Electronic Band Structure Modeling in Strained Si-Nanowires: Two Band $\mathbf{k} \cdot \mathbf{p}$ Versus Tight Binding

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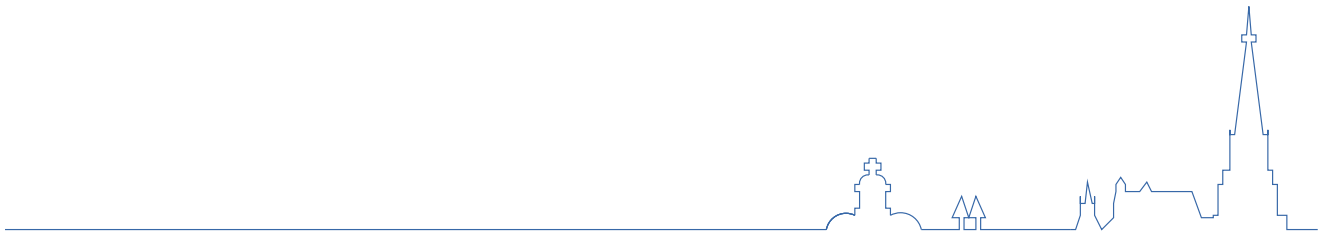


October 27, 2010



Outline

1. Introduction/Motivation
2. The model
3. Results
4. Conclusions



Introduction

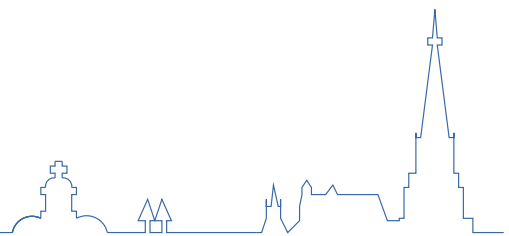
- Subband structures of nanowires are expected to display interesting effects for nanowire diameters below 10 nm:
  - Nonparabolicity
  - Warping
  - Change of effective mass
  - Subband splitting
- These effects have already been investigated using semiempirical tight binding, [1] [2] first principles calculations, [3] and effective mass models with nonparabolicity corrections. [4]
- Tight binding is a well-established method for the analysis of nanowire subband structures.

[1] Neophytou et.al. *IEEE Transactions on Electron Devices*, **55** (2008), 6; 1286–1297

[2] Wang et.al *IEEE Transactions on Electron Devices*, **52** (2005), 7; 1589–1595

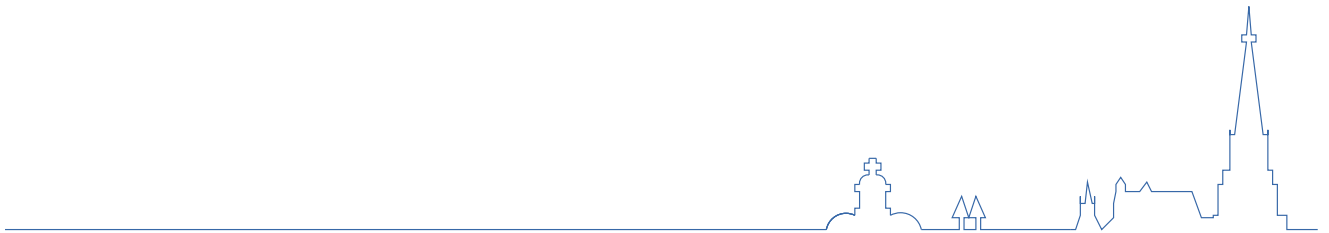
[3] Tsuchiya et.al. *IEEE Transactions on Electron Devices*, **57** (2010), 2; 406–414

[4] Jin et.al. *IEEE Transactions on Electron Devices*, **55** (2008), 11; 2886–2897



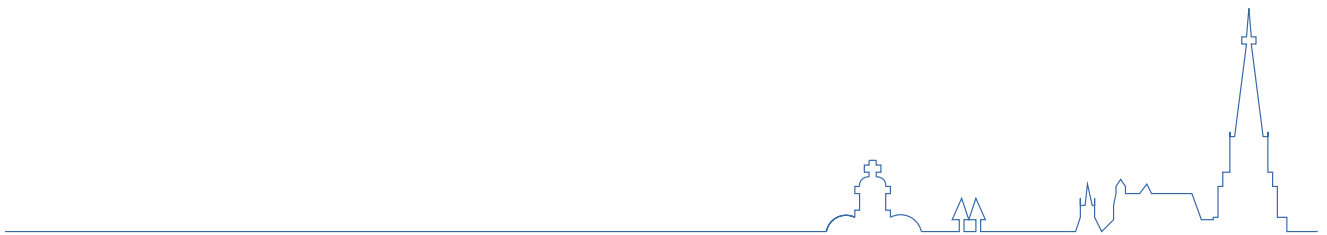
Motivation

- Is there a need for *yet another subband structure tool?*



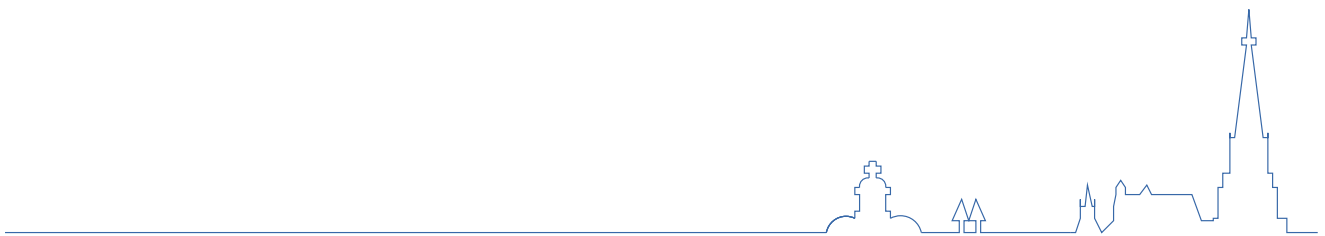
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- The two band $\mathbf{k} \cdot \mathbf{p}$ approach has several benefits...



Motivation

- Is there a need for *yet another subband structure tool?*
- The two band $\mathbf{k} \cdot \mathbf{p}$ approach has several benefits...
- Efficiency
  - Hamiltonian consists only of two bands in contrast to the ten orbitals needed for $sp^3d^5s^*$.
    $\longrightarrow$ smaller system matrix
  - Number of points is independent of crystal orientation.
    $\longrightarrow$ smaller system matrix
  - Continuum model: Number of points is a user choice.
    $\longrightarrow$ tradeoff between speed and accuracy

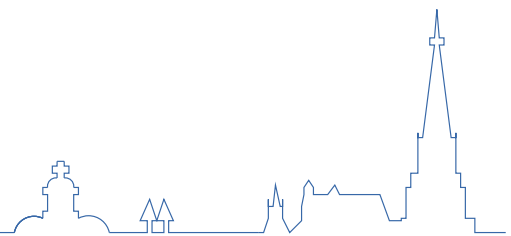


Motivation (cont'd)

- Simplicity and Accuracy
  - We include only one additional parameter with respect to the effective mass model.
  - The parameter describes the coupling between the two bands.
  - Its value has been derived theoretically and confirmed by EPM.
  - Even for ultra-thin films the value has been found to match LCBB calculations. [5]
  - The $\mathbf{k} \cdot \mathbf{p}$ subbands are accurate up to 0.5 eV from the conduction band edge. [6]

[5] Sverdlov et.al. *Solid-State Electronics*, **52** (2008), 10; pp. 1563–1568

[6] Sverdlov et.al. *Journal of Integrated Circuits and Systems*, **4** (2009), 2; 55–60

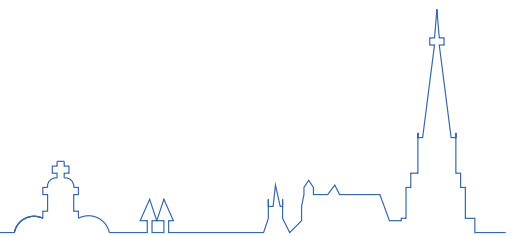


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- Ability to include strain in subband structure calculations

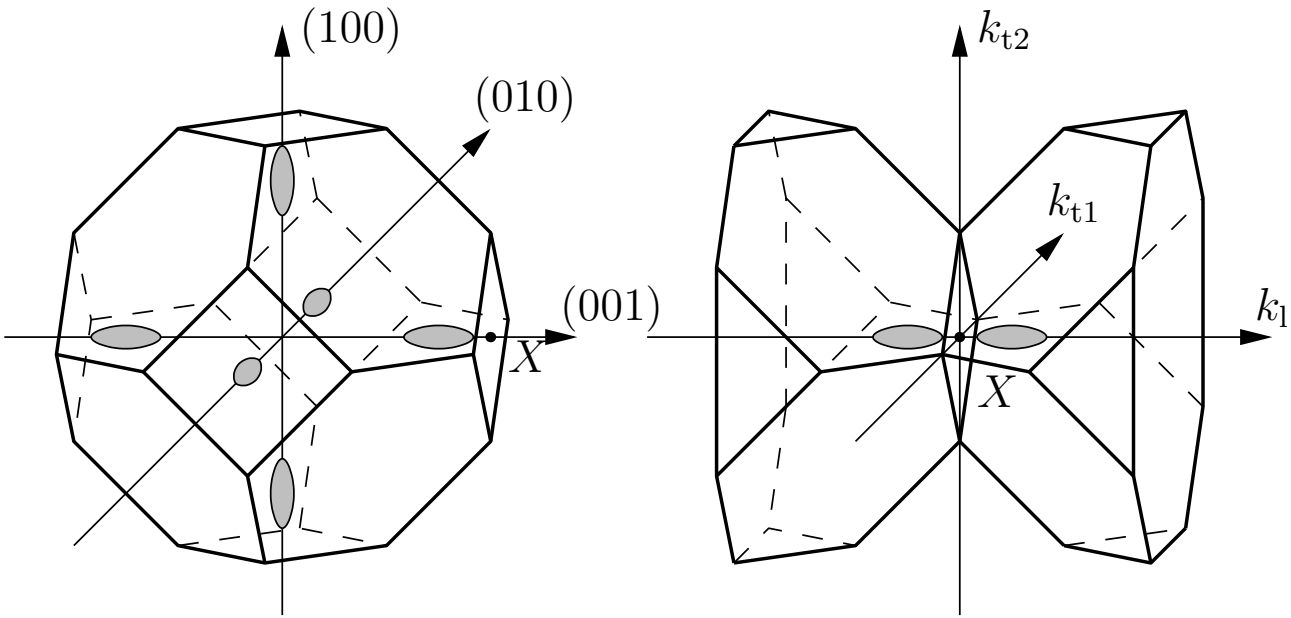
[5] Sverdlov et.al. *Solid-State Electronics*, **52** (2008), 10; pp. 1563–1568

[6] Sverdlov et.al. *Journal of Integrated Circuits and Systems*, **4** (2009), 2; 55–60



Bulk band model

- Description of the conduction band using a two-band, first order $\mathbf{k} \cdot \mathbf{p}$ expansion around the X point
- The two opposing conduction band valleys interact
- The remaining bands are treated as a perturbation



The Hamiltonian

- The resulting Hamiltonian for one valley-pair reads: [7]

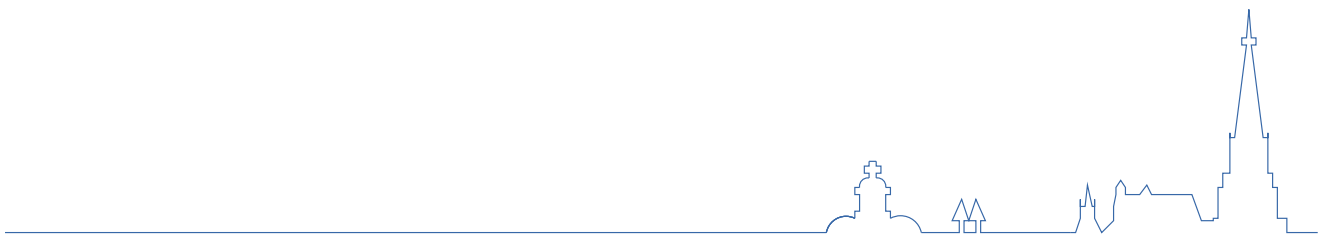
$$\begin{bmatrix} \frac{\hbar^2(k_{\mathrm{t}1}^2+k_{\mathrm{t}2}^2)}{2m_{\mathrm{t}}} + \frac{\hbar^2 k_{\mathrm{l}}^2}{2m_{\mathrm{l}}} - \frac{\hbar^2 k_0 k_{\mathrm{l}}}{m_{\mathrm{l}}} + V + \Xi_u \varepsilon_{\text{l-l}} & -\frac{\hbar^2 k_{\mathrm{t}1} k_{\mathrm{t}2}}{M} + 2\Xi_{u'} \varepsilon_{\text{t1-t2}} \\ -\frac{\hbar^2 k_{\mathrm{t}1} k_{\mathrm{t}2}}{M} + 2\Xi_{u'} \varepsilon_{\text{t1-t2}} & \frac{\hbar^2(k_{\mathrm{t}1}^2+k_{\mathrm{t}2}^2)}{2m_{\mathrm{t}}} + \frac{\hbar^2 k_{\mathrm{l}}^2}{2m_{\mathrm{l}}} + \frac{\hbar^2 k_0 k_{\mathrm{l}}}{m_{\mathrm{l}}} + V + \Xi_u \varepsilon_{\text{l-l}} \end{bmatrix}$$

m_{l}, m_{t}	effective masses in Si	$\Xi_u, \Xi_{u'}$	deformation potentials
$\frac{1}{M} \approx \frac{1}{m_{\mathrm{t}}} - \frac{1}{m_0}$	band coupling parameter	$\varepsilon_{\text{l-l}}$	longitudinal uniaxial strain
$k_0 = 0.15\frac{2\pi}{a_0}$	distance of Δ valley to X	$\varepsilon_{\text{t1-t2}}$	transversal shear strain

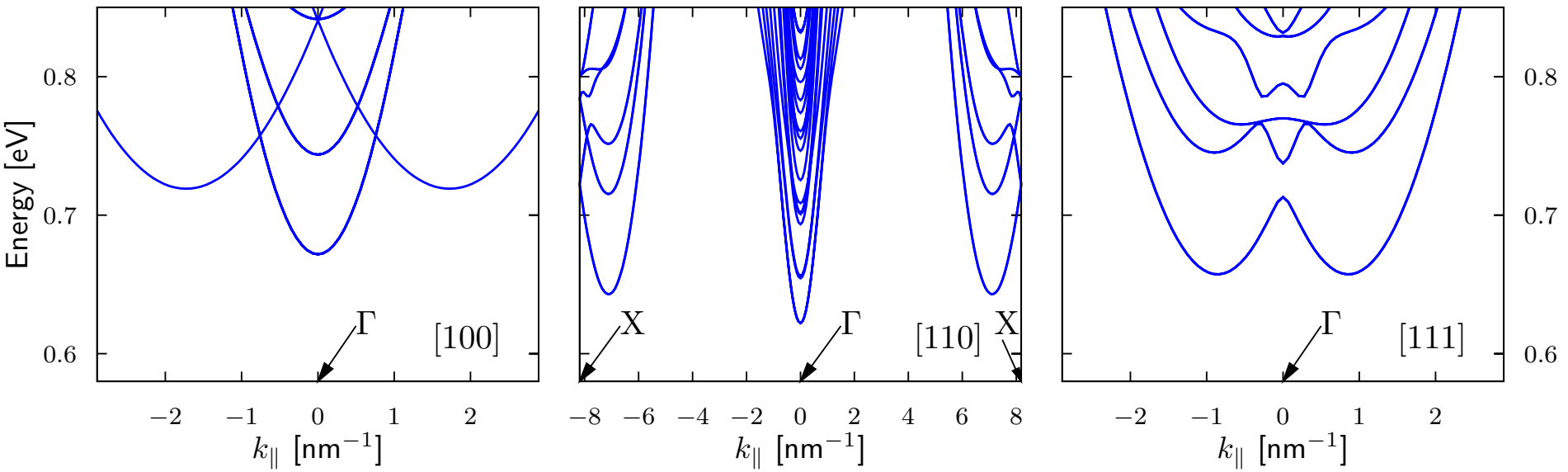
[7] Hensel et.al. *Phys. Rev.*, **138** (1965), 1A; A225–A238

The Hamiltonian (cont'd)

- The Hamlitonian is rotated from the crystal/expansion coordinate system $(\mathrm{l}, \mathrm{t1}, \mathrm{t2})$ to the device coordinate system (x, y, z).
- The wavevector $\mathbf{k}$ expressed in device basis vectors is substituted with $[-i\partial_x \ -i\partial_y \quad k_{\|}]^{\mathrm{T}}$.
- Due to rotation, all kinds of first and (mixed) second order derivaties can be found in the Hamiltonian.
- The eigenvalues of the resulting differential equation are determined numerically using closed boundary conditions.
- The stress tensor given in device coordinates is transformed $(\mathrm{l}, \mathrm{t1}, \mathrm{t2})$ coordinates. Strain is then obtained by applying the mechanical compliance tensor.

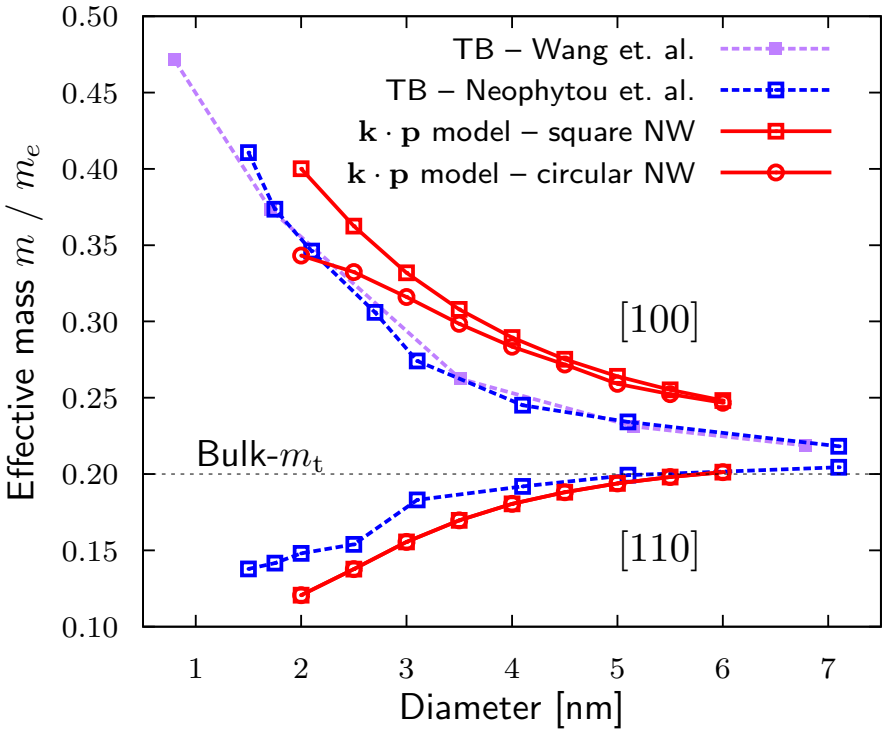


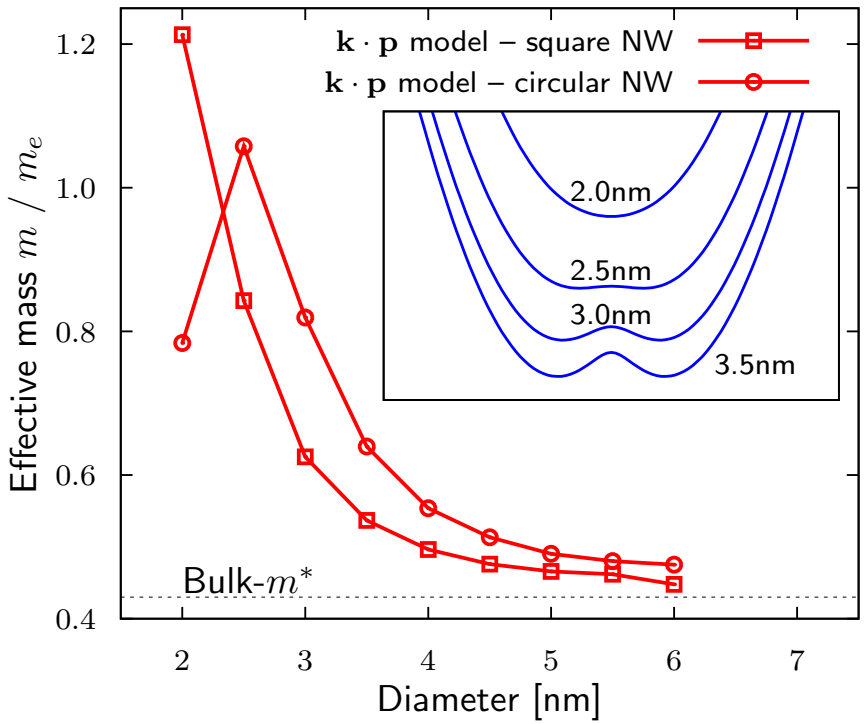
Results



- Subband structures of circular 5 nm thick nanowires with different growth orientations
- For [100] the unprimed subbands are four-fold degenerate.
- For [110] the degeneracy of the unprimed subbands is lifted.
- For [111] confinement dependent splitting occurs at the Γ point.

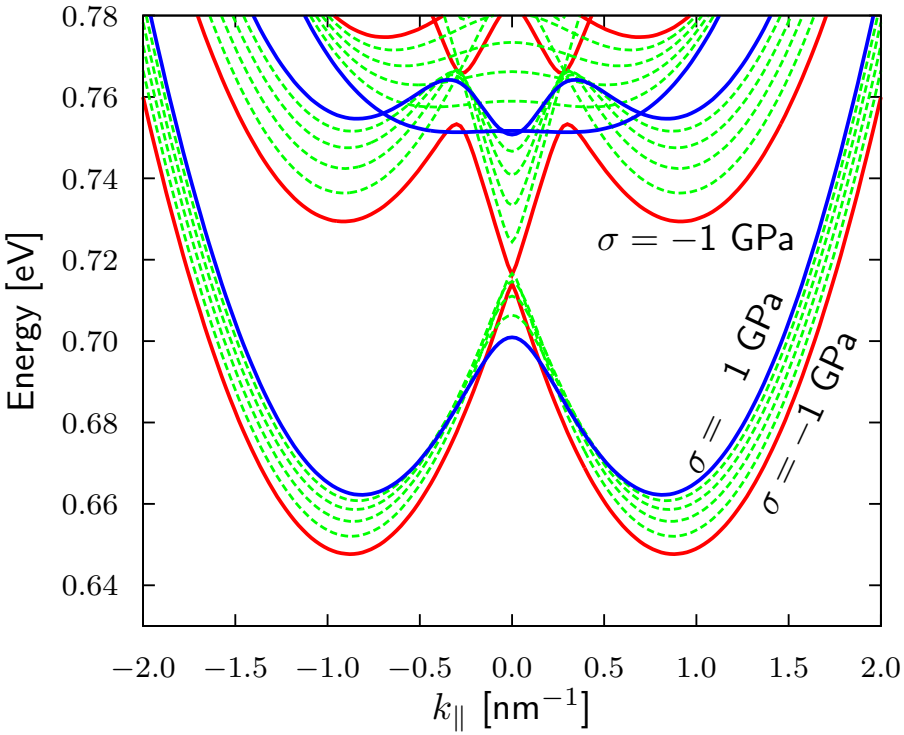
Results (cont'd)

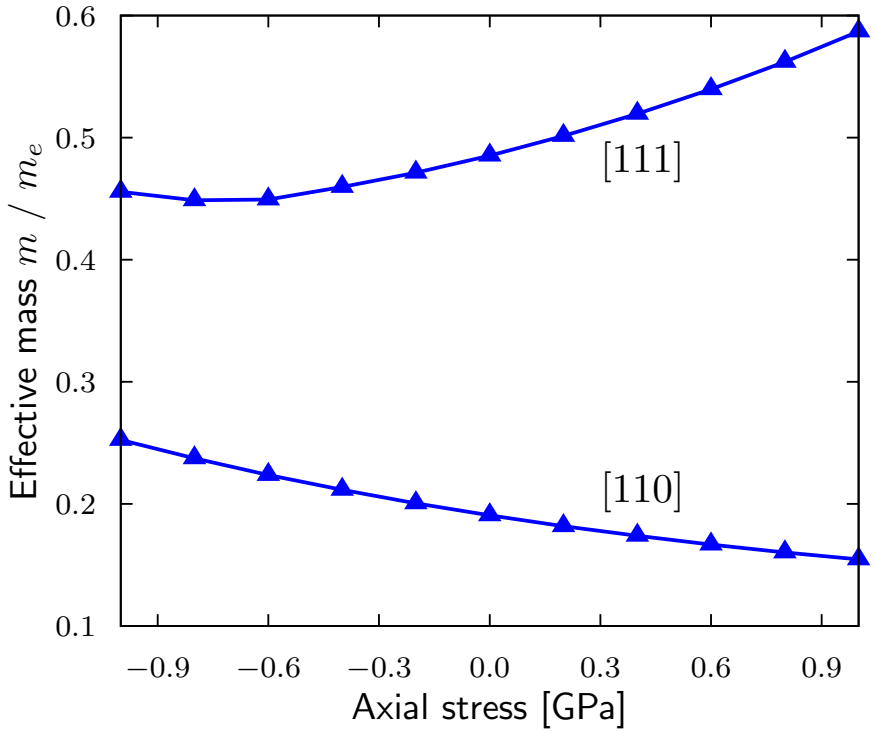




- Results for [100] and [110] agree reasonably well with semiempirical tight binding data.
- For thin [111] nanowires the splitting at Γ becomes so high that the two valleys eventually merge into one.

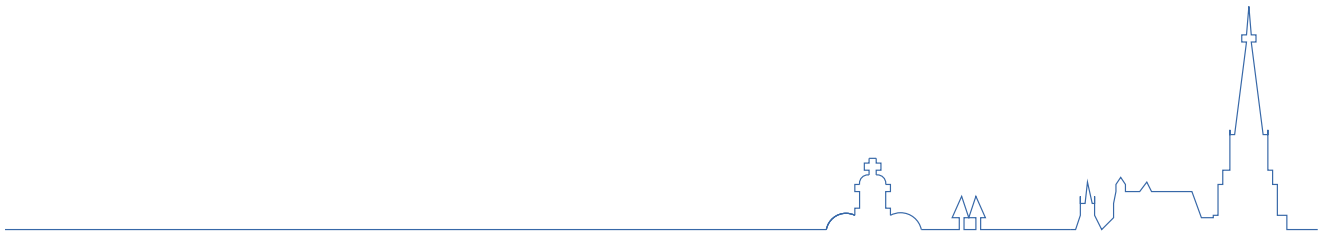
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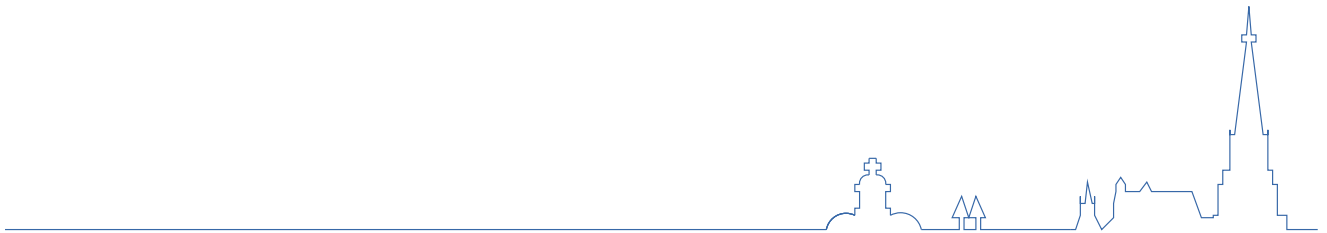
- Results are shown for stressed [111] and [110] nanowires.
- The effect of axial stress is opposite for [110] and [111].
- [100] nanowires show no effective mass change with respect to axial stress, only energy shifts.

Conclusions



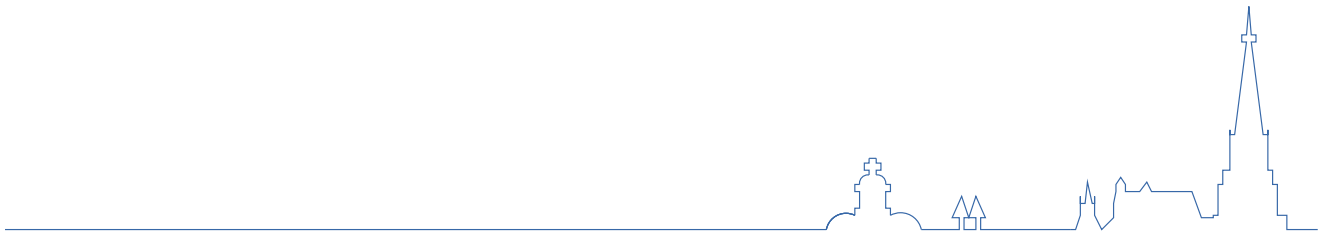
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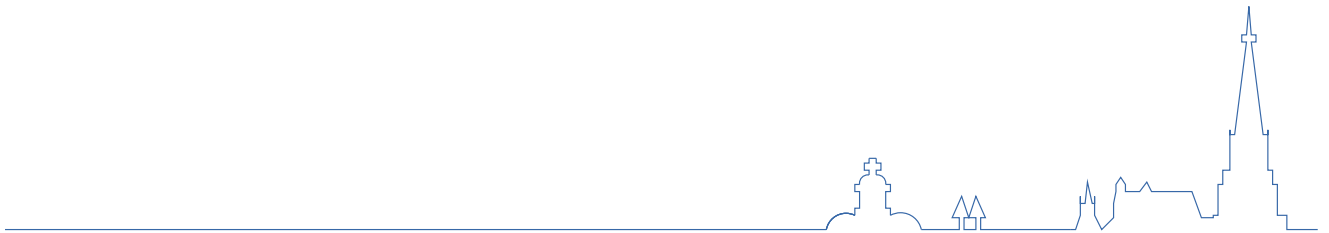
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- These effects depend on orientation, geometry, and stress/strain.



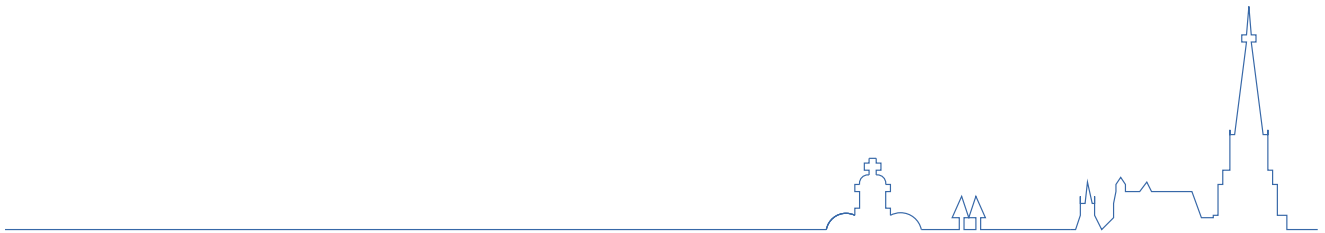
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- This calls for an efficient and reliable band structure modeling and computation tool.



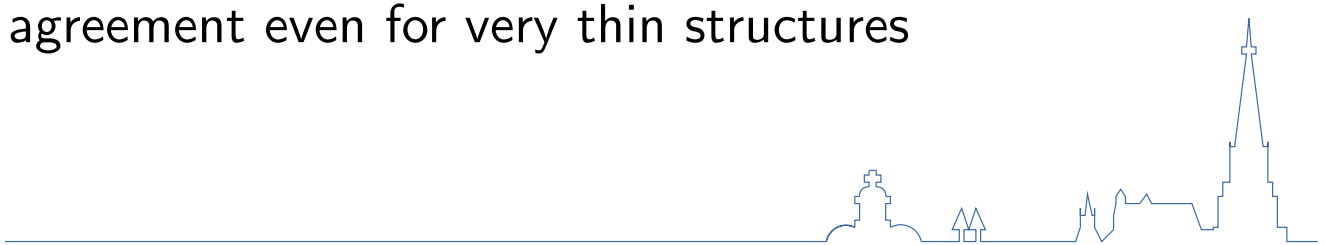
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- This calls for an efficient and reliable band structure modeling and computation tool.
- Semiempirical tight binding can deliver the needed results, however, at the expense of scalability and simplicity (at least ten parameters that have to be fit).
- A $\mathbf{k} \cdot \mathbf{p}$ based approach presents a good alternative:
  - One parameter – calculated analytically and confirmed computationally
  - Smaller system matrix $\longrightarrow$ shorter calculation times
  - First order approximation of strain effects
  - Captures all effects present in tight binding
  - Results in good agreement even for very thin structures



Thank you for your attention!

Questions...

