PHONON MODES IN InAs/AlSb SUPERLATTICES

Josh Matsko *
Department of Physics
Illinois State University
Normal, IL 61761
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ABSTRACT

The InAs/AlSb heterojunction system is a lattice matched semiconductor system with type-II band alignment at the interfaces. This system is attractive to ultra-fast electronic device application due to its high mobility and large conduction-band offset. The superlattice can have two different interfaces: AlAs-like or InSb-like. These interfaces have very different interface roughness, mobility and carrier concentrations. There is experimental evidence showing preferential local arrangements of the interfacial atoms. First principle pseudo-potential calculations indicate that such superlattices with switched layers at the interfaces are more energetically favorable than superlattices with ideal sharp strained interfaces. We theoretically calculate the phonon modes of the InAs/AlSb superlattices using a one-dimensional linear chain model. We compare the interface modes for superlattices with the two different interface structures. We found that there not only are more interface modes in the superlattice with the switched interface layers, but that there also exist bulk modes at the interface, a special feature of this structure.

INTRODUCTION

The InAs/AlSb heterojunction system is a lattice matched semiconductor system with type-II band alignment at the interfaces. [1-3] Depending on the structure of an InAs/AlSb superlattice, two types of interfaces can make up the system: AlAs-like or InSb-like. For instance, in Figure 1, an AlAs-like interface is formed. In a one dimensional linear chain model, the interface is named by the 'adjoining' atoms between the two lattices that make up the superlattice. These interfaces have very different interface roughness, mobility and carrier concentrations.

There is experimental evidence showing a preferential local arrangement of the interfacial atoms. [1,2] First principle pseudopotential calculations indicate that such superlattices with switch layers at interfaces are more energetically favorable than superlattices with ideal sharp strained interfaces. [3]

There are four possible types of switches of atomic layers at the interfaces for In As/AlSb superlattices:
1) the anions around Al
2) the anions around In
3) the cations around Sb
4) the cations around As.

It has been shown that the switch of the cations around an anion is energetically more energetically favorable than non-switched interfaces and when the anions are switched around the cations.[3] In our case, the most favorable switch is that of In and Al around As.

To better understand the characteristics of these superlattices, we theoretically calculated the phonon modes, the vibrational frequencies and vibrational amplitudes. Some of these vibrational amplitudes at certain frequencies are more localized at the interface. They are called interface modes. The interface modes are used as variables to model the behavior of the interface.

THE MODEL

We calculate the phonon modes, including the vibrational

Josh has completed the third year of a five-year program that consists of attending Illinois State University (ISU) for the first three years and then the University of Illinois at Urbana-Champaign (UIUC) for two years. After the five years, he will receive a bachelor's degree in physics from ISU and one in mechanical engineering from UIUC. He also has completed the requirements for a math minor at ISU.

This research was started in December of 1998 and there are plans to continue it. The initial results were presented at the Centennial APS meeting in Atlanta in the spring of 1999. During the summer of 1999 he received a REU award from the NSF and traveled to China for three weeks where he continued this research at the Institute of Semiconductors of the Chinese Academy of Sciences.

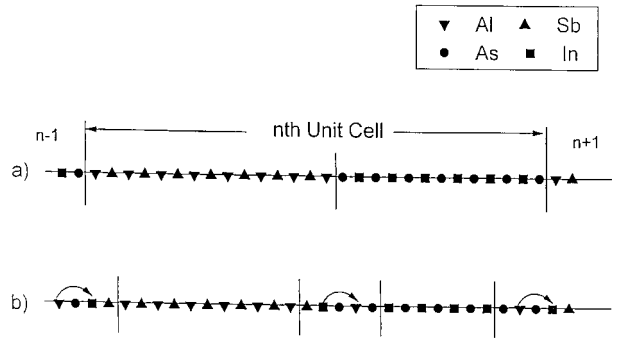

Figure 1
A three-dimensional InAs/AlSb (100) superlattice mapped into a one-dimensional linear chair. (a) the n^th unit cell of the superlattice with ideal AlAs-like interfaces. (b) The superlattice with switched layers of In and Al around As at both AlAs-like interfaces

frequencies and vibrations strengths, of the InAs/AlSb superlattice with both the ideal sharp interfaces and with switches of atomic layers at the interfaces. To do this, we used a one-dimensional linear chain model. [4] The three-dimensional InAs/AlSb(100) superlattice was mapped into a one-dimensional linear chain as shown in Figure 1. [5,6] In Figure 1, each atom represents an atomic plane that has the same atoms as in the real superlattice structure. Since all the atoms on the same plane have the same motion when the wave vector is along the superlattice growth direction, one atom can be used to represent the entire atomic plane. In Figure 1, the reversed triangle represents an Al layer, the triangle an Sb layer, the circle an As layer and the square an In layer.

Following the lead of a similar study[5], we considered twenty-eight atomic layers in the unit cell of our superlattice.

The structure of InAs/AlSb (13,15) superlattice with AlAs ideal interfaces is shown in Figure 1a. The structure of the same superlattice, but with cation layers switches around the As layer at the interfaces is shown in Figure 1b. The vertical lines in this figure show where each interface or interface boundary is located.

Our calculations are performed in a manner similar to a previous study [5] of phonon modes in InAs/GaSb superlattices, which uses one force constant for the longitudinal modes and two for the transverse modes and considers only the nearest neightbor interactions. Since the constituent materials of InAs/AlSb superlattices are similar to those of InAs/GaSb superlattices, we used the same force constants: 0.8 N/cm for longitudinal modes and 1.25 N/cm and 0.12 N/cm for the transverse modes. [5]

CALCULATIONS

The calculations start using the Newton's second law of motion. For the ith atom in the nth unit cell, we have:

$$F_i = \sum_{j \neq i} F_{j,i} = m_i a_i = m_i \frac{d^2 U_{n,i}}{dt^2} \ , \qquad (1)$$

where F_i is the net force on atom i, $F_{j,i}$ is the force from atom j on atom i, m_i is the mass of atom i, and $U_{n,i}$ is the displacement of the i^{th} atom in the n^{th} unit cell. In Equation 1, i goes from 1 to 28, the total number of atomic layers in the superlattice unit cell.

We assume that each atom acts as a harmonic oscillator, so its displacement can be written as:

$$U_{n,i} = A_{0,i}\, e^{i(kna' - \omega t)} \ , \qquad (2)$$

where $A_{0,i}$ is the amplitude of the vibration of the i^{th} atom, k is the wave vector, n is the unit cell number, a' is the total length of the unit cell (in our case 28a where a is the nearest layer distance), ω is the vibrational frequency and t is time.

To find the net force acting on the ith atom, we consider only the nearest neighbor interaction:

$$F_i = \sum_{j \neq i} F_{j,i} = F_{i-1} + F_{i+1} \ . \qquad (3)$$

Equation 3 can be put in terms of displacements by recalling that the harmonic oscillator force depends linearly on displacement:

$$F_i = f_i(U_{n,i+1} - U_{n,i}) + f_i(U_{n,i+1} - U_{n,i}) \ , \qquad (4)$$

where f_i is the force constant between atom i and atom i+1. For the longitudinal modes, all of the force constants are taken to have the same value. For the transverse modes, we have two different force constants.

Substituting Equation 4 into Equation 1 gives:

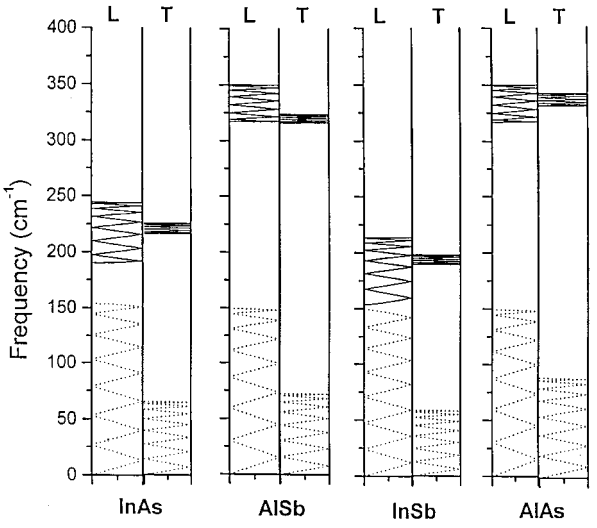

Figure 2
Calculated phonon modes of the four bulk materials: (a) InAs; (b) AlSb; (c) InSb; AlAs. The left panels are for longitudinal (L) modes and the right panels are the transverse (T) modes. The acoustic modes are shown as dotted lines and the optical modes are shown as solid lines.

$$m_i \frac{d^2U_{n,i}}{dt^2} = f_i U_{n,i+1} + f_{i-1} U_{n,i-1} - (f_i + f_{i-1}) U_{n,i} . \quad (5)$$

When $i = 1$, the first atom in the unit cell, we consider its interaction with the last atom in the previous unit cell, n-1. When i is the last atom in the unit cell, we consider its interaction with the first atom in the next unit cell, n+1. The first atom and last atom calculations contain an imaginary part due to the interaction of the previous (n-1) and next (n+1) unit cell.

Substituting Equation 2 into Equation 5 gives:

First atom

$$-m_i\omega^2 A_{0,i} = f_i e^{-ika'} A_{0,i+1} + f_{i-1} A_{0,i-1} - (f_i + f_{i-1}) A_{0,i} \quad (6)$$

Other atoms

$$-m_i\omega^2 A_{0,i} = f_i A_{0,i+1} + f_{i-1} A_{0,i-1} - (f_i + f_{i-1}) A_{0,i} \quad (7)$$

Last Atom

$$-m_i\omega^2 A_{0,i} = f_i A_{0,i+1} + f_{i-1} A_{0,i-1} - (f_i + f_{i-1}) A_{0,i} \quad (8)$$

We use equations 5-8 to calculate the motion of all the atoms. Equations 6-8 can be written in matrix form as:

$$\omega^2 M \boldsymbol{A} = D \boldsymbol{A} , \quad (9)$$

where ω is the frequency, M is a mass matrix where $M_{ij} = m_i$ when $i = j$ and $M_{ij} = 0$ when $i \neq j$, $\boldsymbol{A}$ is a vector with $A_i = A_{0,i}$ and D is a matrix consisting of the force constants. Equation 9 can be rewritten in terms of a Hermitian matrix T as:

$$\omega^2 \boldsymbol{A'} = T \boldsymbol{A'} , \quad (10)$$

where

$$T = M^{-\frac{1}{2}} D M^{-\frac{1}{2}} , \quad (11)$$

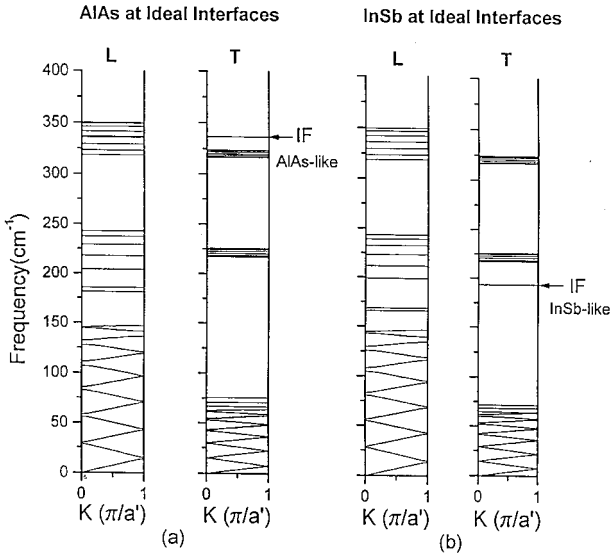

Figure 3
Calculated phonon modes of InAs/AlSb superlattices with two possible ideal interfaces: (a) AlAs-like and (b) InSb-like. The right panels represent transverse modes and the left panels represent longitudinal modes. The interface modes are identified by the letters IF.

and

$$\boldsymbol{A'} = M^{\frac{1}{2}} \boldsymbol{A} . \quad (12)$$

We found the eigenvalues and eigenvectors of the Hermitian matrix, T, using a library subroutine and a FORTRAN 90 program. The eigenvalues, ω^2, of the Hermitian matrix are the squares of the frequencies of the phonon modes. The real and imaginary parts of the eigenvectors are related to the vibration amplitudes by Equation 12.

DISCUSSION

We first calculated the phonon modes for the four bulk materials: InAs and AlSb, the constituent materials of the superlattices and InSb and Al As, two of the possible interface materials. Figure 2 shows the results of our calculations. For each bulk material, we show the longitudinal mode (L) and the transverse mode (T). The frequenices that are below 150 cm^{-1} (in Figure 2 the dotted lines) represent the acoustic modes, the ones above 150 cm^{-1} (in Figure 2 the solid lines) represent the optical modes. When the wavelength is of the mode is much larger than the unit cell and the atoms vibrate in phase with each other it is called an acoustic mode. When the atoms vibrate out of phase with one another, it is called an optic mode.

Because all four of the materials, two bulk materials (InAs and AlSb) and the two interface materials (InSb and AlAs) have similar acoustical frequenicy ranges, the superlattice acoustical frequency range is similar to that of the bulk material. On the other hand, the otical frequency frange for these four materials are quite different. Therefore, the superlattice optical modes will be confined in one of the materials.

Since when we calculate the modes of the bulk material, we took the unit cell to be the same as the superlattices (28 atomic layers), the results are the same as one would get by folding the Brillouin zone for the conventional bulk material fourteen times as the bulk material only has two atoms in the unit cell.

We next studied the superlattices with ideal interfaces and interfaces with switched atomic layers. We followed the techniques used in a previous study of phonon modes in ZnTe/CdSe superlattices. [7,8] The phonon modes calculated for the structure shown in Figure 1(a), (AlAs-like), are shown in Figure 3(a). Figure 3(b) shows the calculated phonon modes for an ideal InSb-like interface. Figure 4 shows the results of the phonon mode calculations for the two possible switches of cation layers about an As layer with two different interfaces: (a) AlAs and (b) InSb.

The possible interface modes are indicated by the label IF in Figures 3 and 4. The interface modes are identified by comparing frequency range of the corresponding bulk material in Figure 2 with the calculated superlattices that have ideal (Figure 3) and switched (Figure 4) interfaces. If the frequency of a superlattice is in the range of either of

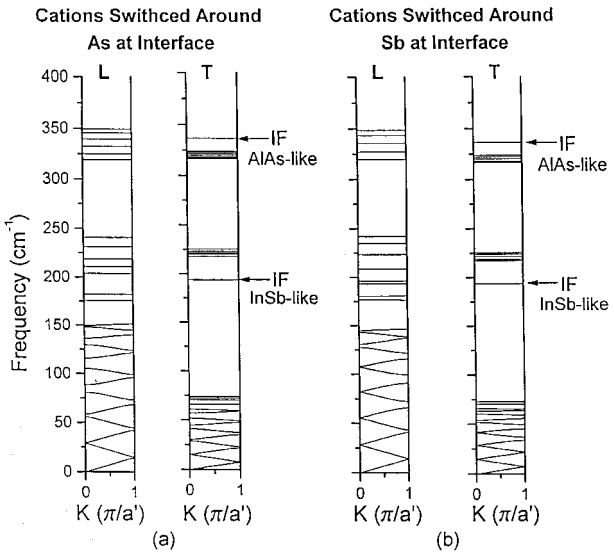

Figure 4
Calculated ;phonon modes of the two possible switches of cation layers around the As layers for superlattices with two different interfaces: (a) AlAs-like and (b) InSb-like. The interface modes are identified for the transverse modes by the letters IF.

the two bulk materials, it is a mode extended to the entire superlattice, and is called an extended mode. If this frequency belongs only to one bulk material, the mode will be confiend to the material and called a confined mode. if the frequency is in the grange of the two of the two interface materials (InSb or AlAs) but not in the range of the bulk material, it is an interface mode. The interface modes of AlAs and InSb are more easily seen in the transverse vibration graphs. Note that there are more interface modes in the superlattices with switched atomic layers than in the superlattices with ideal interfaces.

Figure 5 shows the vibrational amplitudes for particular vibrational frequencies for several different types of phonon modes in InAs/AlSb superlattices. The three displays in Figure 5 are for the superlattice with ideal AlAs interfaces. The top display is for a frequency where the phonon mode is shared by all of the involved material, the vibrational amplitude extends to the entire superlattice. The next display shows a confined mode. The vibrational amplitudes are confined to the InAs layers. The third display shows the transverse interface mode of the superlattice with an ideal AlAs interface. The frequency of this phonon mode is seen in neither InAs or AlSb bulk material. It only belongs to AlAs, so this mode is sharply located at the interface.

When the layers are switched as shown in Figure 1(b), there will be both InSb and AlAs layers at the interfaces. There will also be some thin bulk layers of InAs and AlSb at the interfaces. There will be more interfaces modes in this case, and some bulk modes could also be localized at the interface. Figure 6 shows modes in the superlattice with the switched interface structures shown in Figure 1(b). The first three displays are transverse interface modes, one InSb mode and two AlAs modes where the two AlAs modes have degenerate frequencies and are localized at the two interfaces. The last display shows a confined InAs bulk mode within the thin bulk layers that the switched layers produce at the interface.

We find that the phonon modes for superlattices with ideal sharp interfaces differ from those with switched atomic layers in that the switched superlattices have more interface modes than the ideal interface. This is probably due to the increase in the thickness of the interface due to the switching layers. The phonon modes for the InAs/AlSb superlattice depend on the interface structures.

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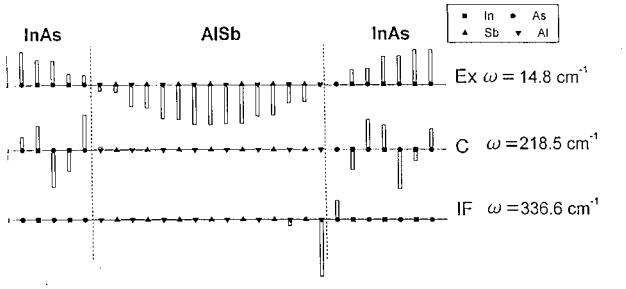

Figure 5
A few different types of modes with both calculated vibrational amplitudes (eigenvectors) and their corresponding vibrational frequencies (eigenvalues) in the InAs/AlSb superlattices. These are for the superlattice with ideal AlAs interfaces where (a) the extended , (b) the confined modes, and (c) the transverse interface modes of the superlattice with AlAs ideal interfaces.

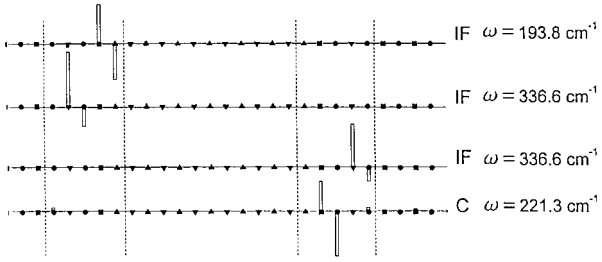

Figure 6
A few different types of modes with both calculated vibrational amplitudes (eigenvectors) and the corresponding vibrational frequencies (eigenvalues) in the InAs/AlSb superlattice. The top three are the transverse interface modes of the superlattice with switched layers of Al and In around As. The bottom display is the confined bulk mode within the bulk layers that are produced by switching layers at the interfaces.

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* current address of author: 3688 Springlake Circle, Loveland, OH 45140 jmatsko@uiuc.edu.
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Dr. Shan-Fen Ren
Department of Physics
Campus Box 4560
Illinois State University
Normal, Il 61790-4560
ren@phy.ilstu.edu