Large scale computer simulations of strain distribution and electron effective masses in silicon $〈100〉$ nanowires

Christian Tuma and Alessandro Curioni

IBM Research – Zurich, Säumerstr. 4, 8803 Rüschlikon, Switzerland

1 Computational details of DFT calculations

Relaxed atom positions and electronic band structures are obtained from plane wave basis set density functional theory (DFT) calculations using the exchange–correlation functional proposed by Perdew, Burke, and Ernzerhof (PBE) in combination with norm conserving atomic pseudopotentials. In the case of bulk silicon the basis set kinetic energy cut-off is set to 35 Rydberg, and the first Brillouin zone is sampled using a 4×4×4 $k$-point scheme. For hydrogen passivated periodic silicon nanowire (SiNW) models the kinetic energy cut-off is increased to 60 Rydberg. Convergence is achieved in structure relaxations when all Cartesian force components are smaller than $2.0 \times 10^{-5}$ atomic units. Unless otherwise noted the SiNW lattice constant $a_0^{\text{DFT}}$ is kept at the bulk silicon DFT (PBE) equilibrium value of 5.472 Å. Periodic images of the nanowires are separated by at least 10 Å. Four $k$-points along the wire axis and one point in perpendicular directions are used for Brillouin zone sampling. All DFT calculations in this work are performed using the CPMD code.

2 DFT electron effective masses of strained bulk silicon

Upon strain along $〈100〉$ the six degenerate $\Delta$-points representing the conduction band minima get energetically separated into a group of two degenerate minima along the direction of strain ($\Delta_2$) and another group of four degenerate minima along the transversal directions ($\Delta_4$), see Fig. 1a. Within the strain interval studied in this work, longitudinal and transversal electron effective masses at the $\Delta_2$ and $\Delta_4$ minima, respectively, $m^*_{\text{l}}(\Delta_2)$ and $m^*_{\text{t}}(\Delta_4)$, show a rather weak and almost linear dependance on strain, see Fig. 1b. To calculate $m^*_{\text{r}}$ we take the reciprocal sum of the six $\Delta$-point electron effective masses in strain direction using weight factors $p_j$ obtained from Boltzmann statistics ($T = 300$ K; $p_1 + ... + p_6 = 1$). The latter serve as a relative measure for corresponding charge carrier densities depending on the valley splitting $\Delta_4 - \Delta_2$. We use the analytic expression shown in Eq. 1 and fit its parameters ($m_i, n_i$) to reproduce $m^*_{\text{r}}$ as a function of strain, see Tab. 1.

\[
y(x) = \frac{a_1 x^2 + b_1 x + c_1}{1 + \exp(m_1 x + n_1)} + \frac{a_2 x^2 + b_2 x + c_2}{1 + \exp(m_2 x + n_2)}
\]

Note, that the numerators in Eq. 1 represent polynomials of second degree which were fitted individually beforehand ($a_i, b_i, c_i$) to reproduce $m^*_{\text{l}}(\Delta_2)$ and $m^*_{\text{t}}(\Delta_4)$ as a function of strain.
Figure 1: Bulk silicon strained along ⟨100⟩. (a) Energetic splitting of the conduction band minima. (b) DFT (PBE) electron effective masses in strain direction.

<table>
<thead>
<tr>
<th>TABLE I: Parameters of Eq. 1 fitted to obtain $m^*_i$ ($m_e$ being the electron rest mass) as a function of strain (in %).</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_i (m_e)$</td>
</tr>
<tr>
<td>$b_i (m_e)$</td>
</tr>
<tr>
<td>$c_i (m_e)$</td>
</tr>
<tr>
<td>$m_i$</td>
</tr>
<tr>
<td>$n_i$</td>
</tr>
<tr>
<td>$m^*_i$</td>
</tr>
</tbody>
</table>

3 Tersoff type interatomic potential calculations

In the present work we determine the structure of strained pristine ⟨100⟩ silicon nanowires of quadratic cross sectional shape employing our recent \textit{ab initio} derived augmented Tersoff type interatomic potential.\textsuperscript{8} Cartesian force components smaller than 2.0×10\textsuperscript{-5} atomic units on atoms allowed to change their position serve as the convergence criterion in all structure optimizations. By construction the surface of our SiNW models corresponds to ideal silicon {100} layers. After geometry optimization this type of surface structure is preserved. We decided to choose this surface type in our calculations instead of, e. g., surface atom dimers because it is more representative of the many configurations the silicon {100} surface can adopt after passivation.

In our original work introducing the \textit{ab initio} derived augmented Tersoff type interatomic potential we have already included examples for the good agreement of experimental or \textit{ab initio} data to results obtained with that potential.\textsuperscript{8} Studies on, e. g., the structure of the Si/SiO\textsubscript{2} interface\textsuperscript{9} or self-diffusion processes in amorphous silica\textsuperscript{10} are further examples where experimental data are reproduced using our Tersoff scheme.
References