Significant Reduction of Phonon Scattering Potential in 1D Si Quantum Dot Array Interconnected with Thin Oxide Layers

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Abstract

Phononic states and the electron-phonon scattering potential in 1D Si quantum dot array interconnected with thin oxide layers are numerically calculated. Significant reduction of the acoustic phonon scattering potential is demonstrated, indicating the possibility of electron-phonon interaction suppression in this system.

Introduction

Recent reports on suppression of electron energy loss in 1D Si quantum dot array interconnected with thin oxide layers (1DSiQDA), illustrated in Fig. 1 (a), provide a new challenge to develop various novel device applications [1]. This new opportunity, however, is subject to thorough understanding of underlying physics. In this work, we present our recent achievements in theoretical analysis of the phononic states and the electron-phonon interaction in the 1DSiQDA. This is the continuation of the previous study on high-energy electron emission from porous silicon [2].

Calculation of Phonon Waves

We numerically calculated the phonon waves in the 1DSiQDA using 1D atomic linear chain model, depicted in Fig. 1 (b). The standing waves were obtained by solving the classical equations of motion for the atoms. Fig. 2 shows the real part of the acoustic phonon waves calculated for the 1DSiQDA (solid line) and the Si quantum wire (SiQW, broken line) as a function of position. The acoustic phonon wave in the SiQW is a plain wave, and that in the 1DSiQDA is slightly modulated. This modulation is caused by the fact that the atomic mass and spring constant in the oxide layers are different from those in the Si regions.

Reduction of Electron-Phonon Scattering Potential

At room temperature, the dominant mechanism of the inelastic electron scattering in the Si system is the acoustic deformation potential scattering (ADP scattering). The scattering potential of the ADP scattering is written as

\[ H_{el-ph} (x) = D_{aco} \frac{\partial S(x)}{\partial x}, \]  

where \( S(x) \) and \( D_{aco} \) denote acoustic phonon wave function and the coupling constant, respectively. The coupling constant is 9eV for Si [3], and 3.5eV for SiO\(_2\) [4]. Fig. 3 shows the derivative of \( S(x) \) in terms of position, also known as ‘strain’, derived from the results shown in Fig. 2. Fig. 4 (a) shows the absolute values of the strain as a function of position. Note that the oxide layers ‘absorb’ the strain in Si regions. Fig. 4 (b) shows the scattering potential, \( H_{el-ph} \), as a function of position. Note that the scattering potential in the 1DSiQDA is reduced by about 20% over all position. This indicates an interesting characteristic of 1DSiQDA as a ‘phononic crystal’ that the oxide layers with smaller coupling constant absorb the strain from the Si regions with larger coupling constant, reducing the overall scattering potential throughout the structure. Fig. 5 shows the scattering potentials averaged over the position as a function of phonon energy. Note that the reduction ratio of the scattering potential is independent of the phonon energy. We speculate that the ratio drastically changes according to the material constants and structure. In the presentation, we show more detailed analysis of the scattering potential reduction in the 1DSiQDA.

Conclusion

The scattering potential of the ADP scattering, the dominant inelastic scattering process in Si, reduces in the 1DSiQDA, indicating the possibility of significant electron-phonon interaction suppression in this system.

References

**Fig. 1** (a) Schematic illustration of the 1D Si quantum dot array interconnected with thin oxide layers (1DSiQDA). (b) 1D atomic linear chain model and parameters used to calculate the phonon waves in the 1DSiQDA.

**Fig. 2** The real part of the acoustic phonon waves calculated for 1DSiQDA (solid line) and Si quantum wire (SiQW, broken line). The phonon energy is set to be 1meV for both phonon waves. The diagram on top of the figure indicates the position of Si regions and oxide layers.

**Fig. 3** The strain caused by the phonon vibrations, defined as the derivative of the phonon wave in terms of position. The strain is an important quantity in this system, because the electron-phonon scattering potential is proportional to the strain, as expressed in Eq. (1).

**Fig. 4** (a) Absolute value of the strain as a function of position, demonstrating that the oxide layers absorb the strain in the Si regions. (b) Scattering potential calculated from (a), showing significant reduction for 1DSiQDA.

**Fig. 5** The scattering potentials averaged over the position as a function of phonon energy. Little dependence on the phonon energy is noticed.