Thermal Conductivty and Scattering Elastic Wave by Integrated Lamellar Nano Structure with Different Thicknesses

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Abstract

In this work, we provide a computational and analytical method to study the scattering properties and associated thermal conductivity generated by embedded nanostructures in inhomogeneous crystalline materials. The nature of the defect and its arrangement also affect the coefficients of reflection, transmission, and conductance of elastic wave spectra in the system waveguide model. This problem is solved by using the matching technique and Newton dynamical equation, which are detailed to represent the entire evanescent and propagating fields in the bulk. The matching approach and the Landauer and Bütikker mathematical framework are applied in tandem by the theoretical formalism to get the reflection and transmission coefficients and the related phononic conductance of the perturbed domain. Furthermore, the corresponding thermal conductivity is derived from the function of temperature and the elastic constant of the behavior of the perturbed region. Furthermore, the numerical calculations are displayed and discussed in connection with the different model parameters. The coherent relationship between traveling phonons and the localized vibration modes at the lamellar structures explains the correlation between changes in the conductance spectra and Fabry Perot resonances.

Keywords: thin films, elastic waves, nanostructures, matching formalism; thermal conductivity; Landauer-Buttiker approach.

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Introduction

The scientific interest of the properties of the vicinal surfaces and of the mesoscopic system is motivated us to study the dynamic phenomena of localization and scattering elastic wave by the different various punctual and extensive defects. This importance derives, for example, from the fact that the development of increasingly miniaturized components in physical devices requires a thorough knowledge of the physics of the actual surfaces of materials [1-2]. In addition, modeling and numerical simulation in materials science is a rapidly developing field of research which concerns all classes of materials and all modeling scales (from nano to macroscopic). On the subjects concerned, the industrial concerns and the fundamental research activities of the laboratories frequently come together (prediction of microstructures, mechanical properties, modeling and simulation of processes or holding in service.) Numerical simulation takes a more and more place Important in the industry

today, with a dual requirement to provide, with sufficient precision, the conditions for the elaboration and processing of materials and the operating behavior of parts with reasonable calculation times. The complexity of the phenomena to be simulated, we can no longer always content ourselves with overly simplified models.

At the same time, many research laboratories have activities related to the development of models of behavior and their validation, in order to establish a realistic description of the materials and their behavior at different scales. In materials science, we can mention: the study of transfer phenomena such as diffusion and segregation, the description of crystalline defects, and the prediction of microstructural evolutions under the action of thermo mechanical fields. The increase in the performance of the calculation means makes it possible to use these models for industrial applications. Development of atomic or molecular systems that can transport information to the nanoscale scale is one of the issues facing modern technology. The study of surfaces is important in this situation because it makes it possible to create nanostructures with precisely regulated geometry. In fact, recent research has demonstrated that the formation of low-dimensional molecular structures is encouraged by the self-organization of surface steps. The development of molecular monolayers trapped between two steps and the synthesis of atomic wires adsorbed near the steps are two prominent instances. The surfaces used are metal or semiconductor vicinal surfaces which have the shape of a staircase as well as certain reconstructed surfaces in the form of crenellations. Besides their ability to generate nanostructures, the surfaces also offer the possibility of working with the latter, using the properties of local probes such as S.T.M or Atomic Force

A.F.M. Indeed, these local probes can act as nanoscopic tools allowing, on the one hand, acting mechanically on the adsorbed molecules and on the other hand to selectively excite a molecule by inducing electronic and / or vibrational transitions. A question of first importance concerns the capacity of such nano-objects to transfer information. In general, this information is conveyed by the collective excitations of the nanostructure which can appear in various forms depending on the nature of the system. The interest lies in two types of excitation (vibrators). On the one hand, the possibility of locally exciting the internal vibrations of the molecules by S.T.M opens up a new path based on their use as a vector of information. Alongside the quick improvement of experimental investigation procedures, there has been a significant advancement in the mathematical tool that is essential to comprehending the various processes surrounding a range of surface imperfections. Our study continues the many efforts on the matching method started by Feuchtwang, which were continued and extended by Jacob Szeftel, Antoine Khater, and others. It also contributes to the development of these theoretical methods. When considering the properties of semi-infinite systems, this approach has some benefits. In addition to providing a satisfactory explanation for the phonon dispersion and surface resonance curves, it also provides a more comprehensive and generic definition of resonances and makes it possible to analyze displacement behavior in the vicinity of Van Hove singularities more transparently.

Its basic principle consists in describing the relationships between the atomic displacements of a semi-infinite system by a finite number of equations, by dividing the initial space of the solid according to three distinct regions, respectively of the bulk, matching and defect region. However, the complete description will be made in the methodology

One basic and interesting subject of solid-state physics is the scattering and localization phenomena caused by structural flaws [3]. A physical system's translational symmetry is broken by inhomogeneities, which can cause a number of effects such localized states, resonant scattering, and wave reflection [4]. Two sorts of challenges that can be found in many different physical problems, such as those related to optics [5], acoustics [6], electronics [7], and magnetics [8, 9], are wave scattering in inhomogeneous media and defect supported localized modes. Defects cause energy to be trapped and limited in the vicinity of the domain defects in all circumstances. This results in spatially localized phonons. The mechanical and elastic characteristics of the low-dimensional system are measured using several experimental methods before the thin film[10,12].

The majority of current studies have focused on the investigation of electronic scattering in nearly one-dimensional systems. [13-17]. The fundamental motivation behind the most recent work has been to better understand the potential restrictions that structural and other types of faults may have on the physical properties of microelectronic devices.been committed to investigating electronic scattering in systems that are almost one-dimensional.

The vibrational scattering features of low dimensional mesoscopic systems of many sorts and of well-controlled intricate geometries are now accessible due to the recent progress in nanotechnologies [18]. Wave propagation through these defect-filled systems has interesting and practical features that have attracted increased attention recently [19, 20]. They are the subject of continuing research because of their fascination in high-tech nanometric devices. The inhomogeneities of the structure scatter the elastic waves of the unperturbed lattice, forming a structure that resembles a waveguide.

Any theoretical inquiry of the vibrational characteristics of perturbed systems must include two fundamental elements. Understanding the interatomic force constants required to create the dynamical matrix is the first step. Second, create a plausible framework to account for the dispersion by disturbing flaws. Within a single mathematical framework, the localization of vibration modes and the wave scattering can be addressed by employing the matching technique methodology [21–27].

We demonstrate in this work the influence of nanostructure on the localization and the scattering events. In the harmonic approximation, the outcomes for the center nearest and next- nearest neighbor force constants are given. An integrated flaw in an inhomogeneous cubic crystalline surface is analyzed. The conductance spectra exhibit resonance characteristics. Specifically, we demonstrate that the spectra exhibit Fabry Perot resonances as a result of the imperfection. These resonances arise from the coherent coupling of the perfect wave-guide's propagating wave and localized modes around the flaw.

There are numerous significant applications for this work in the applied physics fields. especially in the control that hasn't been destroyed.

The structure of the paper is as follows. Section 2 presents the structural theoretical model and the following paragraphs. Section 3 discusses the dynamics vibration technique applied to lamellar structures with different thicknesses in the system wave-guide model. In sec. 4, the thermal conductivity associated with the total

transmittance of the system is displayed. The study's main numerical results are shown in Section 5. Finally, section 6 presents the overall results.

Model of a theoretical system

The system model is shown schematically in Figures 1a–1f. Their two main characteristics are

(1) a structural reorganization of the building block spacings and (2) a change in the elastic constant parameters in a boundary with respect to the ideal 3D lattice, which is caused by the local order of the 3D lattice being reorganized close to a boundary. The perturbed domain is determined by the sort and change of the elastic constants on a boundary.

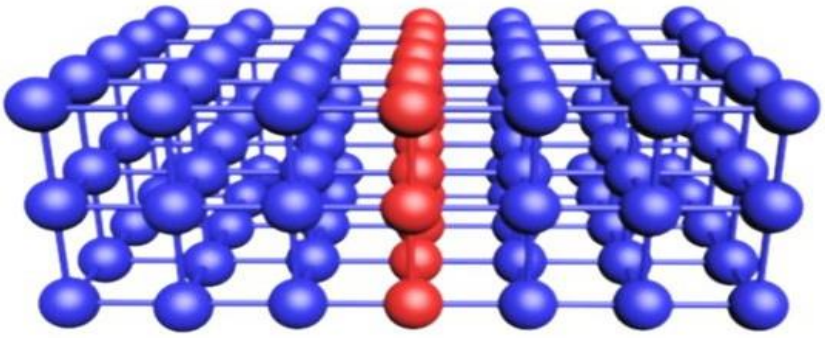


Figure.1a. Schematic representation of crystallographic waveguide showing the configuration identified as the defect nanostructures one integrated layer (red atoms).

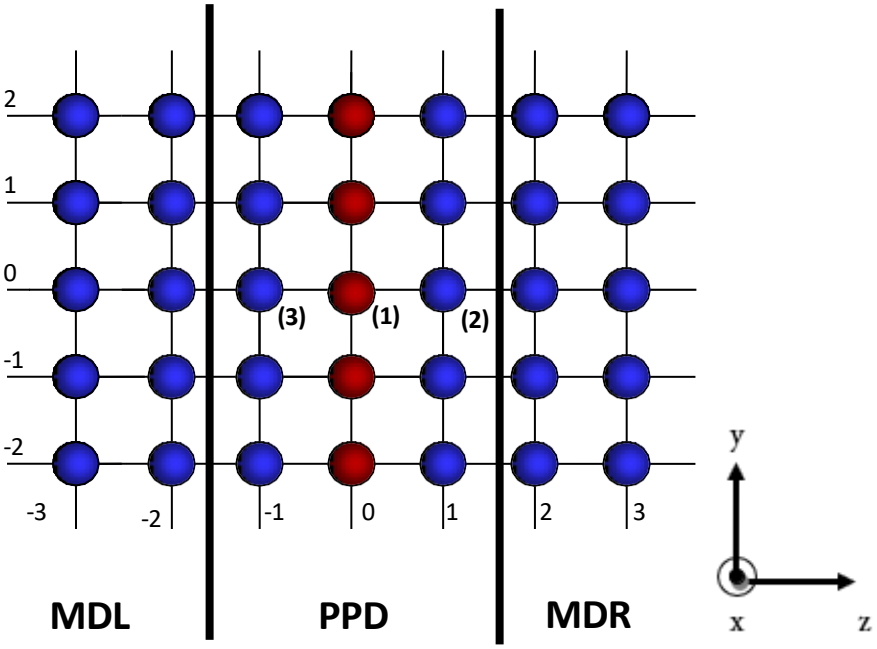


Figure.1b. Projection of system model in plan xoy .

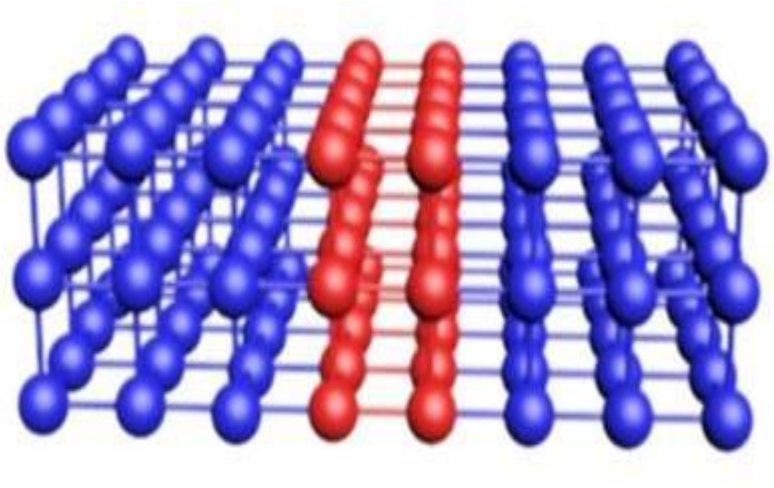


Figure.1c Schematic representation of crystallographic waveguide showing the configuration identified as the defect nanostructures two integrated planes (red atoms).

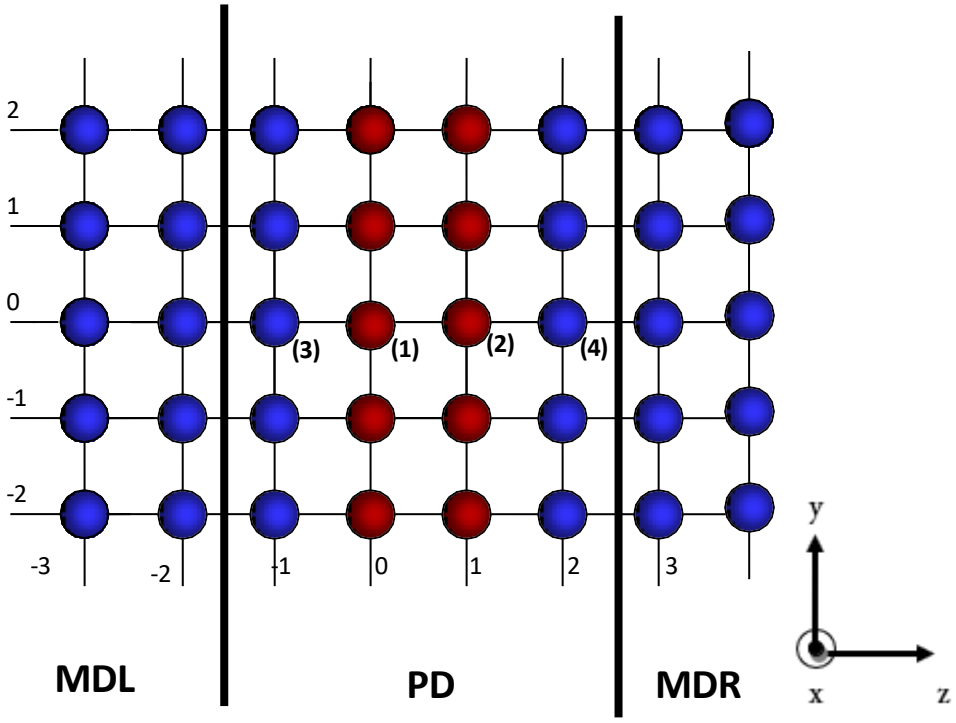
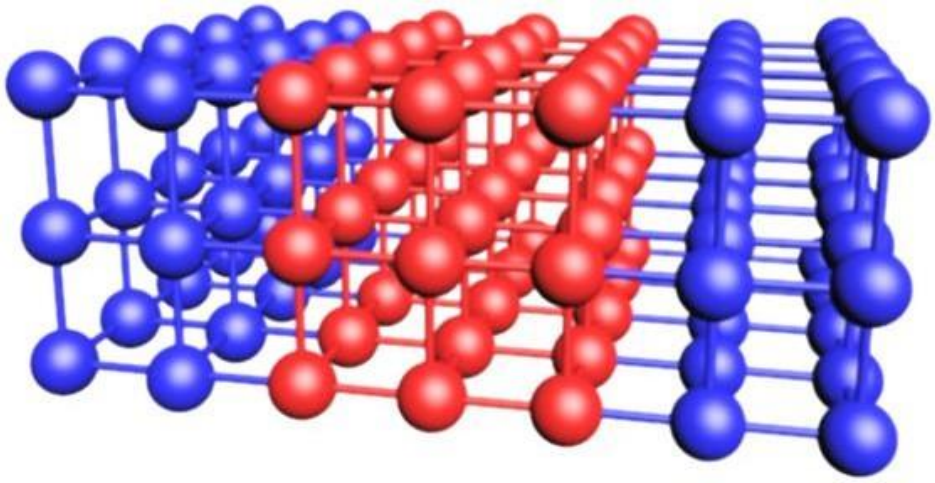


Figure.1d Projection of system model in plan xoy.



Figures.1e Schematic representation of crystallographic waveguide showing the configuration identified as the defect nanostructures three integrated planes (red atoms).

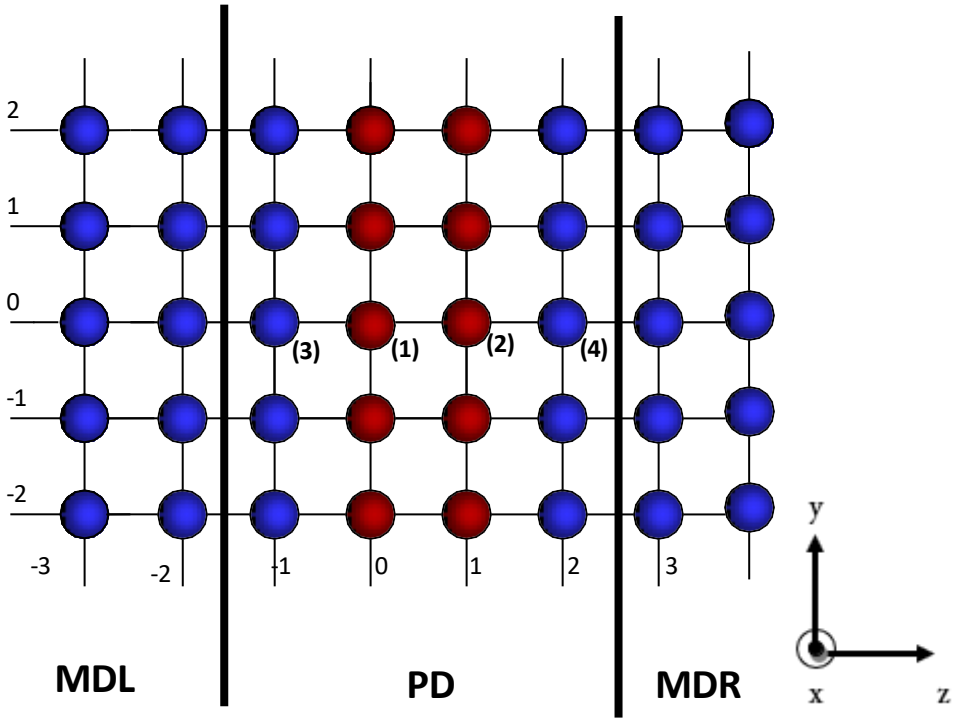


Figure.1f Projection of system model in plan xoy.

Methodology and Applications

The standard harmonic approximation provides the linearized Newton dynamical equation of motion for an atom at location l, [32] by

$$\omega^2 m(l).u_\alpha(l,\omega)=\sum_{l\neq l'}\sum_{\beta} C(l,l')(r_\alpha r_\beta/d^2)_0 x\left[u_\beta(l',\omega)-u_\beta(l,\omega)\right] \qquad (2.a)$$

The l atom's mass is represented by m m(*l*), its associated displacement vector vibration is represented by u (*l*), and the indices and stand for Cartesian co-ordinates. The radius vector's component is described by r , its distance from l to l' is given by d, and the elastic force constant between l and l' is given by C(l,l'). It accepts the values C_1 or C_2, correspondingly, for the nearest and next nearest neighbors, as was previously mentioned. Eq (2) should be applied to the perturbed domain and perfect wave-guides in a methodical and sequential manner.

Assume that *l* and *l'* are inside the ideal wave-guide and away from the borders of the flaw, as seen in Fig. 1. Because of the translational invariance provided by the model's geometry parallel to the defect in the y direction, the factor $_y = ik_y .a$ appears in all of the solutions. This is accomplished by writing the displacement field's wavelike representation in this direction and using Bloch's theorem:

$$u(n_x,n_y\pm1) = e^{\pm iky.a}u(n_x,n_y) \qquad (2.b)$$

The $e^{\pm iky.a}$ in equation (2) are the spatial phase factor of propagating modes, where k_y characterises the phonon wave vector along the y axis and a measures the interatomic distance between nearest neighbor sites. To determine the evanescent field of the vibrational displacement in the two bulk waveguide in the direction normal to the inhomogeneity such as Ox axis, we need to introduce the spacial phase factor doublets

(η,η^{-1}) The atomic motions of indexed sites in the bulk region, as defined in Fig. 1, are:

$$\left[\Omega^2 I - D(\eta,r,\lambda,\varphi_y)\right]|u\rangle = |0\rangle \qquad (3)$$

where D(, r) is the dynamical matrix characteristic of the perfect wave guide lattice, where $_0$ is a characteristic lattice frequency, and $_0^2=C_1/m$. where is the dimensionless frequency provided by $\Omega^2=\omega^2/\omega_0^2$.
I represent the matching unit matrix. D is reduced to a six by six matrix in the arrangement shown in Figs 1a and 1b, for the two inequivalent sites per unit cell and the three degrees of freedom per site. The equivalent vector for a column of the ideal waveguide is denoted by U . The appendix provides a comprehensive breakdown of the matrix members in equation (3) as a function of $_y = k_y\mathbf{a}$. The vector k_y represents the one-dimensional reciprocal lattice wave in the direction of Oy.

As shown in Fig. 1b, the bulk's evanescent and propagating vibrational fields are characterized in the Ox-direction by the phase factor doublets ((i), $^{-1}$(i)). I've labeled the system model's solutions here. Using the

matching technique on Eqs. (2) and (3), the propagating modes are defined by the condition =1, and the evanescent modes are obtained when <1.

Thus, $2I$ $D(\ ,r,\ ,\ y)$ as the derminant of disappears, solutions are reached. One typical secular $\sum_{}^{6} A\eta$. In equation of degrees six (6) in is provided. It can be stated as by in polynomial form case of r = 0.25, the solution of Eq. (3) yields the propagating modes when and the evanescent modes when for the symmetric and asymmetric modes, respectively. The total phase factor, shown in Fig. 2, confirms that bulk dynamics is hermitical, which is analogous to time reversal symmetry in crystalline lattices. This completes the description of the evanescent field vibrations in the bulk of the simple cubic lattice and permits the construction of a basis over the evanescent and traveling modes.

Where there is a defect, as in Fig. 1, in the column interval of [-1, 1], scattering analysis requires consideration of both the propagating modes and the evanescent solutions of the system. Stated otherwise, we need all of the solutions (i) for a given , including the propagating solutions with $_i$ =1 and the evanescent solutions with $_i$ <1.

The phase factor doublets { (i), $^{-1}$(i)}, which reflect the solutions as one proceeds along the wave guides' axis from one column to its nearest neighbors, best characterize the evanescent and propagating vibration fields in the perfect wave guides to the right and left of the defect in Figure 1. These usually complex phase factors are the answers to the equation of motion, Eq(3), which can be determined in a number of methods. Here, the one recommended in Ref.[22] is utilized. Given a fixed r, one can solve the determinant of the matrix of Eq. (3) for the variable frequencies of interest to produce a characteristic polynomial in . Time inversion symmetry allows the lattice solutions to be found in hermitian pairs { (i), $^{-1}$(i)}.

The evanescent modes are not energy-carrying, but they are required for a full description of the multi-channel scattering on the wave-guide. Discrete eigenmodes can tackle the scattering problem for each eigenmode independently since they do not couple between the ideal wave-guide. An entering propagating wave that incidentally occurs from left to right strikes an eigenmode i at frequency . The resulting dispersed waves at are composed of a transmitted and a reflected half.

For an outside atom bordering the defect domain [-1, 1], the Cartesian components of the displacement field U(n,n') can be represented using the matching approach. The sum of the incoming wave and a superposition of the bulk's eigenmodes reflected by the scatter at the same frequency equals the displacement field U (n,n') at a site inside the wave guide to the left of the defect.

$$U_{\alpha}(n,n') = u_i\eta_i^n + \Sigma_j\eta_j^{-n}R_{ij}u_j \text{ with } \quad n<-1 \qquad (4)$$

where the eigenvectors of the dynamic matrix for the ideal wave-guide at frequency are shown by the vectors u_i. The reflection coefficients, R_{ij}, define how an incident wave, i, is scattered into the eigenmodes j = 1. An suitable superposition of the eigenmodes of the perfect wave guide transmitted by the defect at the same frequency can be used to represent the displacement field $U^{+}(n, n')$ for a site inside the wave guide to the right of the defect

$$U^{+}(n,n') = \Sigma_j \eta_j {}^{n}T_{ij}\, u \text{ with } n>1 \qquad (5)$$

For incident wave i, the transmission coefficients into the eigenmodes j = 1 are T_{ij}

For the scattering, consider a Hilbert space. The basis vectors for the reflection and transmission coefficients in this space are indicated by [R>, T>], and the displacements of a set of irreducible sites in the defect domain are indicated by U>. When the defect is connected to the other systems, its equations of motion can be expressed in terms of vectors [U>, R>, T>]. We construct a square linear inhomogeneous system of the equations of the form by applying the transformations between the displacement fields in Eqs (4)–(5).

$$[\Omega^2 I - D(\eta, r)]\, [|U>, |R>, |T>] = -|IH> \qquad (6)$$

Where the inhomogeneous parameters representing the incoming wave are indicated by the vector - IH , when suitably mapped onto the basic vectors.

The displacements U of the irreducible set of atomic sites for the defect domain [-1, 1] and the reflection and transmission coefficients R_{ij} and T_{ij} on the perfect wave-guides are obtained from the solution of Eq (6).

The scattering behavior is typically expressed in terms of the scattering matrix, whose elements at the scattering frequency are determined by the relative reflection and transmission probabilities, r_{ij} and t_{ij}. These are provided by

$$r_{ij} = (V_{gi} / V_{gi})\, |R_{ij}|^2 \text{ and } t_{ij} = (V_{gj} / V_{gi})\, |T_{ij}|^2 \qquad (7)$$

Since the scattering matrix cannot be unitar until the scattered elastic waves are normalized with regard to their group velocity. The group velocity of the eigenmodes, or V_{gs}, should be set to zero for evanescent modes [28–41]. The three eigenmodes' typical group velocity results at r = 0.25 are displayed in Fig. 3.Certain modes show abnormal dispersion zones when the group velocity is negative. These areas require a detailed examination of the ideas behind forward and backward scattering for the waves.

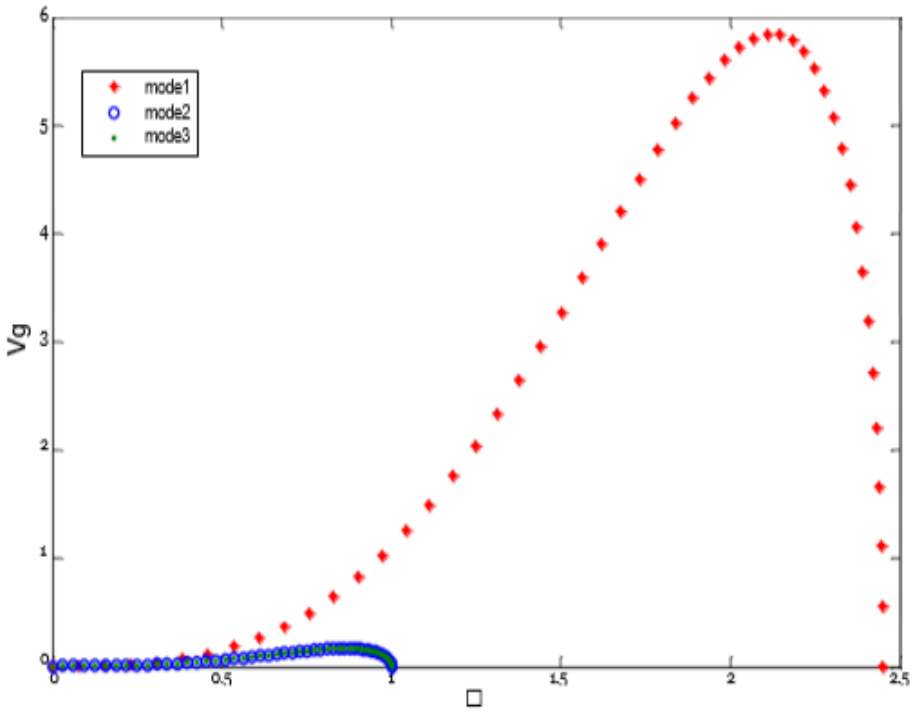


Fig.2 Curves of the group velocities of the different propagating modes (1 to 3) of the perfect crystallographic waveguide V_g, as function of the scattering frequency in the case of ratio ,r = 0.25.

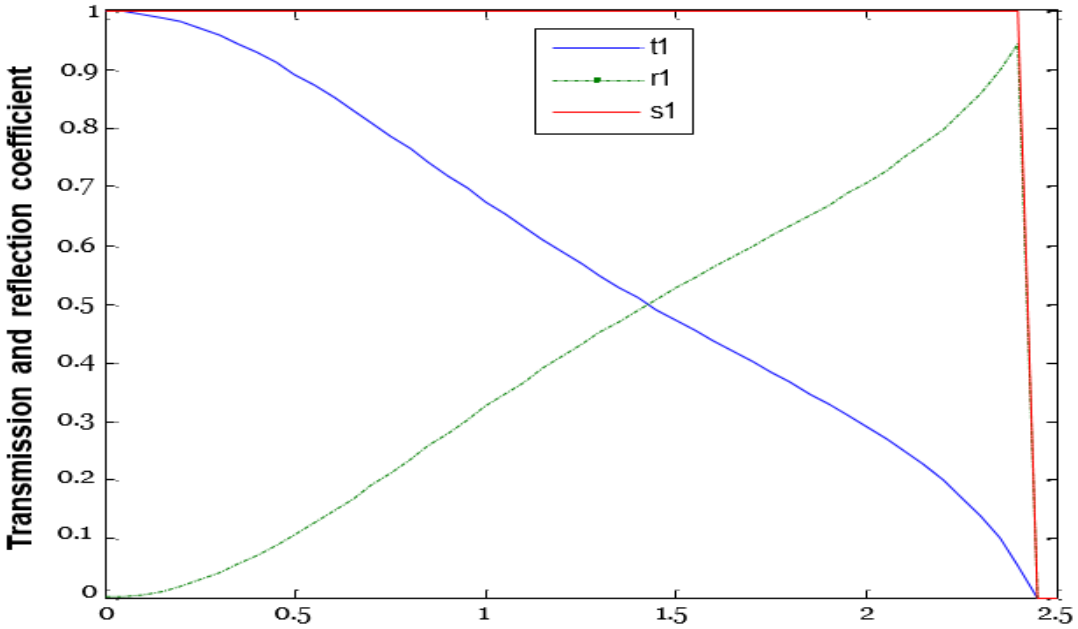


Fig.3a: The curves of transmission t1 (solid lines) and reflection r1 coefficients (dashed lines) and their sum s1 (solid lines) for the system parameters.

Figure.3a: Mode1

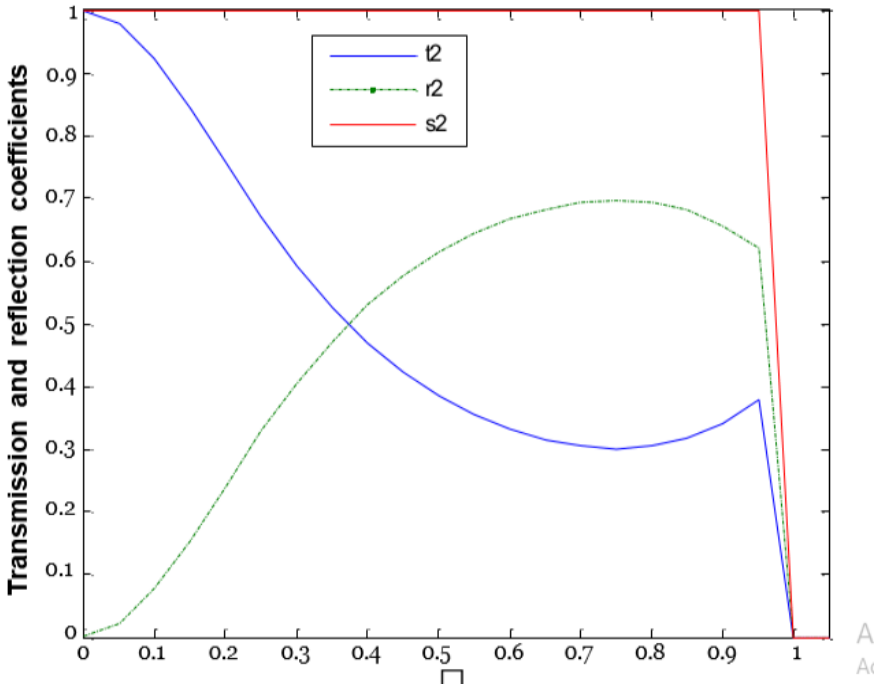


Figure.3b: The curves of transmission t2 (solid lines) and reflection r2 coefficients (dashed lines) and their sum s2 (solid lines) for the system parameters

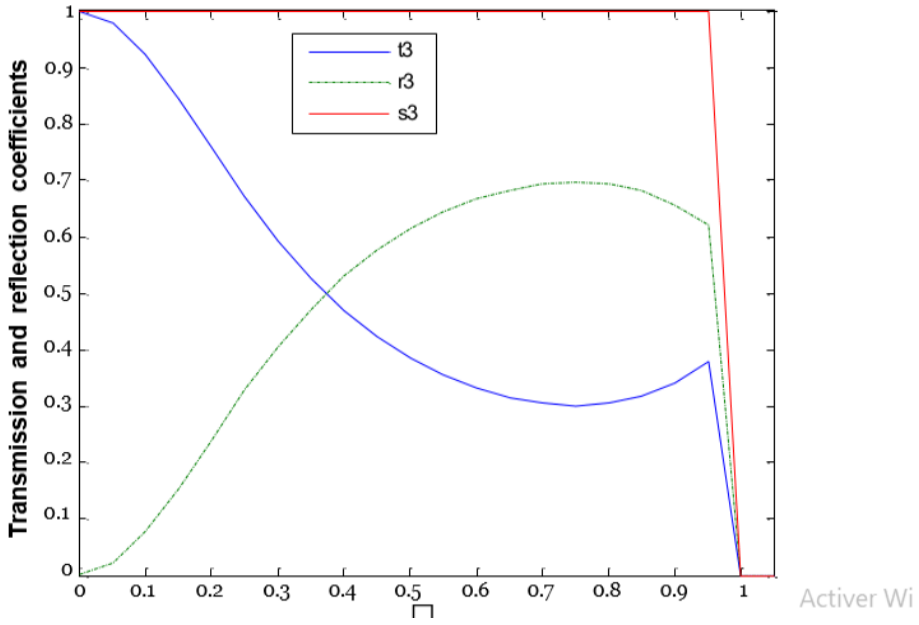


Figure.3c: The curves of transmission t3 (solid lines) and reflection r3 coefficients (dashed lines) and their sum s3 (solid lines) for the system parameters

By adding up all the contributions, we can determine the total reflection and transmission probabilities for a specific eigenmode at scattering frequency .

$$r_i(\Omega) = \sum_j r_{ij}(\Omega) \text{ and } t_i(\Omega) = \sum_j t_{ij}(\Omega). \quad (8)$$

Furthermore, by summing over all input and output channels, it is useful to define the conductance of the system (or the domain defect transmittance) t( ), in order to explain the overall transmission of mesoscopic multichannel systems at a given frequency .

$$t(\Omega) = \sum_i \sum_j t_{ij}(\Omega) \quad (9)$$

where the total is applied across all modes of propagation at frequency . Both the system conductance, t( ), and the transmission probability, t_i( ) per eigenmode i, are crucial to compute since they each correspond to an observable that can be measured experimentally.

Conductivity of Thermal

Numerous intriguing facets of quantum resistance have been discovered as a result of research on electrical transport in mesoscopic systems. The idea of linking charge transport in geometries confined to a quantum transmission problem, developed by Landauer in a series of papers beginning some twenty years ago [38], was a theoretical idea of unification Important. The idea, in its modern understanding [39], can be expressed in terms of formula for conductivity between two ideal electrodes. The thermal conductivity depends mainly on the nature of the material and the temperature. So it related to electrical conductivity. From an atomic perspective, thermal conductivity is associated with two kinds of behavior: the oscillations of atoms about their equilibrium position and the movements of charge carriers, such as electrons or holes. Free electron mobility is more important in metals than in insulators, where phonon contribution is higher. As a result, the thermal conductivity is related to both the material's structure (atom or phonon vibrations) and electrical conductivity (movement of charge carriers).We only take into account the thermal conductivity caused by phonons in our study, and in order to accomplish this, we first calculate the phononic conductance, which is a necessary parameter for calculating the thermal conductivity.

The wave guide conductance t( ), plays an essential role, for example, for the net heat current, Q_{12}, across the defect, between the two ends of the wave guide held at slightly different temperatures T+ T > T. One obtains

$$\partial Q_{12} = L^{-1} \frac{1}{2} \square^2 \frac{\Delta T}{k_\beta T} \int_0^\infty d(\omega_0 \Omega)(\omega_0 \Omega)^2 (\exp(\frac{\square(\omega_0 \Omega)}{k_\beta T})[n(\omega_0 \Omega)]^2 t(\omega_0, \Omega) \quad (10)$$

L is the effective cross linear section of the wave guide, D($_0$) is the phonon density of states on the wave guide, n($_0$) is the Bose-Einstein distribution of the population of phonons at T, and t ($_0$) is the total transmittance of the system , L = **a** in Fig.1a.

Numerical results and discussion

The transmission and reflection scattering cross section numerical results, for $_y$ = 0, are presented in Fig.4 for respectively incident elastic wave modes i = 1, 2, and 3, as a function of the dimensionless frequency ; For the case of integrated nanostructure defect modelled in Fig.1,

The numerical analysis is carried out for r = 0.25 and other elastic force constants in the neighbour of the inhomogeneity atomic region, with respect to the bulk.

In figures 4, the curve of transmission and reflection coefficients i (t1, r1, t2, r2, t3, r3) are presented as function of dimension less frequencies. We show that the transmission and the reflection coefficients verify the unitarity condition s = ti+ri =1 (i =1,2,3) .

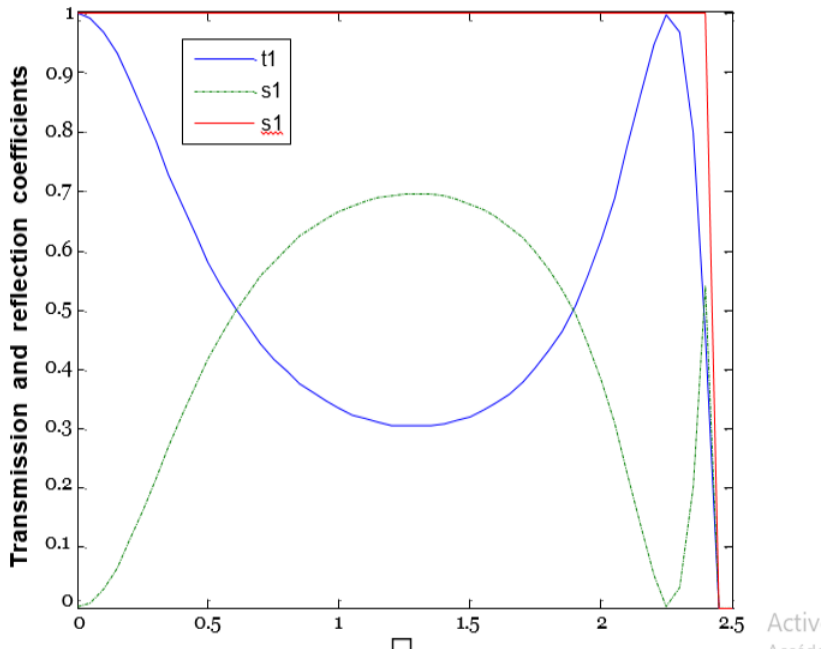


Fig.4a: The curves of transmission t1 (solid lines) and reflection r1 coefficients (dashed lines) and their sum s1 (solid lines) for the system parameters for the system model with two integrate planes.

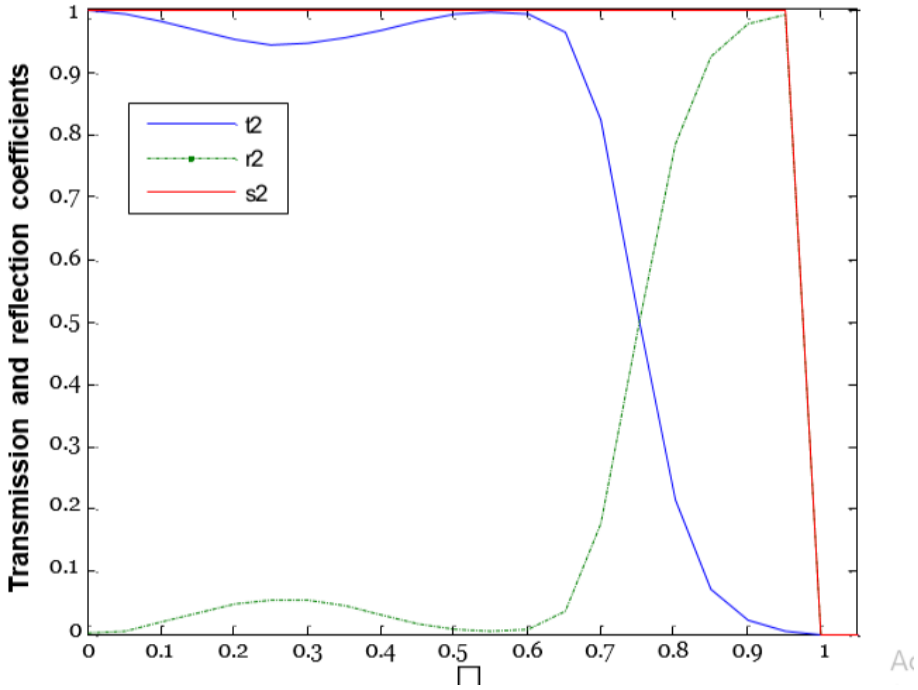


Figure.4b The curves of transmission t2 (solid lines) and reflection r2 coefficients (dashed lines) and their sum s2 (solid lines) for the system parameters

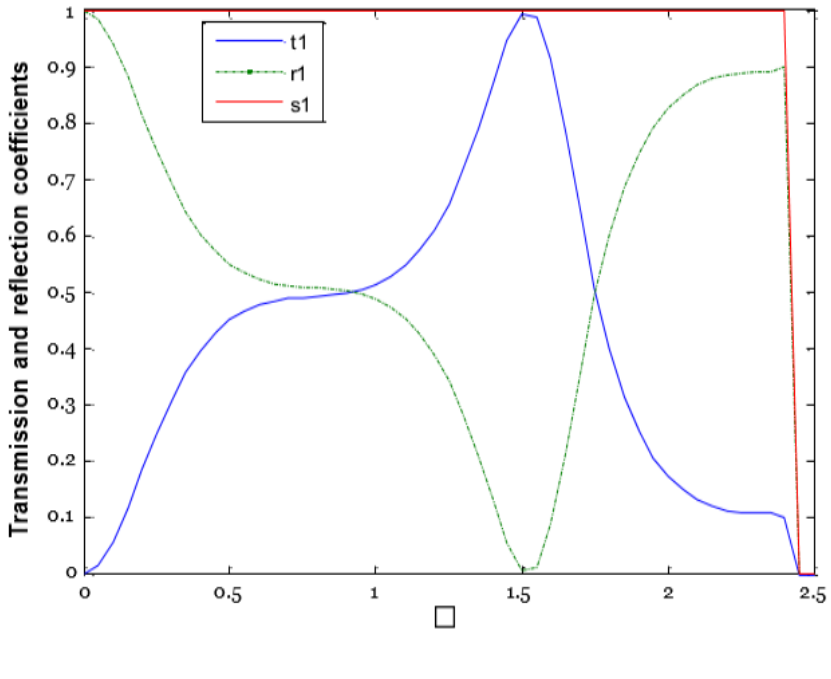


Fig.5a: The curves of transmission t1 (solid lines) and reflection r1 coefficients (dashed lines) and their sum s1 (solid lines) for the system parameters

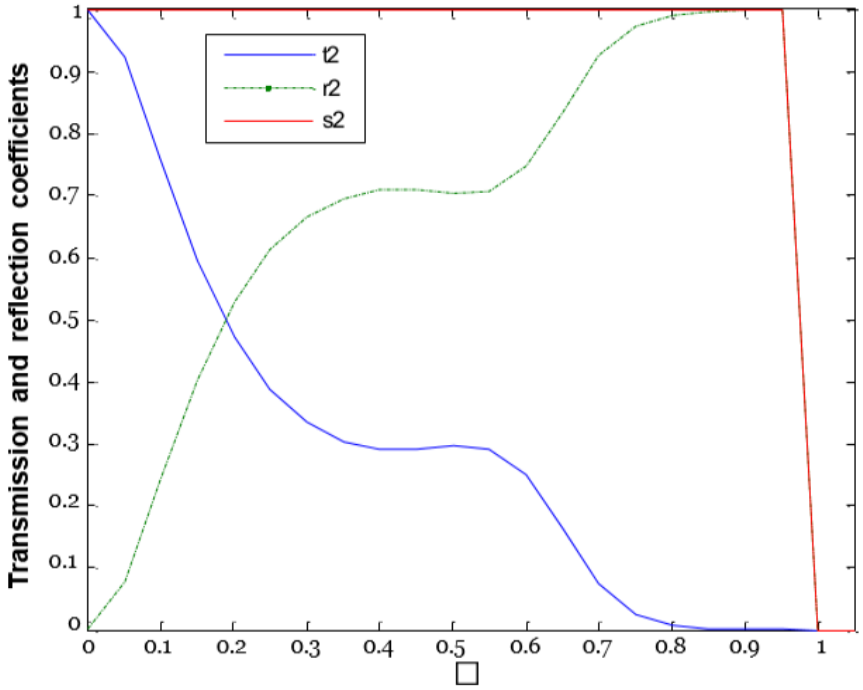


Figure.5b :The curves of transmission t2 (solid lines) and reflection r2 coefficients (dashed lines) and their sum s2 (solid lines) for the system parameters

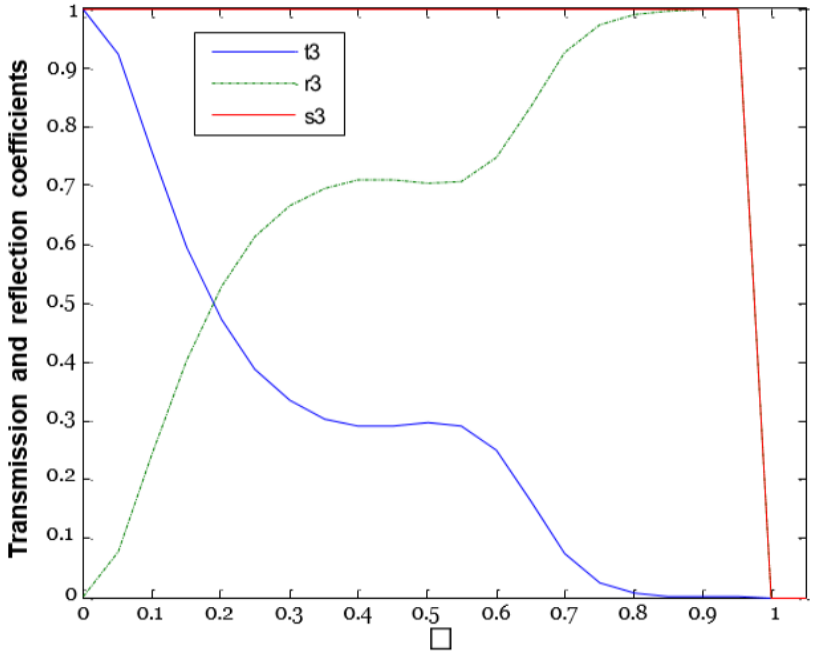


Figure.5c The curves of transmission t3 (solid lines) and reflection r3 coefficients (dashed lines) and their sum s3 (solid lines) for the system parameters

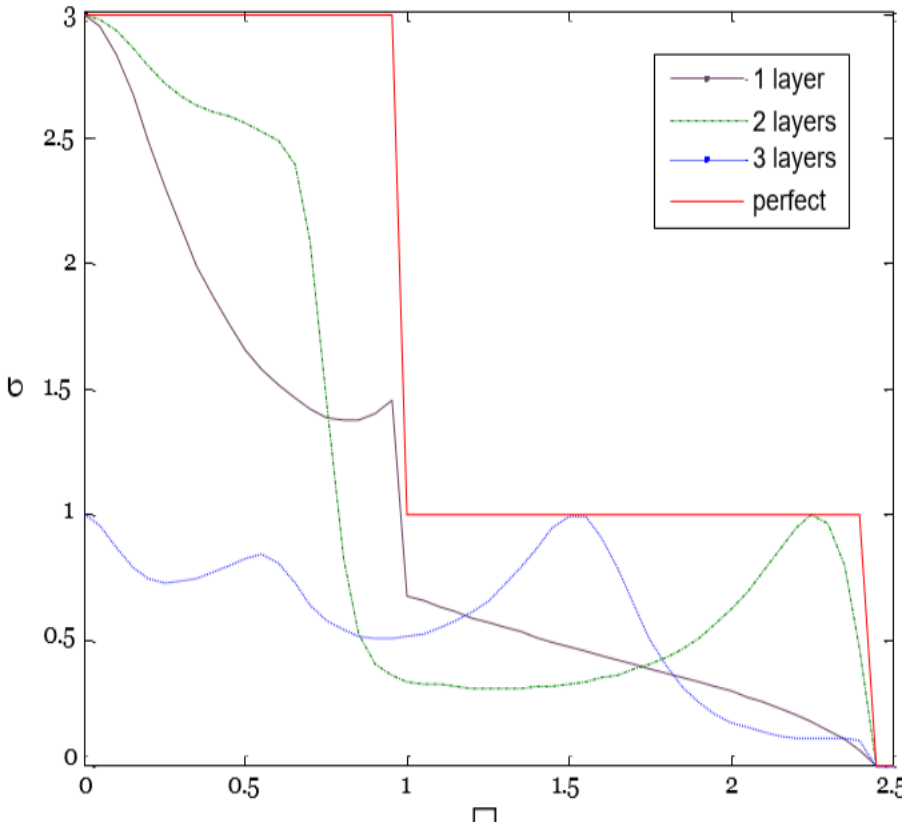


Figure.6 Courbe de la conductance phononiques

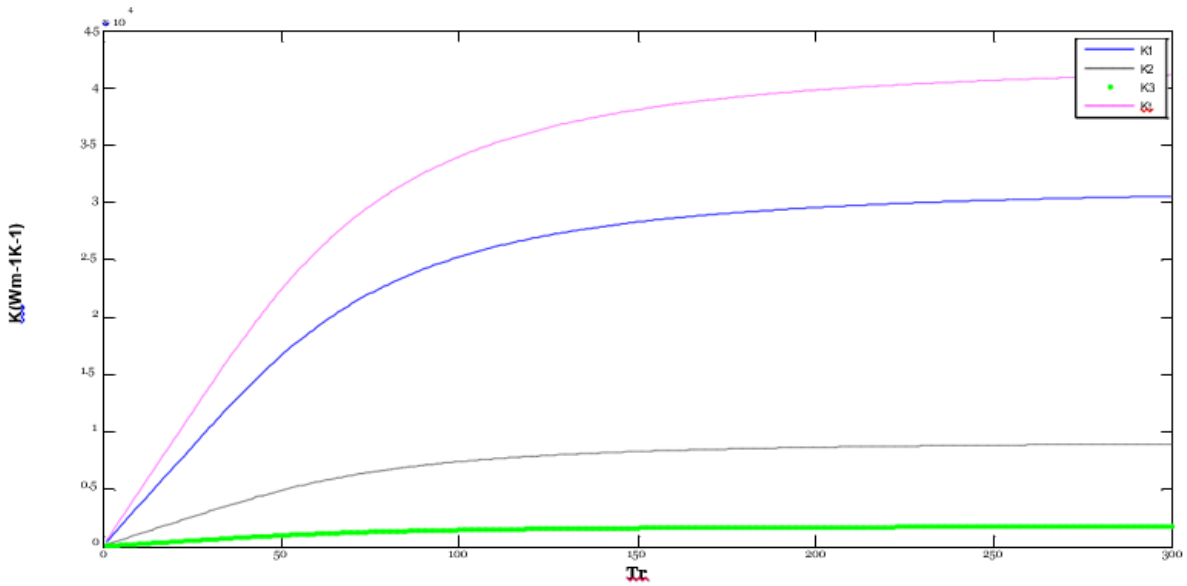


Fig.6 The curves of total conductance respectively for the perfect multichannel waveguide and waveguide with the integrated planes as function of the scattering dimensionless frequency and the system parameters.

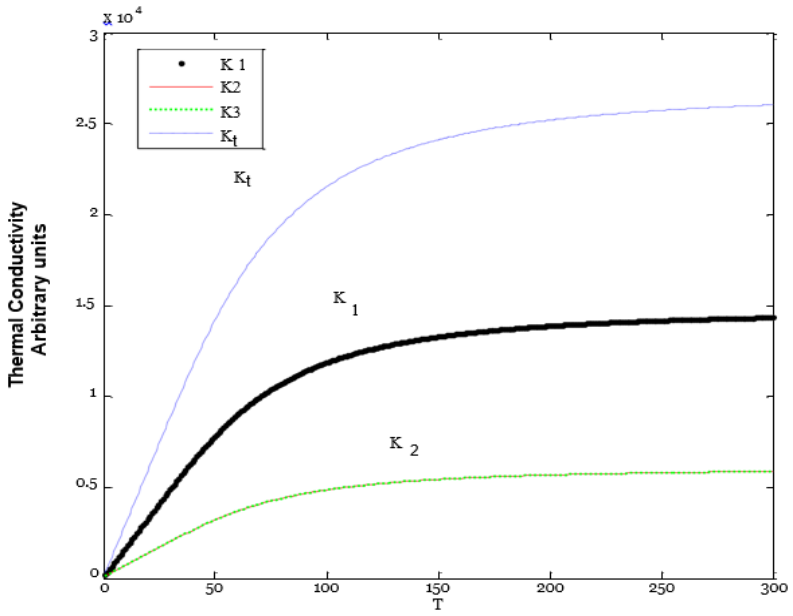


Fig.7: The curves of the thermal conductivity for two integrated layers as the function of the temperature T and the system parameters.

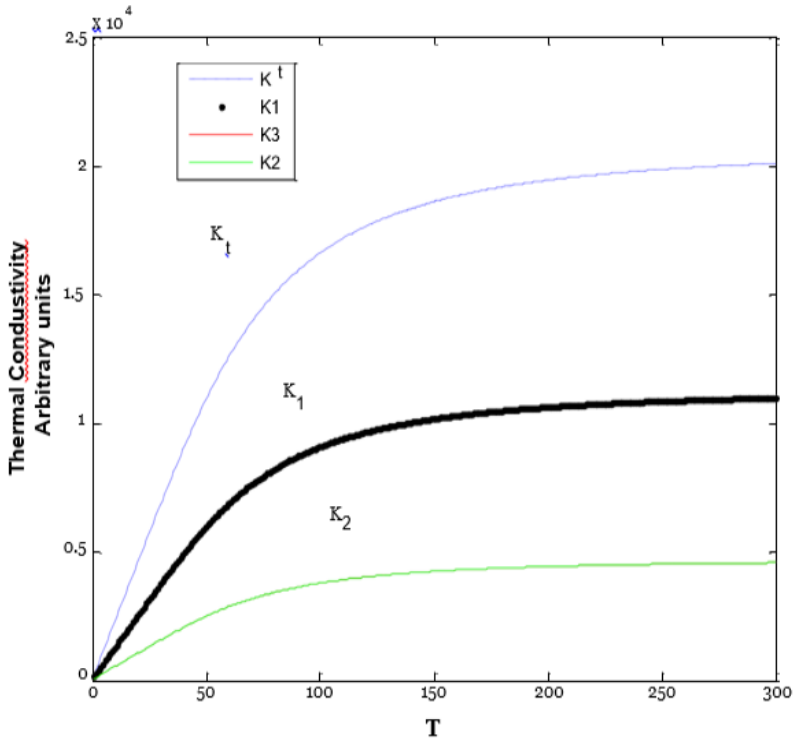


Fig.8: The curves of the thermal conductivity for three integrated layers as the function of the temperature T and the system parameters.

The transmission and reflection coefficients associated with vibrational modes 1 and 3 undergo significant modifications when the system's characteristics are adjusted in the vicinity of the fault.

They dispersed on different frequency bands, accordingly: $0 < \Omega < 2.5$, for the mode 1 and $0 < \Omega < 1$ for the mode two and three which are degenerate. The curve of transmission and reflection coefficients corresponding to the mode 1 is on strip frequencies of $0 < \Omega < 2.5$, which presents the Fabry Perot resonance at $\Omega = 1.85$ induced by the coupling between propagating modes and localized phonons which vary appreciably according to the elastic constants to the neighbourhood of the defect. For superior to 2.5 all coefficients are vanished according to the evanescence of the field vibrationnal modes of the system beyond this frequency.

The conductance t(Ω) of the system misled by sum of the propagating modes of the system which is the signature of the nature of the various defects. It spreads on a beach of frequencies corresponding to 0 < < 2.5, the phonon energy band; the curve of conductance vary according to system parameters and dimension less frequencies.

The conductance spectra always starts with her higher values at low frequencies (tend to zero), and decrease with increasing and vanished at the Brillouin Zone limit at = 2.5. The thermal conductivity is related to the degradation of the performance of the electronic device.

General Conclusions

In this work, using the matching technique in the harmonic approximation, we investigate the general characteristics of phononic scattering at integrated nanostructure in the inhomogeneous system model. The findings demonstrate that the atomic elastic defect parameters and dimension- less frequencies have a substantial impact on the system's conductance as well as the reflection and transmission coefficients. The conductance peaks at lower frequencies, falls as it rises, and disappears at the Brillouin Zone boundary.

From both theoretical and practical perspectives, these spectra could provide valuable insights about the defect's unique geometry and elastic properties surrounding it. Thus, faults in certain nanostructures can be found and investigated using the conductance spectrum, which can subsequently be utilized to characterize such nanostructures. We anticipate that these results can be confirmed in a series of studies that are simple to implement. Even though frequency filters are typically constructed using resonances, the employment of such systems can be very advantageous for transducers and noise-not-destroyed control devices (ultrasonic filters) [42, 43]. Because of the connection between the results and the physical performance degradation of electronic devices, the findings may also be utilized to artificially modify thermal conductivity in those devices.

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