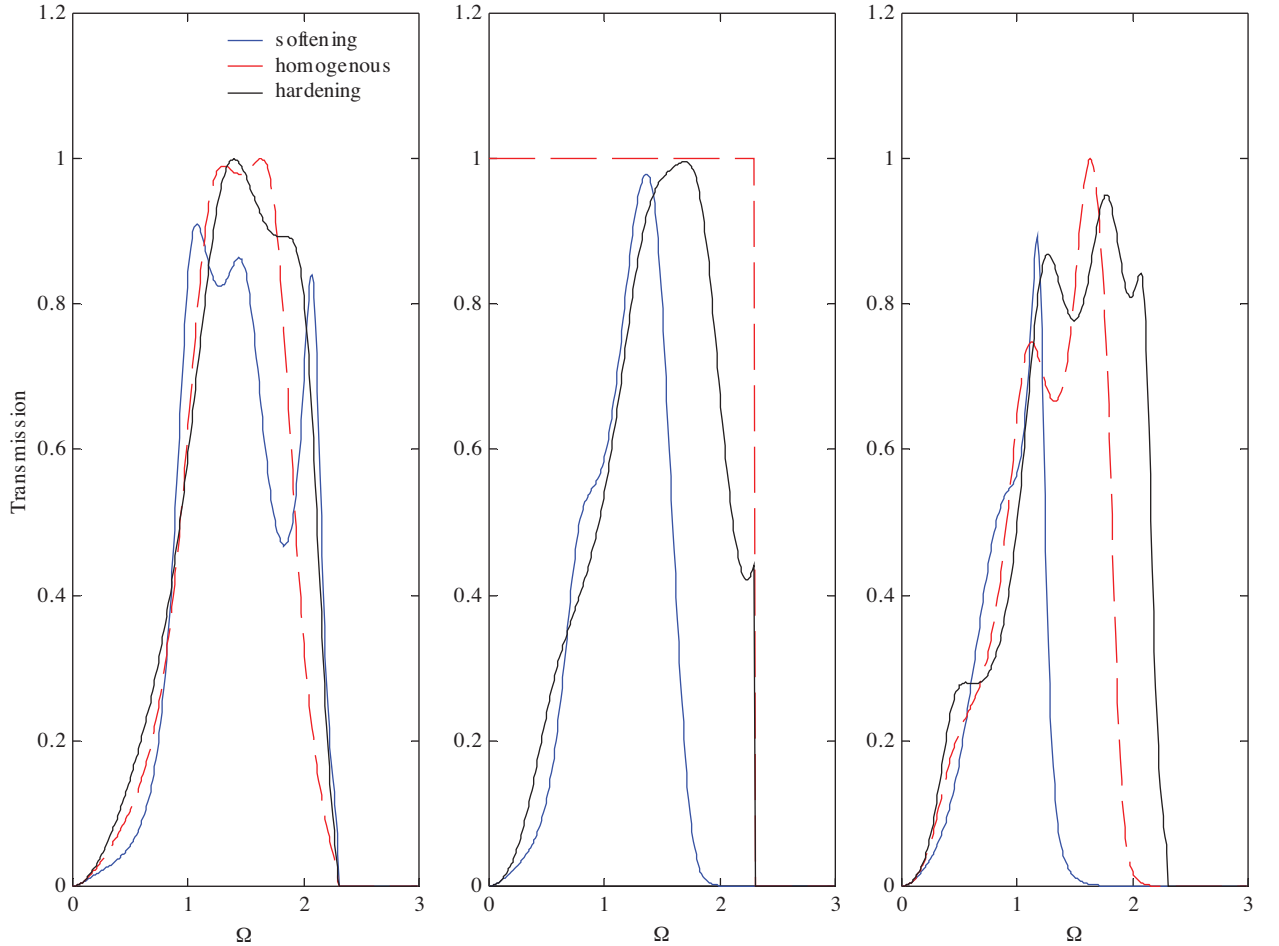


**Figure 3.** Phonon transmission coefficient of the sandwich system A/B/A, at a given incidence angle  $\varphi_x = \varphi_y = 0$ , as a function of frequency. The number of layers for the sandwiched B film is  $m = 1$  layer. Solid lines are obtained when  $r_B = 0.5$  (softening case). The dotted lines correspond to  $r_B = 1.0$  (homogenous case). The dashed lines correspond to  $r_B = 1.5$  (hardening case). In each case, the elastic constant  $k_{AB}$  is taken  $(k_A + k_B)/2$ . The transmission coefficients are arranged in columns from light mass defect at the left to heavy mass defect at the right.

Although this value does not correspond to exact crystalline values, which may be significant in some metals [20], it is a reasonable working value to illustrate the calculation. The purpose of this procedure is to investigate how the local dynamics respond to local changes in the elastic properties. Note that the theory can be tested with arbitrary values via the construction of acoustic models in a laboratory framework.

The results of the examined configurations, corresponding to one layer, three and five layers of the B sandwiched thin film are shown, respectively, in Figure 3, Figure 4 and Figure 5. We have arranged the situations studied in columns, from light defect ( $\mu = 0.5$ ) at the left to heavy defect ( $\mu = 1.5$ ) at the right. The results show some general characteristic, as well as some specific phonon behavior, for all cases in each configuration of the considered number of layers of the bcc B lattice. The spectra are in general sensitive to the changes of the atomic masses and the elastic force constants on the boundary. The phonon transmission is less or equal to the equivalent of one phonon throughout the propagating frequency interval. This illustrates how the B atomic layer at the heart of the defect zone, constricts the transmission to a maximum of one phonon at a time, characteristic of the atomic layer on the interval contact between the bcc lattices.

The transmission and reflection cross sections verify the unitarity condition for the scattering matrix, and this is used throughout as a check on the numerical calculation.

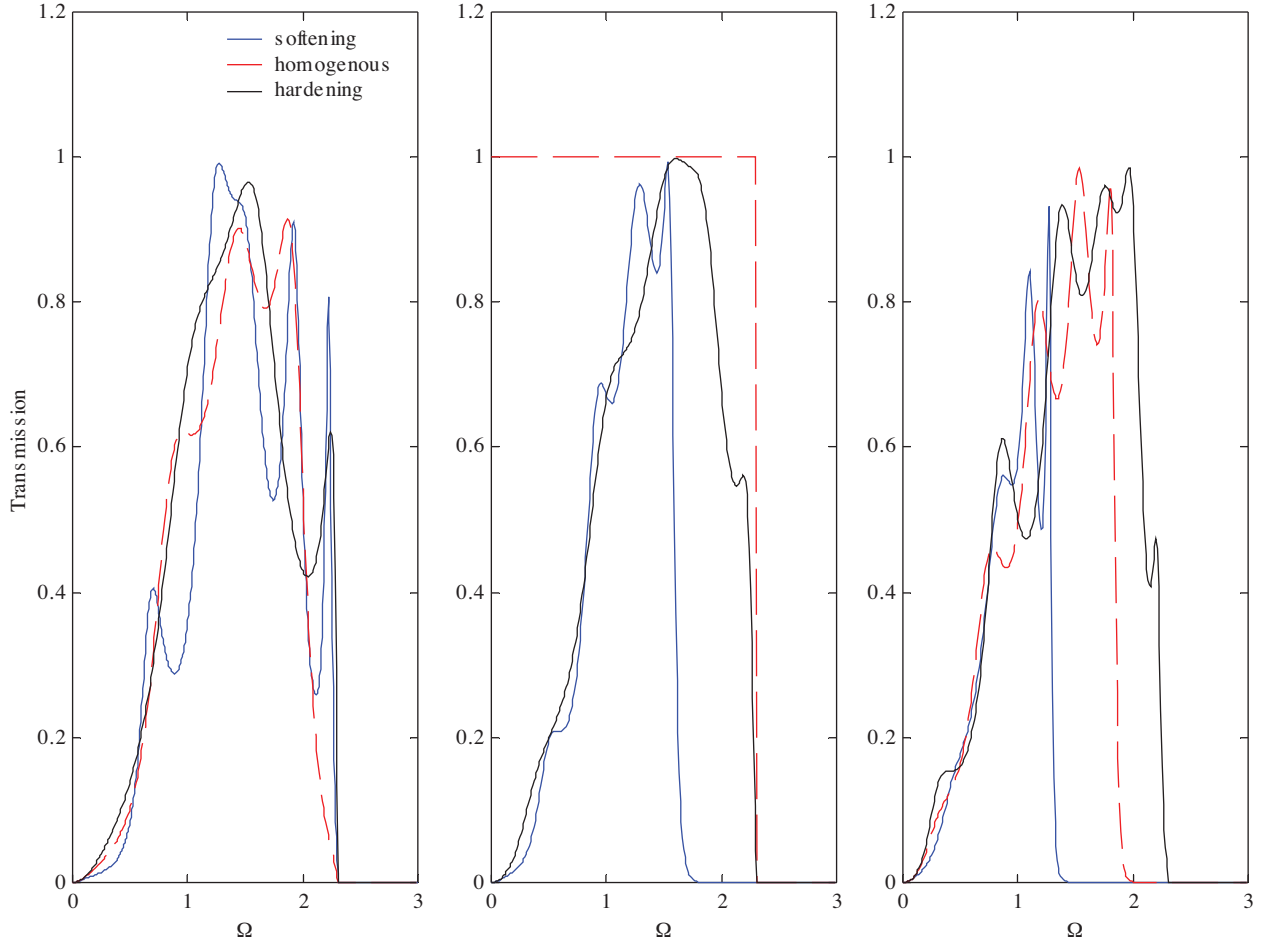


**Figure 4.** As in Figure 3, for the sandwiched B film, in the case where  $m = 3$  layers.



In Figure 3, numerical results are presented for the total phonon transmission for the incident modes, as a function of scattering frequency  $\Omega$ , at a given incidence  $\varphi_x = \varphi_y = 0$ , for the three situations examined of the mass lattice  $m_B$ . As expected, the influence of the mass defect is smallest when the scattering frequency  $\Omega \rightarrow 0$ , leading to a minimum in the transmission  $t \rightarrow 0$ . As one increases the frequency the mass defect leads to a maximum in the transmission. Near the zone boundaries, the transmission gives zero. This is observed in the studied situations, independently of the strength of the boundary. We note that the interaction between the localized modes introduced by the variation of the atomic masses of the B nanostructure and the propagating modes of the perfect A lattice leads to oscillation picks in the vibration spectra. These oscillations shift to higher (lower) frequencies for light (heavy) defect masses. The acoustic modes present no significant transmission for low frequencies, for all cases of the elastic constant considered on the sandwiched domain. The absence is probably due to the relatively long lattice parameter of the modes in this frequency interval, in comparison with the wavelengths, and also due to the interference effects between the modes on the interface zone when modifying the boundary, at a given incidence.

Another general characteristic of the phonon transmission is the displacement of its spectral features to higher frequencies with increasing hardening of the elastic force constants interface interaction in the sandwich domain, in the all cases studied, which is a signature of the nanojunction matching necessary for the transmission.



**Figure 5.** As in Figure 3, for the sandwiched B film, in the case where  $m = 5$  layers.

In a similar manner, the corresponding numerical scattering results for the two other configurations, with three and five layers of the sandwiched lattice B between two A bcc semi-infinite lattices, are presented, respectively, in Figures 4 and 5. The results show some general characteristics, as well as some specific phonon behavior, for each configuration. The spectra are sensitive to the changes of masses and elastic constants. The sensitivity of these results compares to that observed for the vibration spectra at boundaries separating phase domains in fcc interface [21].

## 5. Conclusion

In conclusion, we present a theoretical model to calculate the scattering properties of phonons and coherent transport via A/B/A bcc sandwich system. The purpose is to give an understanding of the relation between the coherent phonon transmission via nanojunction zones and its symmetry properties. The sandwiched thin film is considered to act as elastic joints between two similar groups of bcc semi-infinite lattices, with elastic interactions. It enables one to address questions regarding the mechanical properties of the nanojunction zones in bcc systems. The chosen model is a generic one and it serves to demonstrate the ability of the proposed modeling and analysis tools.

The analysis of the vibration spectra demonstrates the central role of a number of layers of the sandwiched film for the dynamics of the sandwich system. The model is suitable for the study of such a configuration of atomic sandwich systems constructed in an analogous manner on the classical macroscopic scale. The formalism presented is independent of the configuration of the interface of the system, which makes it easy to extend them to study of a variety of problems.

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