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Pressure Effect on Si Quantum-Dot Potential

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Abstract. Application study of the quantum dot potential as a function of hydrostatic pressure for Si has been presented. This study has been calculated by means of our recent model using empirical pseudopotential method. The effect of pressure on the quantum dot potential is noticed. The results are investigated to be used in advanced technologies.

Keywords: Quantum-Dot; Elemental Semiconductor; Pressure Effect
PACS: 73.21.La, 71.20.Mq, 74.62.Fj

INTRODUCTION

Semiconductor quantum dots (QD’s) present considerable advantages over bulk single-crystal semiconductors [1]. They have gained increasing attention of scientists and engineers of various disciplines in the past decade due to their flexible processibility and unique properties [2–4]. For a number of optoelectronic applications, e.g., light-emitting diodes (LED) [5,6], strongly luminescent semiconductor nanocrystals are highly desirable. However, due to the large surface-to-volume ratio of nanoparticles, the most common reason for poor luminescence efficiency is non-radiative recombination of light-generated charge carriers at surface-traps [7]. Elimination of these traps can be achieved either by proper chemical modification of the particle surface [8,9] or by growing hetero-epitaxially an inorganic passivation shell around the semiconductor cores [10,11].

So band gaps, pressure dependence of electronic structure, optical constants, photoemission spectra, dielectric functions depending on frequency and wavevector, alloy properties, bonding and chemical properties, etc. can in principle be and have been evaluated for many materials using the pseudopotential approach.

The most remarkable aspect of tetrahedral coordinated structures is their low density. Therefore, under pressure a tetrahedral coordinated semiconductor can be transformed to a structure with high density. The zinc-blende structure (ZB) has the lowest minimum total energy. It is the most stable phase of these compounds at ambient pressure. If pressure is applied, the volume decreases and a transition to the β-Sn (or NaCl) phase occurs at relatively low pressure.

Udipi et al. [12] presented semiclassical simulation results for the potential energy profile and electron density distribution in a 200 nm silicon quantum dot. For the solution of the continuity equation, the efficient difference approximations, proposed by Scharfetter and Gummel [13] extended to three dimensions. In essence, they followed the two-dimensional approach due to Selberherr et al. [14] to extend two to three dimensions.

The investigation of chemical trends in solid state properties appears thus as an extremely useful part of new materials research. This is interesting when one tries to...
gain some information about the many properties of the group of binary compounds under pressure. It seems more fundamental to relate the high pressure behavior of the compounds to the type of bonds between nearest atoms. By controlling the evolution with pressure of the bond character in terms of the band structure, we can attempt to link the effect of high pressure to the quantum dot potential. In this context, we have used this procedure for testing the validity of our model [15] of QD's potential. The aim of this paper is to extend this method for calculating the high pressure effect on QD's potential.

Calculations and Results

The band gaps between the top valence energy level at Γ and lower conduction energy level at X are computed on the basis of the empirical pseudopotential method (EPM). The pseudopotential form factors are found by using a non-linear least-square method [16–18], in which all the parameters are simultaneously optimized under a definite criterion of minimizing the root-mean-square deviation. Optical, ultraviolet photoemission spectroscopy (UPS), and X-ray photoemission spectroscopy (XPS) data are used. Table 1 gives the adjusted pseudopotential form factors for both ambient and transition pressure. We have evaluated the quantum dot potential by means of our recent model [15], according to the formula

$$P_{\text{QD}} = \frac{b}{a} \cdot E_{\text{grx}} \cdot 10^{-3} \cdot \lambda$$

where $\frac{b}{a}$ is constant (in eV$^{-1}$) [see table 4 in Ref. 15] and $\lambda$ is a parameter appropriate for group-IV ($\lambda = 6$), III-V ($\lambda = 4$) and II-VI ($\lambda = 2$) semiconductors (in V).

<table>
<thead>
<tr>
<th>Pressure</th>
<th>$a_0$</th>
<th>$V_s(3)$</th>
<th>$V_s(8)$</th>
<th>$V_s(11)$</th>
<th>$V_a(3)$</th>
<th>$V_a(4)$</th>
<th>$V_a(11)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>10.2646</td>
<td>-0.21</td>
<td>0.04</td>
<td>0.08</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$p_t$</td>
<td>8.9997</td>
<td>-0.351030</td>
<td>0.119031</td>
<td>0.027508</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

At normal pressure, the covalent semiconductors are four-fold coordinated. The reason that the density is so low is that nearest neighbors are bound by overlapping hybridized orbitals, which are the well-known sp$^3$ hybrids with tetrahedral direction. Therefore, these covalent compounds can be transformed either through chemical shifts or under pressure into a denser structure, which may be ionic or metallic. The transformation can be reached by decreasing the lattice volume of these compounds.

By analyzing the variation of the band structure with pressure on the basis of the bonding properties, one can establish at least the first order phase transformations as a result of the change of the nature of the binding and the type of structures. We present in Fig. 1 the results of our calculations of band structure of the material, Si, used in QD's at ambient pressure and the transition one. The transition occurs when the Ewald contribution dominates over the covalent electronic contribution.
FIGURE 1 Calculated band structure of Si at $p = 0$ kbar (a) and at $p = p_t$ (b).

If pressure is applied, the volume decreases and the strong $sp^3$ covalent bonding, which characterizes the covalent structure at normal pressure, is destroyed, resulting in a new structure. From our point of view, this discrepancy at very high pressure is an immediate consequence of the difference in the corresponding quantum dot potential. The effect of hydrostatic pressure is to transform the compounds from a four-fold coordinated structure to a denser structure. In table 2, we compare the calculated transition pressure with experimental and other theoretical values.

The critical transition pressure is the pressure value which separates the decrease and the increase of the QD's potential. The transition pressure $P_t$ is important to be computed from difference in molar free energies of compounds. The Gibbs free-energy difference $\Delta G_t$ between a compound which has the tetrahedral coordination at $p=0$ and at high pressures is nearly given by $P_t \Delta V/V_t$ (in kJ/mol). This is because the
compressibility is nearly equal in the two structures. All energies are larger for smaller bond lengths. The stable phase at a given pressure is the one with lowest Gibbs free energy. The increase of the QD's potential under pressure is confirmed by the change of the positions of the last valence and first conduction bands at points Γ and X, respectively as shown in table 3.

**Table 2** The calculated quantum dot potential for Si (in mV) at 0 and at the critical transition pressure (pt in kbar). The latter are compared to the other theoretical and experimental values. *: The used data. a: Ref. [19].

<table>
<thead>
<tr>
<th>P_{QD} at p=0</th>
<th>P_{QD} [12]</th>
<th>P_{QD} at p=pt</th>
<th>pt</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.65</td>
<td>≤ 1</td>
<td>0.79</td>
<td>100*, 119.5(^a), 125(^a)</td>
</tr>
</tbody>
</table>

**Table 3** The calculated energy level along Γ \(\rightarrow\) X at 0 and the critical transition pressure (pt in kbar) for Si.

<table>
<thead>
<tr>
<th>Pressure</th>
<th>E_{\text{eF}}</th>
<th>E_{\text{gX}}</th>
<th>E_{\text{gF}}</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>10.57671</td>
<td>11.47451</td>
<td>0.9</td>
</tr>
<tr>
<td>pt</td>
<td>13.39944</td>
<td>14.49925</td>
<td>1.09</td>
</tr>
</tbody>
</table>

The QD's potential increases as pressure increases until a critical value is reached, characterized by random behavior (Table 2). A new atomic arrangement is then more appropriate than the ZB structure. As a consequence, fluctuations of the QD's potential appear. Our critical values of pressure are of the same order as the experimental ones. Therefore, we may reach to the fact that the sudden variation of the QD's potential is an indication of the structural phase transition and a more control of tunneling electron across the quantum dot. In conclusion, the simple method provides an easy way to calculate the structural phase transition and confirms its validity for IV compounds, expecting new phase transformations for other compounds and new realization for quantum dot techniques.

**ACKNOWLEDGMENT**

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**REFERENCES**

15. Y. Al-Douri, Quantum dot modeling of semiconductors, in: Ali H. Reshak (Editor), Advances in Condensed Matter Physics, Research Signpost, Kerala, India (2009)