Strain Effects and Temperature-Dependent Phase Stability of II-VI Semiconductor Nanostructures

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Abstract. We report strain and strain-induced piezoelectric effects in arbitrary shaped CdTe/ZnTe quantum wire (QWR) and temperature-dependent phase stability of CdS nanostructures. Strain field distributions are obtained by using analytical expressions derived from inclusion theory, whereas strain-induced piezoelectric fields are obtained for rectangular box shaped CdTe/Znte QWR with a continuum model based on coupled electric and mechanical balance equations. CdTe/ZnTe QWRs are observed to be greatly relaxed despite of higher lattice mismatch. Strain-induced piezoelectric effect is relatively small. First principle molecular dynamic simulations are performed to determine the relative stability of wurtzite, graphitic and rocksalt phases of the CdS nanostructure at various temperatures. In the temperature range from 300 K to 450 K, the phase stability sequence for the CdS nanostructure is observed to be rocksalt, wurtzite and graphitic phase.

Keywords: Nanostructures, Strain, Molecular Dynamics, Phase stability
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INTRODUCTION

III-V GaN-based materials are the leading materials for fabrication of blue-green light-emitting devices. However, large internal piezoelectric field and spontaneous polarization leads to higher carrier densities to generate optical gain [1]. Group II-VI semiconductors, such as CdTe and CdS based nanostructures may serve as alternative materials to resolve this problem. Among these, CdTe/ZnTe nanostructures are particularly important for light emitting devices in green region of spectrum. On the other hand, CdS is important material in optoelectronic and biorelated applications, where it may be operated at high temperature conditions [3]. Relatively less work has been done on these potentially applicable materials.

In this contribution we report, strain effects in different shapes of highly strained CdTe/ZnTe QWR (lattice mismatch -5.89%) by using analytical solution of Eshelby cylindrical inclusion problem and the strain-induced piezoelectric effects with full 3D coupled electromechanical continuum model. Also we study temperature-dependent phase stability of CdS nanostructures with first principle MD simulations for wrutzite, rocksalt and graphitic phases.

DESCRIPTION

Strain field distributions are obtained for triangular, crescent and half-ellipsoidal shaped CdTe/ZnTe QWRs by using inclusion theory [4]. We use a full 3D coupled electromechanical model based on balance equations of elasticity and electrostatics with which strain induced piezoelectric fields are obtained for rectangular box shaped CdTe/Znte QWR with dimensions of $10 \times 10 \times 70$ nm.

In MD simulations, CPMD package is used to calculate the total energy of CdS nanostructures under temperature range from 300 K to 450 K. Interactions between the valence electrons and the ion cores are modeled by the HSC norm-conserving methodology and by the SGS norm- conserving pseudopotentials for Cd and S elements, respectively. The CPMD calculations are performed in a cubic box with 20 Å side with periodic boundary conditions. Maximum dimension of CdS nanostructure is about 13 Å and the vacuum region between each nanostructure is about 7 Å are taken as the test calculations indicated that the interaction between nanostructures is negligible when the vacuum region is larger than 6 Å. The kinetic energy cutoff of the plane wave basis was set to 20 Ry. The time step for Born-Oppenheimer molecular dynamics is 0.12 fs in the NTP ensemble, and the simulation time is 12 ps.

RESULTS

Values of the strain tensor components at the center of the triangular, crescent and half-ellipsoidal shaped CdTe/ZnTe QWR are tabulated in Table 1. The individual strain tensor component's magnitudes are higher in all geometries. The hydrostatic strain component is relatively small $\sim$3.65% (in un-relaxed case, $3\varepsilon_0 = \sim$17.67%) signifying great amount of relaxation and is independent of geometry and dimensions [4]. The geometry independence of hydrostatic strain components is due to the assumption of homogeneity of

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TABLE 1. Values of strain tensor components at the center of the QWR: Inclusion theory

	Triangular*	Crescent†	Half-ellipsoidal**
$\varepsilon_{xx}(\%)$	-1.5	-2.0	-3.25
$\varepsilon_{yy}(\%)$	3.5	4.0	5.25

* Base = 20 nm and height = 7 nm
† Maximum thickness is 10 nm and two ends are separated by 40 nm
** Diameter = 55 nm and height = 7.5 nm

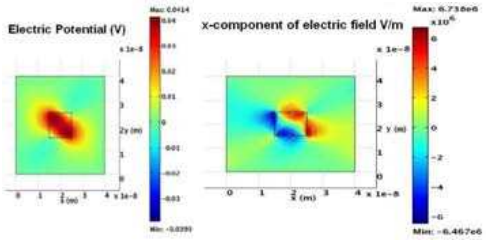

FIGURE 1. Electric potential and z-component of Electric field

the QWR system for determination of strain fields. The significant modification in the band states is expected because of relatively higher magnitudes of individual strain components.

Figure 1 shows the results obtained from 3D simulations of CdTe/ZnTe QWR. The strain fields are similar to those obtained from inclusion theory. The potential difference across the QWR ends is 0.08 V and the magnitude of the electric field is fractions of MV/m inside the QWR. The potential difference and electric fields are smaller by orders of magnitude than those of typical GaN based nanostructures (V = 2 V, E_z=600 MV/m)[1].

Figure 2 shows snapshots for various phase structures of nanosized $Cd_{48}S_{48}$ after relaxation at different temperatures. With an increase in temperature, the number of broken bonds increases. Rocksalt CdS nanostructure is stable in the temperature range of 300-450 K and also it is more stable at higher temperatures. The phase stability sequence for the CdS nanostructure at higher temperature is rocksalt, wurtzite, and graphitic phase, which coincides with the stability sequence for bulk CdS crystals under high pressure [3]. At 300 K, only the rocksalt phase of CdS nanostructure could maintain its initial input structure compared to wurtzite and graphitic phases as it has less numbers of broken bonds. However, it begins slowly to be corrupted as temperature goes beyond 450 K.

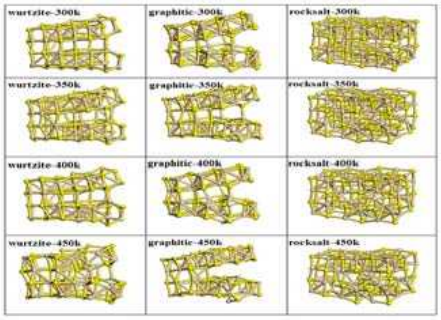

FIGURE 2. Snapshots of CdS nanostructure at different temperature conditions

CONCLUSIONS

The strain distributions for triangular, Crescent and half-ellipsoidal shaped CdTe/ZnTe QWRs are analyzed. CdTe/ZnTe QWRs are greatly relaxed despite of higher initial misfit. As a consequences higher value of hydrostatic strain and that of individual strain components, the and edge shift is large and the significant modification in valence band states, respectively, is expected. Strain-induced piezoelectric fields are analyzed with full 3D coupled electromechanical model. CdTe/ZnTe materials can serve as an alternative material to GaN with advantage of order of magnitude smaller magnitudes of electric quantities, in respective applications. First principles MD simulations were carried out for wurtzite, graphitic, and rocksalt phases of the CdS nanostructure in the temperature range of 300-450 K. The phase stability sequence for the CdS nanostructure is rocksalt, wurtzite, and graphitic phases.

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