Vibration dynamics of single atomic nanocontacts

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Abstract. The motivation for this work is to introduce a model for an atomic nanocontact, whereby its mechanical properties can be analysed via the local spectra. The model system consists of two sets of triple parallel semi-infinite atomic chains joined by a single atom in between. We calculate the vibration spectra and the local densities of vibration states, in the harmonic approximation, for the irreducible set of sites that constitute the nanocontact domain. The nanocontact observables are numerically calculated for different cases of elastic hardening and softening, to investigate how the local dynamics can respond to changes in the microscopic environment on the domain. We have also calculated the phonon scattering and coherent conductance at the nanocontact, derived in a Landauer-Büttiker matrix approach. The analysis of the spectra, of the densities of vibration states, and of the phonon conductance, identifies characteristic features and demonstrates the central role of a core subset of sites in the nanocontact domain.

1. Introduction

Different experimental techniques are used to measure the elastic and mechanical properties of low dimensional system, in particular surface Brillouin light scattering [1], and surface acoustic wave (SAW) spectroscopy [2]. There are also a number of theoretical methods to deal with the effects of different type of nanostructures or defects embedded in low dimensional systems. The matching method that we employ in this work has previously been extended with success to study the diffraction of waves at isolated nanostructures in quasi-one-dimensional disordered systems [3-5].

In the present work, we present a simple model for the study of the vibration spectra and of the phonon transmission on an atomic nanocontact that acts as a joint between two sets of semi-infinite monatomic chains. In a first approximation the system is considered to be reposing on a solid surface with no interactions with the substrate. The results are presented for central nearest and next-nearest neighbor force constants in the harmonic approximation.

The analysis is carried out for triple chains integrated to the nanocontact as in figure 1. In particular we show that the nanostructure leads to Fano resonances in the vibration spectra. These resonances result from the coherent coupling between localized modes on the nanocontact domain and the continuum of propagating phonons of the perfect wave-guide.

The case of an asymmetric nanocontact, as in figure 1, is analyzed in depth to illustrate the model in the next section, where we also present the general dynamics model. In the final section some numerical results are presented with conclusions.
2. Model dynamics

The elastic interactions between nearest and next nearest neighbours in the domains to the left and the right of the nanocontact are represented respectively by the constants $k_1$ and $k_2$, where the shaded area in figure 1 constitutes the effective nanocontact domain. The elastic constants in this inhomogeneous boundary may differ from bulk values, and are hence labelled $k_{1d}$ and $k_{2d}$. It is convenient next to define the following ratios: $r = k_2/k_1$, $r_{1d} = k_{1d}/k_1$, $r_{2d} = k_{2d}/k_1$.

![Figure 1](image_url)

**Figure 1.** Schematic representation for an atomic nanocontact between quasi-one-dimensional lattice waveguides each composed of three semi-infinite chains on either side. The shaded zone denotes an effective nanocontact domain.

The dynamics of the system in the harmonic approximation [6], are described by the equations of motion of atomic sites $l$, where $u_{\alpha}(l)$ is the corresponding vibration displacement vector for site $l$. The indices $\alpha$ and $\beta$ denote Cartesian co-ordinates, $m(l)$ is the atomic mass for site $l$.

For sites $l$ and $l'$ distant from the inhomogeneous boundary to the left and right of the interval $n \in [-2, 2]$ of figure 1, the equations of motion may be cast, in the matrix form

$$[\Omega^{2} I - D(\eta, k_1, k_2)] |u\rangle = 0$$

$D$ is a $(6 \times 6)$ matrix, $|u\rangle$ is the corresponding displacement vector for a column of the perfect waveguide, and $\eta$ is the phase factor.

To illustrate the model, the propagating modes for the perfect waveguides are calculated for a choice of $r = 0.75$, as a function of the normalized wave vector $\varphi = k_0a$, where $\varphi_0$ runs in the interval $[-\pi, \pi]$ over the first Brillouin zone and $a$ is the inter-atomic distance between adjacent sites. There are two acoustical modes 1 and 2, and four optical modes 3, 4, 5, 6, ranging from bottom to top in numerical order.

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 nanocontact domain from the rest of the system. This irreducible set is comprised as in figure 1, from the sites labelled (1), (2), (3), (4), (5), (6), (7), (8), (9), (10) and (11). To decouple the infinite set of equations, the matching method procedure [7–9] is used, and we obtain a system of linear homogeneous equations

$$[\Omega^{2} I - D(\eta, r, r_{1d}, r_{2d})] |u, R\rangle = 0$$

The corresponding dimensions of this matrix $(34 \times 34)$ and of the vector $|u, R\rangle$ are characteristic of the irreducible set of sites in the nanocontact domain.

The most direct manner to calculate the spectral densities is via the Green’s functions, which may be expressed formally as in [10]. The vibration density of states (DOS) per atomic site $l$, is obtained next as a sum over the trace of the spectral density matrix.
3. Numerical applications and conclusions

The numerical analysis is carried out for three different cases determining a choice of the elastic properties of the atomic nanocontact domain.

(i) Softening \( r_{1d} = 0.9, \ r = 0.75, \ r_{2d} = 0.65 \)

(ii) Homogeneous \( r_{1d} = 1.0, \ r = 0.75, \ r_{2d} = 0.75 \)

(iii) Hardening \( r_{1d} = 1.1, \ r = 0.75, \ r_{2d} = 0.85 \).

The vibration spectra, and the localized density of states DOS, are calculated for the different sites of the nanocontact domain. There is evidence with reference to the DOS, as in figure 2, for a localized collective resonance about \( \Omega \approx 0.5 \) for the ensemble of the irreducible sites of the nanocontact domain.

![Figure 2](image)

**Figure 2.** The DOS vibration spectra of the nanocontact sites as identified in Figure 1, and their variations with the elastic constants on the boundary, from softening to hardening.

It is observed that the energy line of this mode goes to higher frequencies with increasing hardness of the elastic constants, namely \( \Omega = 0.45 \) for (i), \( \Omega = 0.50 \) for (ii), \( \Omega = 0.55 \) for (iii). The changes in \( \Omega \) are of the order of magnitude of the changes considered for the elastic constants of the nanocontact domain, which leads us to the conclusion that this mode would correspond primarily to a collective vibration of the nanocontact domain in the potential well.
The corner sites (8, 11) do not present any other features attesting to more of a role of confinement for the nanocontact domain. The symmetric sites along the y-axis of the system, namely (2, 4), (3, 5), (6, 9), (7, 10), show a richer DOS than the other sites (1) and (3, 5). The analysis of their DOS yields a number of further conclusions. The pair of sites (3, 5) present, for example, a specific resonance line at $\Omega = 1.25$, that does not show up for any of the other sites in the nanocontact domain. We interpret this by assigning the resonance line to collective localized vibration mode of the pair of sites (3, 5) against the rest of the system where all sites remain stationary.

![Image](image_url)

**Figure 3.** The total phonon transmittance spectra via the nanocontact, as a function of the variation of the elastic constants on the boundary, from softening to hardening. The histogram (green) shows the phonon conductance spectra for the ideal waveguide.

We have also calculated the total phonon conductance, by summing over all the contributions of transmission probabilities at incident phonon frequencies, $\Omega$, for the three cases of elastic constraints on the atomic nanocontact domain. The conductance spectra are briefly presented in figure 3, for the three cases of interest, namely softening (blue), homogeneous (red), and hardening (black). The histogram (green) shows the phonon conductance spectra for the ideal waveguide. By comparing these conductance spectra it is possible to conclude that there are spectral features which, invariant with the change of the nanocontact boundary force constants, are associated to the critical behaviour of the waveguide phonons at their cut-off frequencies in their propagating intervals. The other critical features are Fano resonances, which peak positions vary with elastic boundary conditions; these arise effectively due to the interaction of bulk waveguide phonons with the localized boundary states. In particular we retrieve the DOS resonance line of the pair of sites (3, 5) at $\Omega \sim 1.25$, as shown in figure 2, via a Fano resonance in a comparable frequency interval. It shifts to relatively higher frequencies with increasing boundary elastic hardening.

**4. Conclusion**

In conclusion, we have presented a model calculation for the study of the vibration spectra of an atomic nanocontact which acts as the joint between two sets of semi-infinite monatomic chains. This analysis enables one to address questions regarding the mechanical properties of nanocontacts. The analysis of the vibration spectra and of the DOS of the set of irreducible sites in the nanocontact domain demonstrates the central role of a core subset of these sites for the dynamics of the
nanocontact. It can also serve towards the study of granular chains constructed in an analogous manner on the classical macroscopic scale.

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