Residual Stress Modeling In Quantum Dots

B. Vlahovic, K. Wang, V.M. Suslov, S.L. Yakovlev, C. Otieno, A. Soldi, and J. Dutta

Department of Physics, North Carolina Central University
Durham, NC 27707

ABSTRACT

One of the possible applications of the quantum dots is in a new generation of photovoltaic cells. Theory predicts the efficiency of these based solar cells to be up to 63 percent, which is substantially higher than the theoretical limits existing in mono crystal solar cells (34%) or hetero junction (39 % three junctions and 42 % four junctions). The differences in thermoelastic properties between the quantum dots and substrate materials, such as thermal expansion and lattice mismatch, will cause residual stresses. These stresses in turn will affect the electronic and transport properties in the quantum dots. With the available thermoelastic properties and finite element modeling method, the residual stress distribution will be studied. Various factors, such as geometry, thickness and size, will be discussed.

Keywords: Quantum Dots, Lattice Mismatch, Thermal Expansion, Critical Thickness, Residual Stress.

1. INTRODUCTION

Quantum dots considered here are fabricated by growing nanometer-sized metallic materials on various semiconductor substrates. They have broad area of applications as for instance theoretically they are the most promising in photovoltaic cells with a potential of 63% efficiency [1,2]. Due to the differences in materials properties used in their creation, residual strain and stresses are usually generated at the interfaces and inside the quantum dots. These stresses consequently modify the electronic and transport properties in quantum dots. There are two main sources that contribute to the residual stresses, one is the lattice mismatch between substrate and a quantum dot, the other is the difference of the coefficient of thermal expansion between quantum dots and substrate materials. Here, we will discuss the effects of these two major factors on the distribution of residual stresses in quantum dots. The effects of size, geometry, and deposition temperature will also be discussed.

2. LATTICE MISMATCH

For quantum dots with lattice parameter a_q grown on a substrate with lattice parameter a_S, the in-plane strain at the interface is [3]

$$\varepsilon_{\parallel} = \frac{a_S - a_q}{a_S} \qquad (1)$$

If the thickness is less than the critical thickness, the quantum dots remain pseudomorphic. If the thickness is larger than the critical thickness, misfit dislocations are generated in the interface to relax the misfit strain [3]. For isotropic materials, distribution of residual stresses/strains sometimes can be found in closed form for high symmetric geometries [4]. In most cases, in materials with anisotropic thermoelastic properties and irregular shapes, distribution of residual stresses can not be found in closed form. Numerical methods, such as finite element or finite difference method, have to be employed to solve the problem. Bimberg et al. [4] have provided a comprehensive review on the modeling work published in literature prior to 1998. Here, an estimate of the maximum residual stress caused by the lattice mismatch in a gold dot grown on silicon substrate with cylindrical geometry will be provided.

3. THERMAL RESIDUAL STRESSES

For quantum dots fabricated at high temperatures, after the sample is cooled down to the room temperature, the differences in the coefficient of thermal expansion between the dots and the substrate materials will introduce residual stresses within the sample. The strain tensor can be described by [5]

$$\varepsilon_{ij} = s^{T}_{ijkl}\sigma_{kl} + \alpha_{ij}\Delta T \qquad (2)$$

Where $\varepsilon_{,ij}$ is the strain tensor, σ_{kj} is the stress tensor, α_{ij} is the thermal expansion tensor, s^{T}_{ijkl} are the compliance of the crystal, and ΔT is the temperature drop in the system. The equilibrium equations of the system are

$$\frac{\partial \sigma_{ij}}{\partial x_j} + f_i = 0 \qquad (3)$$

where f_i are the body forces per unit volume acting on the system. In equations (2) and (3), the indices i, j, k, l have values 1, 2, and 3. The thermal residual stresses for arbitrary shape with isotropic or anisotropic material properties can be calculated by numerical modeling approaches, such as finite element method or finite difference approximation.

Here, a finite element code PDE2, developed and distributed by Macsyma, is utilized to model the thermal residual stress distribution. The effects of fabrication temperature, the size of the quantum dot have also been investigated.

4. CONCLUSIONS AND DISCUSSION

In this paper, the residual stresses existed in quantum dots have been studied. The two major sources of residual stresses in quantum dots were separately examined. The effects of these two sources will be compared and the dominant factors will be identified. The distribution of residual stresses within the quantum dot has also been calculated by a finite element method. This provides a base for further work on the calculation of electronic and transport properties within the quantum dots. In order to accomplish this, the potential field induced by the residual strain can be calculated from the distribution of residual strain. This extra potential caused by the residual strain and the original potential field of the valance band both can then be included in the time-independent Schrödinger equation to calculate the energies and wave functions of the valance band. Johnson et al. [6] have applied finite element method to calculate both the residual stress and the electronic and transport properties in Si_xGe_{1-x} quantum wires and quantum dots. Their calculations were consistent with experimental results [7,8]. They also demonstrated that the densities of state for electrons in Si_xGe_{1-x} quantum wires and quantum dots indeed change with the residual stresses [6]. In our next step, the residual stress distribution for a gold quantum dot grown on silicon substrate calculated by the finite element method will be incorporated in our newly developed approach for solving a time-independent Schrödinger equation. The energies and wave functions of the valance band can then be calculated. Our final goal is to understand the effects of size, strain, composition and other parameters on the electronic and transport properties in order to improve the quality of the devices.

ACKNOWLEDGMENT

This work is supported by the DoD through Grant contract No DAAD19-01-1-0795

REFERENCES

[1] A. Luque and A. Mart í, Phys. Rev. Lett. **78**(26), 5014(1997).

[2] A. Mart í and A. Luque, IEEE Trans. Electron Devices **48**(10), 2394(2001).

[3] S. Jain, M. Willander and R. Van Overstraeten, "Compound Semiconductors Strained Layers and Devices", Kluwer Academic Publishers, 2000.

[4] D. Bimberg, M. Grundmann and N. N. Ledentsov, "Quantum Dot Heterostructures", John Wiley & Sons, 1999.

[5] J. F. Nye, "Physical Properties of Crystals", Oxford University Press, 1985.

[6] H. J. Johnson, L.B. Freund, C. D. Akyuz, and A. Zaslavsky, *J. Appl. Phys.*, **84**(7), 3714(1998).

[7] M. –E. Pistol, N. Carlsson, C. Persson, W. Seifert, and L. Samuelson, *Appl. Phys. Lett*. **67**(10), 1438(1995).

[8] C. D. Akyuz, A. Zaslavsky, L. B. Freund, D. A. Syphers, and T. O. Sedgwick, *Appl. Phys. Lett*. **72**(14), 1739-1741, 1998.