Effect of Anharmonicity of Interatomic Potential on Strain Distribution in Semiconductor Nanostructures

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Large lattice mismatch in semiconductor nanostructures

Large built-in strain affects most of the QD properties

Parameters of the simulated InAs/GaAs QD structure:
- Dimer size: 2 nm, height 3.5 nm
- Width of the wetting layer 1 nm
- Periodicity: lateral 17 nm, along growth direction 8.5 nm

Electronic structure

Equilibrium atomic positions

Usually used – Keating’s Valence Force Field Model (VFFM)

\begin{equation}
E = \frac{3}{8} \sum_{\text{neighbors}} \frac{a_{\text{nn}}}{d_{\text{nn}}^6} (r_{\text{nn}} \cdot r_{\text{nn}} - d_{\text{nn}} \cdot d_{\text{nn}}) + \sum_{\text{couplets}} \frac{\beta_{\text{mm}} \beta_{\text{nn}}}{d_{\text{mm}} d_{\text{nn}}} (r_{\text{mm}} \cdot r_{\text{nn}} - d_{\text{mm}} d_{\text{nn}})
\end{equation}

Notations:
- \(d_{\text{nn}}\) – unstrained bond
- \(r_{\text{mm}}\) – strained bond
- \(\beta\) – unstrained inter-bond angle
- \(\theta\) – inter-bond angle

Anharmonicity corrections to VFF parameters:

\begin{align}
\alpha &= \alpha_0 \left[ 1 - A \frac{d_{\text{nn}}^2}{d_{\text{nn}}^2} \right] \\
\beta &= \beta_0 \left[ 1 - C \frac{d_{\text{nn}}^2}{d_{\text{nn}}^2} \right] \left[ 1 - B \cos\theta - \cos\theta \right]
\end{align}

\(A, B,\) and \(C\) were obtained by fitting the experimental phonon spectra of strained materials

\begin{tabular}{|c|c|c|c|c|c|}
\hline
Material & \(\alpha_0\) (N/m) & \(\beta_0\) (N/m) & \(A\) & \(B\) & \(C\) \\
\hline
Si & 48.5 & 13.8 & 7.67 & 4.67 & 4.53 \\
Ge & 38.0 & 12.0 & 8.33 & 4.80 & 5.08 \\
GaAs & 41.49 & 8.94 & 7.20 & 7.62 & 6.40 \\
InAs & 35.18 & 5.49 & 7.61 & 4.78 & 6.45 \\
GaSb & 33.16 & 7.22 & 7.96 & 6.54 & 6.07 \\
InSb & 29.61 & 4.77 & 7.53 & 9.62 & 6.46 \\
AlSb & 35.35 & 6.77 & 8.28 & 7.58 & 7.17 \\
\hline
\end{tabular}

Conclusions

- Built-in strain strongly affects the electronic structure of nanostructures
- Anharmonicity in valence-force-field results in a strain distribution leading to a 100 meV improvement of computed (within tight binding sp\textsuperscript{3}d\textsuperscript{5}s\textsuperscript{3}d\textsuperscript{10} band offsets compared to experiment

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