Microscopic interface phonon modes in structures of GaAs quantum dots embedded in AlAs shells

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By means of a microscopic valence force field model, a series of novel microscopic interface phonon modes are identified in shell quantum dots (SQDs) composed of a GaAs quantum dot of nanoscale embedded in an AlAs shell of a few atomic layers in thickness. In SQDs with such thin shells, the basic principle of the continuum dielectric model and the macroscopic dielectric function are not valid any more. The frequencies of these microscopic interface modes lie inside the gap between the bulk GaAs band and the bulk AlAs band, contrary to the macroscopic interface phonon modes. The average vibrational energies and amplitudes of each atomic shell show peaks at the interface between GaAs and AlAs. These peaks decay fast as their penetrating depths from the interface increase.

Keywords: A. Nanostructures; A. Semiconductors; C. Crystal structure and symmetry; D. Phonons
1. Introduction

Interesting results have been reported on the surface and interface modes of phonons and polaritons in layered or spherical structures by means of macroscopic continuum model. By using the Rosenzweig model, G. Armand et al. \cite{1} have found that there are surface phonon modes in the gap of the bulk phonon modes and below the lowest bulk band. Maradudin et al. \cite{2} have predicted that there are surface phonon waves propagating in the gap between the bulk phonon bands and below the lowest bulk phonon band in structures that a semi-infinite GaAs/AlAs superlattice is in contact with a thin film of GaAs or AlAs. The amplitudes of some surface modes show strong decaying or variation as their penetrating depths from the surface increase. At about the same time, Quinn et al. predicted that there are surface plasmon modes without suffering Landau damping surviving below, above or between the bands of bulk plasmon frequencies in both type-I and type-II semi-infinite semiconductor superlattices. \cite{3, 4}. Interface and surface modes in shell quantum dots (SQDs) composed of a spherical core of one material (core material) embedded in a matrix of another material (shell material) have been studied by many authors. \cite{5, 6, 7}. However, most of the theoretical treatments on shell QDs are performed in the framework of mechanical continuum model, continuum dielectric model, or continuum model coupling both the mechanical vibrational amplitudes and the electrostatic potential. \cite{5}. Their regions of validity is limited to modes whose effective wavelength is large compared to the interatomic spacing. In the case of surface plasmons the continuum dielectric approach is limited to dots whose size is large enough that the plasma frequency greatly exceeds the differences between the single-particle energies. \cite{8}. After surveying systematically the validity of the dielectric approximation in describing electron-energy-loss spectra of surface and interface phonons in thin films of ionic crystals, Lambin et al. \cite{9} demonstrated
that the dielectric approximation reproduces the essential features of the phonon response when the layer thickness exceeds 20-30 Å. Approximation can no longer be applied to thinner films as the concept of bulk dielectric function, the only input required in this approach, breaks down. Even for films in above thickness range, small contributions of microscopic surface phonons survive and they may not be neglected. The eigenvectors of the microscopic surface phonons are found to be large at the first surface layer and rapidly decreasing as the distance from the surface increases. Therefore to describe phonon modes in semiconductor SQDs with small dots size and thin shells, an anisotropic microscopic model is especially needed.

2. The theoretical formalism

We have developed a microscopic valence force field model (VFFM) in recent years to investigate phonon modes in QDs [10, 11, 12]. In this model, the change of the total energy due to the lattice vibration is considered as two parts, \( \Delta E = \Delta E_s + \Delta E_c \), where the energy changing due to short-range interactions describes the covalent bonding, and the long range part approximates the Coulomb interactions [17, 14, 15]. For the short range part, we employed a VFFM as [16], \( \Delta E_s = \sum_i \frac{1}{2} C_0 (\Delta d_i)^2 + \sum_j \frac{1}{2} C_1 (\Delta \theta_j)^2 \), where \( C_0 \) and \( C_1 \) are two parameters to describe the energy change due to the bond length and the bond angle respectively, and the summation runs over all the bond lengths and bond angles. Because each of these two parameters has a simple and clear physical meaning, this model allows us to treat the interaction between atoms at the surface and interface appropriately.

In our model, the projection operators of the irreducible representations of the group theory is employed to reduce the computational intensity [18, 19, 20]. For example, the dynamic matrix for a 8.0 nm GaAs/AlAs SQD is in the order of 35,565. This can be reduced to five matrices in five different representations of \( A_1, A_2, E, T_1, \) and
T_2, with the sizes of 1592, 1368, 2960, 4335, and 4560 respectively. This approach further allows us to investigate phonon modes with different symmetries in QDs in detail.

By employing this model, we have investigated phonon modes in GaAs/AlAs SQDs composed of a spherical GaAs core of radius d_s embedded in an AlAs shell with external radius d_L \cite{12}. Our theoretical formalism has considered every details in the SQDs. it is suitable to deal with SQDs that the the core material and the shell material have totally different parameters. But for calculations of GaAs/AlAs SQDs, the parameters C_0, C_1, and e^* for both GaAs and AlAs are taken to be the same for simplicity, and only the mass difference is considered. The C_0, C_1, and e^* are taken as 38.80, 0.858, and 0.6581, and the masses of Ga, As and Al are taken as 69.723, 74.922 and 26.982 respectively in atom unit.

When considering the interaction between atoms, special attention is paid to atoms near the surfaces and interface of the shell QDs. More specifically, for the short range interaction, when an atom is located near the surface, interaction from its nearest neighboring atom is considered only if that specific nearest atom is within the QD, and interaction from its second neighboring atom is considered only if that specific second neighbor atom is in the QD as well as the nearest neighboring atom that makes the link between them.

3. Results and discussion

By employing this model, the frequencies and vibrational strengths of phonon modes of GaAs/AlAs SQDs are calculated as functions of the size of internal dot and the thickness of the external shell of SQDs in each of five representations of A_1, A_2, E, T_1 and T_2 \cite{12}. The results of our model shows that the entire optical frequency range of SQDs is divided into two nonoverlapping bands, which are originated from
bulk AlAs band and bulk GaAs band respectively, so named as AlAs-like band and GaAs-like band respectively. The lowest and highest frequency of the bulk AlAs (GaAs) optical band is 318.48 cm\textsuperscript{-1} and 396.00 cm\textsuperscript{-1} (268.80 cm\textsuperscript{-1} and 292.13 cm\textsuperscript{-1}) respectively evaluated from the VFFM. We have also noticed that there are many phonon modes inside the gap between bulk GaAs band and the bulk AlAs band in SQDs, especially in SQDs covered by thin shells to which the concept of bulk dielectric function is no longer available. In this letter, we concentrate our attention on the study of phonon modes in SQDs with shells of a few atomic layers by using VFFM.

Fig. 1 is a plot of density of states of phonon modes for 10 selected symmetries and scales of SQDs with thin shells. It is plotted by taking half width of the Gaussian broadening $\sigma = 0.4 cm^{-1}$ and the frequency step $\Delta \omega = 0.2 cm^{-1}$. Two thin vertical lines are used to show the upper edge of the bulk GaAs band and the lower edge of the bulk AlAs band. According to the dielectric model, all the interface modes corresponding to different angular quantum number $l$ fall within the bulk AlAs band or bulk GaAs band respectively, no matter the shell thickness of the GaAs/AlAs SQD is infinite or finite (for the latter case, we suppose that the SQD is enclosed by vacuum). Therefore, all the modes with frequencies inside the gap between GaAs and AlAs bulk bands (with $292.13 cm^{-1} \leq \omega \leq 318.48 cm^{-1}$) should be categorized into microscopic interface modes, since they are novel modes that could be revealed only by microscopic models. Indeed these modes have obvious characteristics of the interface modes as we will show below. To distinguish with these microscopic interface modes, we call other modes with frequencies within the bulk AlAs band or the bulk GaAs band internal modes.

It is seen from Fig. 1 that for QDs with $d_S = 21.70 \ \AA$ and $d_L = 26.95 \ \AA$ (or a 21.70 Å/26.95 Å SQD), there are two $T_2$ modes with frequencies of 299.13 cm\textsuperscript{-1} and 304.64 cm\textsuperscript{-1} and a single $A_1$ mode with frequency of 305.71 cm\textsuperscript{-1} in the gap between the GaAs-like phonon band and the AlAs-like phonon band. Similarly in that frequency range, for a 31.34 Å/34.26 Å SQD, there are two modes of $A_1$ and $T_2$ symmetries, no
mode of $A_2$ symmetry, and one single mode of $T_1$ and $E$ symmetries, respectively. These are microscopic interface modes that are caused by the microscopic bonding condition at the interface that completely fail to survive in macroscopic continuum dielectric model. In this letter main attention is paid to exam the characteristics of these microscopic interface modes.

We first exam the average vibrational amplitudes (AVA) of these atomic shells for the microscopic interface phonon modes. The AVA of the $l$-th atomic shell is defined as $A_l^i = \frac{1}{n} \sum_{k=l}^{n} |a_{lk}^i|$, where $a_{lk}^i$ is the vibrational amplitude of the $k$-th atom in the $l$-th shell in the $i$-th phonon mode, and $n$ is the total number of atoms in the $l$-th shell. In our spherical QD, the center of the QD is chosen on an atom, and the shells consist of atoms with the same distance to the center of the QD. Two sets of plots are shown in Fig. 2 to investigate the behavior the AVA of microscopic interface modes. These plots show the AVA of atoms in the $l$-th shell as a function of the shell’s diameter. The mode order number and the frequency of the mode are indicated in each mode. The upper four subfigures in Fig. 2 are for four modes of $T_2$ symmetry in a 21.70 Å/26.95 ÅSQD with the frequency range from 286.92 cm$^{-1}$ to 331.92 cm$^{-1}$, while the lower four are for the four modes of $A_1$ symmetry in a 31.34 Å/34.26 ÅSQDs with the frequency range from 286.43 cm$^{-1}$ to 330.44 cm$^{-1}$. It is seen that the peaks of AVA of the 164-th and 165-th modes of $T_2$ symmetry with frequencies of 299.13 and 304.64 cm$^{-1}$ appear exactly at the vertical thin line which indicate GaAs/AlAs interface of diameter 21.70 Å. These are typical microscopic interface modes. The 163-th mode and the 166-th mode of $T_2$ symmetry have frequencies inside the bulk GaAs and bulk AlAs bands, so their AVA show the basic characteristics of GaAs bulk modes and AlAs bulk modes [11]. Similarly, for modes of $A_1$ symmetry in a 31.34 Å/34.26 ÅSQD, the AVA of the 131-th and 132-th modes have peaks at or near the interface shell indicated by a vertical line. Here we want to add another important effect: due to the quantum confinement effect discussed in detail in Ref.s [10], [11], [12], the highest frequency
of the GaAs-like modes decreases and the lowest frequency of the AlAs-like modes increases as the core size and the shell thickness decrease, which makes the gap between the top of the GaAs-like band and the AlAs-like band much wider than the gap between two bulk materials. Therefore, some modes appear outside the gap but near the gap may still be microscopic interface modes. The AVA of the 130-th mode (with frequency of 286.43 \(cm^{-1}\)) of \(A_1\) symmetry for the 31.34 Å/34.26 ÅSQD is certainly this case, because it has also a highest peak located exactly at the interface.

To reveal more characteristics of the microscopic interface modes in SQDs, we have further calculated a few other physical properties of these interface modes. These include the average vibrational energy, the total vibrational energy, the total vibrational amplitudes, and the radial projection of the vibrational amplitude of the \(l\)-th shell. These properties are defined as the following: for the \(i\)-th mode, the average vibrational energy of the \(l\)-th shell, \(E_{i,l}\), is defined as 

\[
E_{i,l} = m_l \tilde{A}_{i,l}^2 = m_l \left[ \frac{1}{n} \sum_{k=1}^{n} (a_{ik})^2 \right]^{\frac{1}{2}};
\]

where \(a_{ik}\) and \(n\) are the same as defined above. The total vibrational energy of each shell, \(E_{l,T}^{i}\), is defined as 

\[
E_{l,T}^{i} = E_{i,l} \cdot n;
\]

The total vibrational amplitude of each shell in the \(i\)-th mode is defined as 

\[
A_{l,T}^{i} = A_{i}^{i} \cdot n,
\]

where \(A_{i}^{i}\) is the AVA defined before. The radial projection of the vibrational amplitude in the \(l-th \) shell is defined by

\[
\frac{A_{L}^{i}}{A_{i}} = \frac{1}{n} \sum_{k=1}^{n} \frac{|a_{ik} \cdot r_k|}{(|r_k| \cdot |a_{ik}|)},
\]

where \(a_{ik}\) denotes the vibrational amplitude of the \(k\)-th atom in the \(i\)-th mode, and \(r_k\) is the position vector of the \(k\)-th atom relative to the center of the QD. The quantity \(A_{L}^{i}/A_{i}\) describes to what extent a phonon mode is radial-like.

In Fig. 3, these four physical quantities as well as the AVA defined earlier are plotted as functions of the shell diameters for an microscopic interface mode with frequency of 294.20 \(cm^{-1}\), that is an \(A_1\) mode in 44.76 Å/48.85 ÅSQDs. The five subfigures from top to bottom are the plots of the average vibrational energy, the total vibrational energy, the average vibrational amplitude, the total vibrational amplitude, and the radical projection of the vibrational amplitude. In Fig. 3, these five physical quantities of the \(l\)-th atomic shell for the same phonon mode are plotted.
as functions of the shell diameter. These figures are useful to value how important
the corresponding mode is in experiments. It is seen that the first four quantities
all have peaks at the interface of GaAs/AlAs and the peaks decay with oscillatory
manner as the distance from the interface increases. The fifth subfigure show that
for this A₁ microscopic interface modes, the radial projections of the inner shells are
almost equal to 1. In this 44.76Å/48.85ÅSQD, this is true for shells with diameter
less than 30Å. The radial projections of shells close to the interface and surface
are fluctuating, indicating that the vibrational motion of atoms in these shells are
disturbed by the influence of the interface and surface. The average radial projection
of the entire SQD for this A₁ mode, \(< A_L/A >\), is equal to 0.7829.

To distinguish the interface modes from other modes in SQDs, we have introduced
another useful physical quantity: the k-space projection strength of SQDs. Suppose
that the eigen states of a phonon mode in the SQDs can be written as \(\phi_{\alpha,j}\),
where \(\alpha = A_1, A_2, E, T_1, \text{ or } T_2\), is the symmetry index, and \(j\) is the serial number
of this mode in the \(\alpha\) – th representation. On the other hand, the eigen states
of bulk phonon modes can be written as \(\chi_{i,k}\), where \(k\) is the wave vector in k-
space, and \(i = 1 \text{ to } 6\) corresponding to six bulk phonon states (three optical modes
and three acoustic modes). Then, the k-space projection strength is defined as
\(P_{i,k}^{\alpha,j} = |\langle \chi_{i,k}, \phi_{\alpha,j} \rangle|^2 \cdot C_{l,c}^{\alpha,j} \cdot \exp\). In Fig. 4(a), we plot the k-space projection strenght
of the microscopic interface mode with frequency \(\omega^{T_2} = 299.13\ \text{cm}^{-1}\), that is a mode
with T₂ symmetry in a 21.70 Å/26.95 ÅQD. It is seen that the projection strength
of this mode covers a wide range from Γ-X-Γ-L, and it has significant components
for bulk LO, TO₂, and LA modes and a slightly weaker components for bulk TO₁,
TA₁, and TA₂ modes. As a comparison, we have also plotted the k-space projection
strength of an internal mode of the same QD with frequency \(\omega = 286.92\ \text{cm}^{-1}\) that
falls inside the bulk GaAs band. We can see that even for this small SQD, the char-
acteristics of a bulk mode is still shown as a sharp peak in the k-space. In general
our results show that for internal modes of SQDs with larger scale, the k-space pro-
jections strength always show narrow and sharp peak on one or a few bulk modes.
Furthermore, the SQD modes with $A_1$ symmetry usually has dominant projection in bulk longitudinal mode, while the SQD modes with $T_1$ symmetry usually has dominant projection in bulk transverse mode.

In summary, it is pointed out that by employing a microscopic valence force field model, many microscopic interface phonon modes with frequencies in the gap between the bulk AlAs band and the bulk GaAs band can be identified in SQDs with thin shells. These interface modes are unable to be described by means of the continuum dielectric model. The average vibrational amplitude and the average vibrational energy of each atomic shell show peaks at the GaAs/AlAs interface, and the peak value decay in oscillatory manner as the its distance from the interface increases. The k-space projection of the microscopic interface modes shows diverse distributions for all six bulk modes, which are a typical characteristics of an interface mode.

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Figure 1: The density of states of phonon modes of selected ten kinds of SQDs with thin shells

Figure 2: The average vibrational amplitudes as function of the radius of atomic shells for phonon modes of two kinds of SQDs with the frequencies covering the whole range from the upper region of bulk GaAs band to the lower region of bulk AlAs band

Figure 3: The vibrational energy, the total vibrational energy, the average vibrational amplitude, the total vibrational amplitude, and the radial projection of the vibration amplitude as function of the radius of atomic shells for microscopic interface mode with frequency $294.20 \text{ cm}^{-1}$ of $A_1$ symmetry in SQDs with $d_s=44.76 \ \text{Å}$ and $d_L=48.85 \ \text{Å}$

Figure 4: The k-space projection of vibrational amplitudes for modes of $T_2$ symmetry in SQDs with $d_s=21.70 \ \text{Å}$ and $d_L=26.95 \ \text{Å}$. 
FIG. 1

Density of States (arb. units)

Frequency (cm⁻¹)

- $75.54 \, \text{A/79.66 \, \text{A}}$
- $44.76 \, \text{A/48.85 \, \text{A}}$
- $31.34 \, \text{A/34.26 \, \text{A}}$
- $21.70 \, \text{A/26.95 \, \text{A}}$

- $\Delta E$
- $T_2$
- $T_1$
- $E$
- $A_1$
- $A_2$
- $A_1$
- $A_1$
- $A_1$
- $A_1$
GaAs/AlAs

$E_{L}$

$E_{L,T}$

$A_{L}$

$A_{L,T}$

$\frac{A_{L}}{A}$

Diameter (Å)

$NPM = 363$

$\omega = 294.20 \text{ cm}^{-1}$

$A_{1}$

$\langle A_{L}/A \rangle = 0.7829$

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\( \omega = 299.13 \text{ cm}^{-1} \)
NPM = 164
nksp = 1

\( \omega = 286.92 \text{ cm}^{-1} \)
NPM = 163
nksp = 1

Fig. 4