Numerical simulation of the longitudinal dispersion bands of phonons in a $(GaAs)_1/(AlAs)_1$ superlattice

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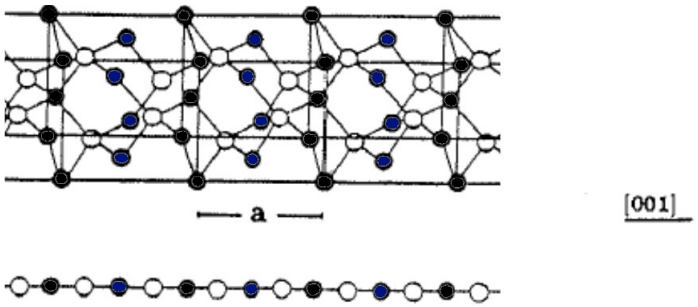

Figure 1: The superlattice used in this study and its projection on the [001] direction. Gallium atoms are painted black, Aluminium ones are blue and Arsenic is white. Note that, when projecting on the [001] direction, each of the planes can be treated as a single atom.

1 Abstract

2 Introduction

Normal vibrational modes of a of quantized elastic system are called phonon. They are collective excitation - i.e. bosonic quasiparticles - and their dispersion relation are related to a number of properties of the system itself.
A superlattice is a kind of metamaterial made up from two (or more) materials, in a periodic structure. An ideal $(GaAs)_1/(AlAs)_1$ superlattice is made up from one layer of $GaAs$ followed by one of $AlAs$ in a periodic matter (see Figure 1.

In general, the vibrational properties of a crystalline solid can be studied trough lattice dynamics; thanks to the periodicity of the system the problem can be further reduced to the solution of the dynamics of the atoms in the unitary cell.
Three more approximations will be employed:

1. **The harmonic approximation**, which consider the atomics cores as simple harmonic oscillator

2. **The nearest neighbour approximation**, where for each atom the interaction between anything other than the closest atoms next to it are neglected.

3. **The Born-Oppenheimer approximation** where ionic and electronic motions can be treated indipendently.

Thanks to these approximation it is possible to reduce in a the quanto-mechanical problem of vibration in a solid to the classical one of finding the normal modes to then find the dispersion bands (how the frequency depends on $\vec{q}$, the wavevector of the mode).
Only the [0,0,1] direction will be considered, so that the materials' layers follow

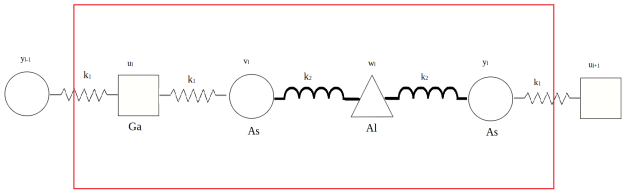

Figure 2: The 4-atom unitary cell analysed in this work.
k_1 is the elastic constant between Ga and As and k_2 is the elastic constant between Al and As. Considering an infinite linear chain u_l represent the displacement of the l-th (arbitrary origin) atom of Ga, v_l the displacement of the l-th atom of As of the GaAs molecule, w_l the displacement of the l-th atom of Al, y_l the displacement of the l-th atom of As of the $AlAs$ molecule.

each other orthogonally with respect to this direction. Only longitudinal vibrations have been taken into account.

3 Physical Problem

Because of the approximation used in this study, the relevant physical model is a linear chain of atoms in which the unit cell is made up by 4 atoms, *Ga-As-Al-As* as in Figure 2, and- at least in first approximation - only interaction with nearest neighbour needs to be taken into account.
The following system results (see Figure 2 for the meaning of each symbol):

$$\begin{cases} M_{Ga}\ddot{u}_l = -k_1(u_l - v_l) - k_1(u_l - y_{l-1}) \\ M_{As}\ddot{v}_l = -k_1(v_l - u_l) - k_2(v_l - w_l) \\ M_{Al}\ddot{w}_l = -k_2(w_l - v_l) - k_2(w_l - y_l) \\ M_{As}\ddot{y}_l = -k_2(y_l - w_l) - k_1(y_l - u_{l+1}) \end{cases} \tag{1}$$

To solve this system we impose that every displacement has the form of a plane wave:

$$\begin{cases} u_l = Ue^{i(qla-\omega t)} \\ v_l = Ve^{i(qla-\omega t)} \\ w_l = We^{i(qla-\omega t)} \\ y_l = Ye^{i(qla-\omega t)} \end{cases} \tag{2}$$

where a is the lattice parameter of the superlattice (sum of the lengths of the respective unit cells). Solving the system for ω and then varying $\vec{q}$ will lead to the dispersion bands; because the unit cell has 4 atoms the system to solve is 4-dimensional and so 4 dispersion bands are expected.

4 Numerical solution

The problem of the dispersion bands of GaAs/AlAs reduces to the solution of the system showed in Equation 1.
Substituting in the system the solution for the plain wave in Equation 2, after some algebra one gets:

$$\begin{cases} (-\omega^2 M_1 + 2k_1)U - k_1 V - (k_1 e^{-iqa})Y = 0 \\ (-\omega^2 M_3 + 2K2)W - k_2 V - k_2 Y = 0 \\ -k_1 U - k_2 W + (-\omega^2 M_2 + k_1 + k_2)V = 0 \\ -(k_1 e^{iqa})U - k_2 W + (-\omega^2 M_2 + k_1 + k_2)Y = 0 \end{cases} \tag{3}$$

This is convenient as the system's associated matrix is already written in the form $[-\omega^2 I + A]$, where

$$A = \begin{pmatrix} \frac{2k_1}{M_{Ga}} & 0 & -\frac{k_1}{M_{Ga}} & -\frac{k_1}{M_{Ga}} e^{-iqa} \\ 0 & \frac{2k_2}{M_{Al}} & -\frac{k_2}{M_{Al}} & -\frac{k_2}{M_{Al}} \\ -\frac{k_1}{M_{As}} & -\frac{k_2}{M_{As}} & \frac{k_1}{M_{As}} + \frac{k_2}{M_{As}} & 0 \\ -\frac{k_1}{M_{As}} e^{iqa} & -\frac{k_2}{M_{As}} & 0 & \frac{k_1}{M_{As}} + \frac{k_2}{M_{As}} \end{pmatrix} \tag{4}$$

so it is possible to solve the secular equation and find ω^2. Varying q inside the first Brillouin Zone one arrives at the dispersion relation. The eigenvectors of A are instead the displacement of the single atoms in the chain.

To obtain the solution of the problem a numerical approach was undertaken: a program in C++ has been written which, after discretising the Brillouin Zone in a selected number of points, calculate appropriate wavevector q for each points, and then fills the matrix in Equation 4 with the appropriate values. Finally, using a subroutine of the *Eigen* linear algebra package, it finds eigenvectors and eigenvalues for each matrix.
The result is a discretized version of the dispersion relation, which is then plotted with GNUPLOT.

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1 CODICE
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Listing 1: Subroutine norma
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