Electronic Band Structure

The band structure is modeled in the envelope function approximation, using either the single-band effective mass approximation or a multiband model.

To describe non-parabolicity, 2- or 3-band models are needed. The 3-band modeled is strongly recommended for structures based on electrons in III-V heterostructures.

Single-band model

The single-band model is the default case, or can also be specified explicitly by using:

```
  <Materials>
     ...
     <Number_of_bands>1</Number_of_bands>
    ...
  </Materials>
```

In this case a 1-dimensional Schrödinger equation is solved:

$$-\frac{\hbar^2}{2m_{\perp}^*(z)} \frac{\partial^2}{\partial z^2} \psi(z) + V(z) \psi(z) = E \psi(z)$$

where $m_{\perp}^*(z)$ is a position-dependent effective mass along the growth direction.

Effective mass

Effective mass from k.p parameters

If the following option is used, the effective mass is calculated from the k.p parameters

```
  <Materials>
    <Material>
      ...
<Effective_mass_from_kp_parameters>yes</Effective_mass_from_kp_parameters>
    </Material>
   </Materials>
```

using the following equation:

$$ \frac{m_0}{m_{\perp}^*} = S + \frac{E_P(E_g+2\Delta_{\text{SO}}/3)}{E_g(E_g+\Delta_{\text{SO}})} $$

where E_P is the Kane energy, E_g the band gap and Δ_{SO} is the spin-orbit splitting [Vurgaftman2001]. The effective mass of the database is ignored in this case.

Effective mass without k.p parameters

On the other hand, if

```
<Effective_mass_from_kp_parameters>no</Effective_mass_from_kp_parameters>
```

is specified, the effective mass is taken directly from the nextnano.NEGF database. Note that the database can be overwritten in the input file.

```
<Materials>
  <Material>
      ...
<Effective_mass_from_kp_parameters>no</Effective_mass_from_kp_parameters>
      <Overwrite>
        <ElectronMass>0.07</ElectronMass>
      </Overwrite>
  </Material>
</Materials>
```

Overwitting in-plane effective mass

For anisotropic effective masses, the axial $m_{\perp}^*$ and in-plane $m_{\parallel}^*$ effective masses can be individually overwritten in a separate way in the following way:

```
<Materials>
  <Material>
      ...
<Effective_mass_from_kp_parameters>no</Effective_mass_from_kp_parameters>
      <Overwrite>
        <ElectronMass>0.07</ElectronMass>
        <ElectronMass_inPlane>0.12</ElectronMass_inPlane>
      </Overwrite>
  </Material>
</Materials>
```

Non-parabolicity within single-band approach (not recommended)

If the non-parabolicty flag is specified

```
<NonParabolicity>yes</NonParabolicity>
```

the effective mass is evaluated at the energy of the lowest miniband: $$ \frac{m_0}{m^*} = S + \frac{E_P((E_g+E_0)+2\Delta_{\text{SO}}/3)}{(E_g+E_ 0)((E_g+E_0)+\Delta_{\text{SO}})} $$ where E_0 is the energy difference between the lowest miniband and the conduction band edge.

Note, however, that in this case the effective mass is not state-dependent, i.e. higher energy states

have the same effective mass than the lowest miniband. A full nonparabolic description is provided by 2- or 3-band models described below.

2-band model

The two-band model allows for a more accurate description of the nonparabolicity. It can be activated by using the following syntax:

```
<Materials>
   ...
   <Number_of_bands>2</Number_of_bands>
  ...
</Materials>
```

In this case, a conduction band is coupled to an effective valence band. The 2-band Hamiltonian describing the 1-D Schrödinger equation along the z-axis reads $$ H(z) = \left({\begin{array}{cc} E_c(z) + S(z)\frac{\hbar^2 k_z^2}{2 m_0} & i P(z) k_z \\ - i P(z) k_z & E_v(z) + (1+L(z))\frac{\hbar^2 k_z^2}{2 m_0}\\ \end{array} } \right) $$

where P is the interband momentum matrix element, which is related to the Kane energy E_p through: $$ P(z) = \sqrt{\frac{m_0 E_p(z)}{2}} $$ L correponds to the Dresselhaus parameter L' used in 8-band k.p parameters of nextnano3/nextnano++. By default, this value is set to -1. Note that when $S<0$ **and** $L\neq-1$, spurious solutions are likely to occur. Hence it is recommended either (i) to let $L=-1$ (default value), or (ii) to use renormalized k.p parameters E_p, S and L given by nextnano++ with $S=1$.

If

```
<Effective_mass_from_kp_parameters>yes</Effective_mass_from_kp_parameters>
```

is specified, the band structure is calculated from the parameters E_p, S, E_g, and band offsets. The effective mass of the database is not used.

Input from effective mass and non-parabolicity

If

```
<Effective_mass_from_kp_parameters>no</Effective_mass_from_kp_parameters>
```

is specified, the effective mass m^*_0 of the database (or overwritten in the input file) is used as an input to calculate the k.p parameters. In this case, the parameter S is set to $S=0$, and the interband energy is overwritten using: $$ E_p = \frac{m_0}{m^*} E_g $$

In this case, non-parabolicity is controlled by the value of the bandgap.

To further modify non-parabolicity, a non-parabolic coefficient a_{np} can be further specified in the database or in the input file (optional):

```
<NonParabolicityRelative>0.02</NonParabolicityRelative>
```

The parameters E_g and E_p are then modified according to: $$ E'_g = E_g (1- a_{np}) $$ and $$ E'_p = E_p (1- a_{np}) $$

In this case, the dispersion relation is given by: $$ E(k) = \frac{\hbar^2 k^2}{2m^*_0} \frac{1}{1 + \frac{(1-a_{np}) E}{E_g}} \simeq \frac{\hbar^2 k^2}{2m^*_0} \left[1 - \frac{(1-a_{np}) E}{E_g} \right] $$

3-band model

The 3-band model can be activated using:

```
  <Materials>
     ...
     <Number_of_bands>3</Number_of_bands>
    ...
  </Materials>
```

Its aim is to account accurately for the nonparabolicity of the conduction band. It accounts for the 3 following bands:

- conduction band
- light-hole (lh) band
- split-off (so) band

In this basis, the considered Hamiltonian reads:

$$ H = \left({\begin{array}{ccc} E_c(z) + S(z)\frac{\hbar^2 k_z^2}{2 m_0} & i \sqrt{\frac{2}{3}} P(z) k_z & -i \sqrt{\frac{1}{3}} P(z) k_z\\ - i \sqrt{\frac{2}{3}} P(z) k_z & E_{lh}(z) + (1+L(z)) \frac{\hbar^2 k_z^2}{2 m_0} & 0\\ i \sqrt{\frac{1}{3}} P(z) k_z & 0 & E_{so} + (1+L(z))\frac{\hbar^2 k_z^2}{2 m_0}(z) \end{array} } \right) $$

Input from effective mass and non-parabolicity

When

```
<Effective_mass_from_kp_parameters>no</Effective_mass_from_kp_parameters>
```

is specified, the effective mass m^*_0 of the database (or overwritten in the input file) is used as an input to calculate the k.p parameters. In this case, the parameter S is set to $S=0$, and the interband energy is overwritten using: $$ E_p = \frac{m_0}{m^*} \frac{E_g(Eg+\Delta_{SO})}{Eg+\frac{2}{3}\Delta_{SO}} $$

Output of the effective mass in the multiband case

In the multiband case (2 or 3 bands), a position and state-dependent effective mass is output in the file “EffectiveMassesPosition.dat”. Note that this effective mass is only an output in order to allow comparison with other models and to analyze the multiband calculation.

In the 2-band case, its value is given for the level i by:

$$ \frac{m_0}{m_{\perp}^*(z,i)} = S(z) + \frac{E_P(z)}{\epsilon_i-E_{v,av}(z)} = S(z) + \frac{E_P(z)}{\epsilon_i-\left(E_{g}(z)+\frac{1}{3}\Delta_{SO}(z)\right)} $$

In the 3-band case, it reads $$ \frac{m_0}{m_{\perp}^*(z,i)} = S(z) + \frac{2}{3} \frac{E_P(z)}{\epsilon_i-E_{lh}(z)} + \frac{1}{3} \frac{E_P(z)}{\epsilon_i-E_{SO}(z)}$$

where ϵ_i is the energy of level i. Note that this formula accounts for nonparabolicity as the effective mass depends on the energy difference between the energy level and the valence bandedges.

From this position-dependent effective masses, an averaged effective mass can de defined for each level, accounting for nonparabolicity. The state-dependent effective mass $m_{\perp}^*(i)$ is output in the file “EffectiveMasses.dat” and is defined by the following averaging: $$ \frac{m_0}{m_{\perp}^*(i)} = \int dz \frac{m_0}{m_{\perp}^*(z,i)} |\Psi_i(z)|^2 $$

In-plane nonparabolicity

In the multiband models, to account that the in-plane effective mass depends on both the energies along the growth axis z and the in-plane directions (x,y), the following command has to included in <Materials>:

```
<Materials>
   ...
   <InPlaneNonParabolicity>yes</InPlaneNonParabolicity>
   ...
</Materials>
```

If no is specified, the dispersion will be nonparabolic along the growth axis, while parabolic in the plane.

Rescaling of k.p parameters (for multiband)

It is possible to rescale the $S = 1+2F$ parameter (where F is the remote-band contribution) by using the following command:

```
<Material>
            <Name>In(x)Ga(1-x)As</Name>
            ...
<Effective_mass_from_kp_parameters>yes</Effective_mass_from_kp_parameters>
            <Rescale_S>yes</Rescale_S>
```

```
            <Rescale_S_to>1.0</Rescale_S_to>
        </Material>
```

The effect on S and Ep of rescaling is the following: $$S \rightarrow S'$$ $$E_p \rightarrow E_p' $$ while the effective mass at bandedge is conserved. For 2 bands this corresponds to: $$ S + \frac{E_P}{E_g} = S' + \frac{E'_P}{E_g}$$ while for 3 bands it corresponds to: $$ S + \frac{E_P(E_g+2\Delta_{\text{SO}}/3)}{E_g(E_g+\Delta_{\text{SO}})} = S' + \frac{E'_P(E_g+2\Delta_{\text{SO}}/3)}{E_g(E_g+\Delta_{\text{SO}})}$$

Note that the effective mass is conserved at the bandedge energy, but that the nonparabolicity will be affected by such rescaling.

In the above example, rescaling S to 1, means that only the free electron kinetic energy term will remain (i.e. no remote-band contribution, $F=0$).

Smoothing of the k.p parameters (2 or 3 band case)

In the multiband case, spurious solutions can occur at the interface in the case of a discontinuity of the k.p parameters E_p and/or S. To avoid this, a smoothing of the k.p parameters is done. The smoothing length can be set manually using the following command (otherwise it is set automatically);

```
    <Simulation_Parameter>
       ...
       <Smoothing_Length_kp unit="nm">0.2</Smoothing_Length_kp>
       ...
   </Simulation_Parameter>
```

In any case, the used value is displayed in the log file:

```
Calculating axial electronic structure...
00:00:07   46.2  Smoothing of k.p parameters: auto mode
00:00:07   46.1  Smoothing length for Ep (Kane) parameter =
0.274702188030413 nm
00:00:07   46.1  Smoothing length for S (remote bands) parameter =
0.260335418344245 nm
```

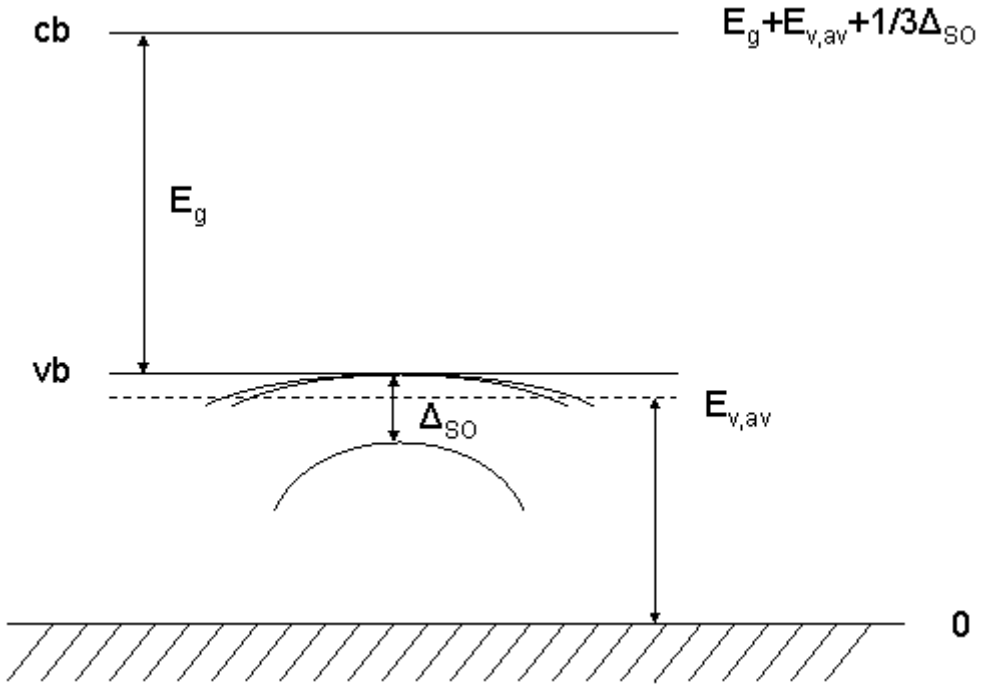
The smoothing is performed by performing a convolution of the $E_p(z)$ and $S(z)$ spatial functions by a Gaussian e^{-z^2/L_s^2} where L_s is either the E_p or S smoothing length.

Definition of band offsets

There are two options to define band offsets:

- Option a) Specify conduction band offset (CBO) directly, and then the valence band offset (VBO) is calculated.
- Option b) Specify valence band offset (VBO), and then the conduction band offset (CBO) is

calculated.



$E_{\rm v,av}$ is the average energy of heavy hole (hh), light hole (lh) and split-off hole (so). $\Delta_{\rm so}$ is the spin-orbit split-off energy.

- Option a) Specify conduction band offset (CBO) $E_{\rm c}$
  `<UseConductionBandOffset>yes</UseConductionBandOffset>`

The valence bandedges are then defined according to $$E_{\rm lh}(T) = E_{\rm c} - E_{\rm g}(T)$$ $$E_{\rm so}(T) = E_{\rm c} - E_{\rm g}(T) - \Delta_{\rm so} = E_{\rm lh}(T) - \Delta_{\rm so} $$

- Option b) Specify valence band offset (VBO) $E_{\rm v,av}$
  The conduction band edge $E_{\rm c}$ is calculated and depends on temperature.
  `<UseConductionBandOffset>no</UseConductionBandOffset>` (default)

\begin{align*} E_{\rm lh} & = E_{\rm v,av}+\frac{1}{3}\Delta_{\rm so}\\ E_{\rm so} & = E_{\rm v,av}-\frac{2}{3}\Delta_{\rm so}\\ E_{\rm c}(T) & = E_{\rm lh} + E_{\rm g}(T) \end{align*}

Note that the band gap $E_{\rm gap}$ is temperature dependent (Varshni formula), $$E_{\rm gap}(T)=E_{\rm gap}(T=0 {\rm ~K})-\frac{\alpha T^2}{T+\beta},$$ where α and β are the Varshni parameters. On the other hand, the bandoffsets of the database don't have any tabulated temperature dependence. Hence the two options lead to different temperature dependence, as the temperature dependence of the bandgap is attributed to the conduction band if `<UseConductionBandOffset>no</UseConductionBandOffset>` is used, and to the valence band in the `<UseConductionBandOffset>yes</UseConductionBandOffset>` case.