Physics-based Device Simulation

C. Jungemann

Institut für Theoretische Elektrotechnik
RWTH Aachen University
52056 Aachen

A European Project supported within the Seventh Framework Programme for Research and Technological Development

Outline

- Motivation
- Pros & Cons
- Semiclassical transport
- Results
- Conclusions

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models

Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models

Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models

Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models

Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models

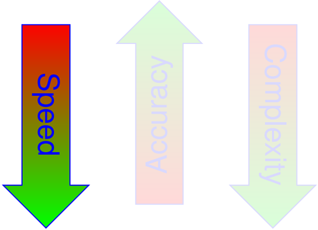
Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models



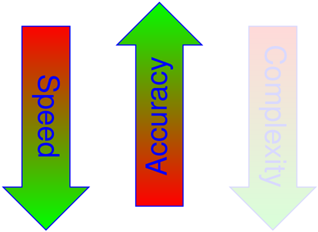
Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models



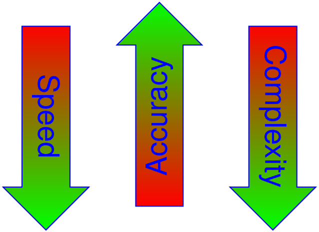
Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models



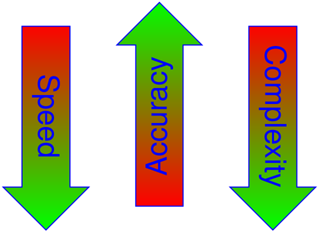
Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models



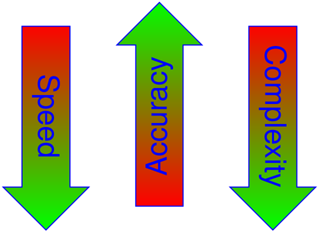
Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models



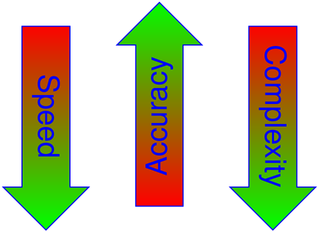
Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models



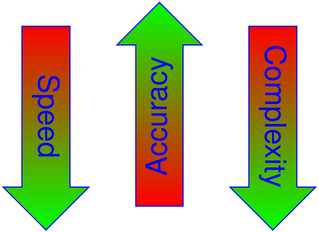
Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models



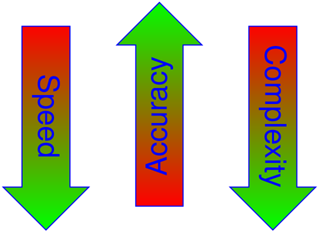
Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models



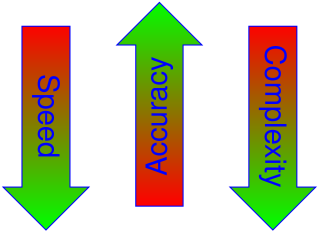
Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Motivation

Simulation hierarchy

- Quantum transport
- Semiclassical transport
- TCAD
- Compact models



Why semiclassical transport simulation (Boltzmann equation)?

- Complex band structures
- Detailed scattering models
- Only material-dependent parameters
- DC, AC and noise analysis
- No adjustable parameters in the RF noise model

Pros & Cons

- Realistic device structure
- Microscopic, accurate physics (Boltzmann equation)
- Detailed physics
- Consistent modeling of transport and noise
- Numerically challenging
- Very slow (a CPU day per bias point for a 2D device)
- Limited device detail (2D, only few parasitics)
- Only as good as the models

Pros & Cons

- Realistic device structure
- Microscopic, accurate physics (Boltzmann equation)
- Detailed physics
- Consistent modeling of transport and noise
- Numerically challenging
- Very slow (a CPU day per bias point for a 2D device)
- Limited device detail (2D, only few parasitics)
- Only as good as the models

Pros & Cons

- Realistic device structure
- Microscopic, accurate physics (Boltzmann equation)
- Detailed physics
- Consistent modeling of transport and noise
- Numerically challenging
- Very slow (a CPU day per bias point for a 2D device)
- Limited device detail (2D, only few parasitics)
- Only as good as the models

Pros & Cons

- Realistic device structure
- Microscopic, accurate physics (Boltzmann equation)
- Detailed physics
- Consistent modeling of transport and noise
- Numerically challenging
- Very slow (a CPU day per bias point for a 2D device)
- Limited device detail (2D, only few parasitics)
- Only as good as the models

Pros & Cons

- Realistic device structure
- Microscopic, accurate physics (Boltzmann equation)
- Detailed physics
- Consistent modeling of transport and noise
- Numerically challenging
- Very slow (a CPU day per bias point for a 2D device)
- Limited device detail (2D, only few parasitics)
- Only as good as the models

Pros & Cons

- Realistic device structure
- Microscopic, accurate physics (Boltzmann equation)
- Detailed physics
- Consistent modeling of transport and noise
- Numerically challenging
- Very slow (a CPU day per bias point for a 2D device)
- Limited device detail (2D, only few parasitics)
- Only as good as the models

Pros & Cons

- Realistic device structure
- Microscopic, accurate physics (Boltzmann equation)
- Detailed physics
- Consistent modeling of transport and noise
- Numerically challenging
- Very slow (a CPU day per bias point for a 2D device)
- Limited device detail (2D, only few parasitics)
- Only as good as the models

Pros & Cons

- Realistic device structure
- Microscopic, accurate physics (Boltzmann equation)
- Detailed physics
- Consistent modeling of transport and noise
- Numerically challenging
- Very slow (a CPU day per bias point for a 2D device)
- Limited device detail (2D, only few parasitics)
- Only as good as the models

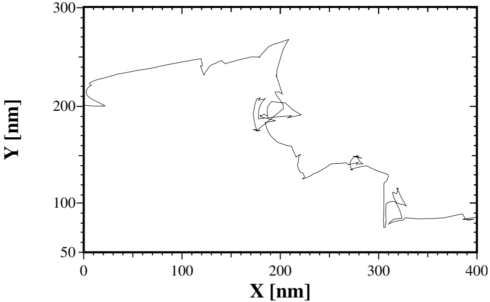
Pros & Cons

- Realistic device structure
- Microscopic, accurate physics (Boltzmann equation)
- Detailed physics
- Consistent modeling of transport and noise
- Numerically challenging
- Very slow (a CPU day per bias point for a 2D device)
- Limited device detail (2D, only few parasitics)
- Only as good as the models

Semiclassical transport

Semiclassical transport

Path of an electron in a semiconductor



Newton's equations of motion

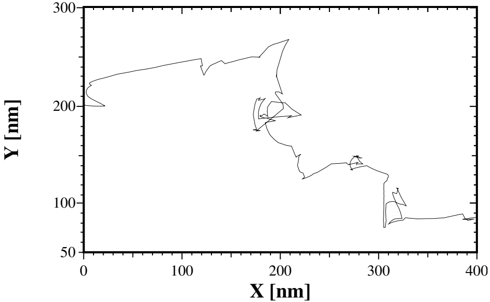
$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = \vec{F}\,, \qquad \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \vec{v}$$

Two first order ODEs

Two initial conditions (position, momentum)

Semiclassical transport

Path of an electron in a semiconductor



Newton's equations of motion

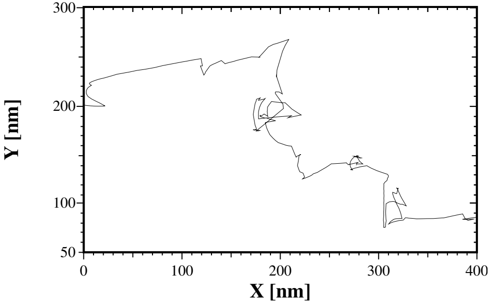
$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = \vec{F}\,, \qquad \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \vec{v}$$

Two first order ODEs

Two initial conditions (position, momentum)

Semiclassical transport

Path of an electron in a semiconductor



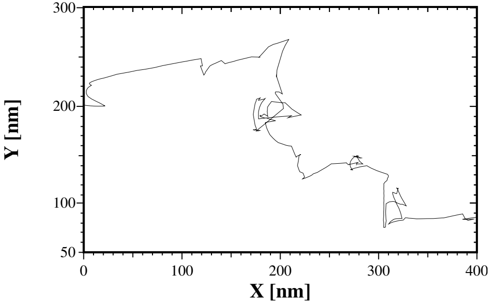
Newton's equations of motion

$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = \vec{F}\,, \qquad \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \vec{v}$$

Two first order ODEs
Two initial conditions (position, momentum)

Semiclassical transport

Path of an electron in a semiconductor



Newton's equations of motion

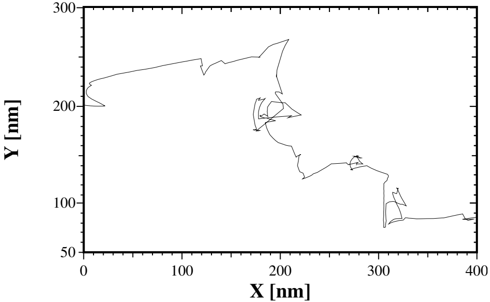
$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = \vec{F}\,, \qquad \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \vec{v}$$

Two first order ODEs

Two initial conditions (position, momentum)

Semiclassical transport

Path of an electron in a semiconductor



Newton's equations of motion

$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = \vec{F}\,, \qquad \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \vec{v}$$

Two first order ODEs

Two initial conditions (position, momentum)

Semiclassical Transport

Particle ensemble described by a distribution function ($\vec{p} = \hbar\vec{k}$)

$$f(\vec{r}, \vec{k}, t)$$

Number of particles in a volume of phase space

$$dN = \frac{2}{(2\pi)^3} f(\vec{r}, \vec{k}, t) d^3r d^3k$$

Equilibrium (Boltzmann distribution)

$$f_0 = c \exp\left(-\frac{\varepsilon(\vec{r}, \vec{k})}{kT}\right)$$

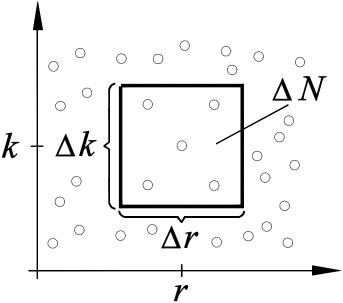
Semiclassical Transport

Particle ensemble described by a distribution function ($\vec{p} = \hbar\vec{k}$)

$$f(\vec{r}, \vec{k}, t)$$

Number of particles in a volume of phase space

$$dN = \frac{2}{(2\pi)^3} f(\vec{r}, \vec{k}, t) d^3 r d^3 k$$



Equilibrium (Boltzmann distribution)

$$f_0 = c \exp\left(-\frac{\varepsilon(\vec{r}, \vec{k})}{kT}\right)$$

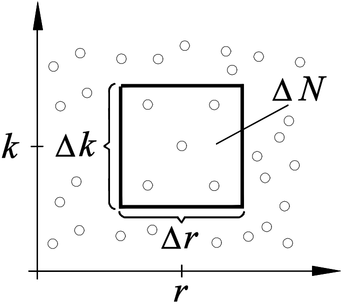
Semiclassical Transport

Particle ensemble described by a distribution function ($\vec{p} = \hbar\vec{k}$)

$$f(\vec{r}, \vec{k}, t)$$

Number of particles in a volume of phase space

$$dN = \frac{2}{(2\pi)^3} f(\vec{r}, \vec{k}, t) d^3r d^3k$$



Equilibrium (Boltzmann distribution)

$$f_0 = c \exp\left(-\frac{\varepsilon(\vec{r}, \vec{k})}{kT}\right)$$

Semiclassical Transport

Boltzmann Transport Equation

$$\frac{\partial f\left(\vec{r},\vec{k},t\right)}{\partial t} - \frac{q}{\hbar}\vec{E}(\vec{r})\cdot\nabla_{\vec{k}} f\left(\vec{r},\vec{k},t\right) + \vec{v}\left(\vec{k}\right)\cdot\nabla_{\vec{r}} f\left(\vec{r},\vec{k},t\right) =$$

$$\frac{\Omega_{\mathrm{sys}}}{(2\pi)^3}\int W\left(\vec{r},\vec{k}|\vec{k}'\right) f\left(\vec{r},\vec{k}',t\right) - W\left(\vec{r},\vec{k}'|\vec{k}\right) f\left(\vec{r},\vec{k},t\right) d^3k'$$

Integro-differential equation

Direct discretization of the 6D phase space is not possible

Spherical Harmonics Expansion solver (SHE) for the BTE
(Bologna group, Maryland group et al.)

Semiclassical Transport

Boltzmann Transport Equation

$$\frac{\partial f\left(\vec{r},\vec{k},t\right)}{\partial t} - \frac{q}{\hbar}\vec{E}(\vec{r})\cdot\nabla_{\vec{k}} f\left(\vec{r},\vec{k},t\right) + \vec{v}\left(\vec{k}\right)\cdot\nabla_{\vec{r}} f\left(\vec{r},\vec{k},t\right) =$$

$$\frac{\Omega_{\mathrm{sys}}}{(2\pi)^3}\int W\left(\vec{r},\vec{k}|\vec{k}'\right) f\left(\vec{r},\vec{k}',t\right) - W\left(\vec{r},\vec{k}'|\vec{k}\right) f\left(\vec{r},\vec{k},t\right) d^3k'$$

Integro-differential equation

Direct discretization of the 6D phase space is not possible

Spherical Harmonics Expansion solver (SHE) for the BTE
(Bologna group, Maryland group et al.)

Semiclassical Transport

Boltzmann Transport Equation

$$\frac{\partial f\left(\vec{r},\vec{k},t\right)}{\partial t} - \frac{q}{\hbar}\vec{E}(\vec{r})\cdot\nabla_{\vec{k}} f\left(\vec{r},\vec{k},t\right) + \vec{v}\left(\vec{k}\right)\cdot\nabla_{\vec{r}} f\left(\vec{r},\vec{k},t\right) =$$

$$\frac{\Omega_{\mathrm{sys}}}{(2\pi)^3}\int W\left(\vec{r},\vec{k}|\vec{k}'\right) f\left(\vec{r},\vec{k}',t\right) - W\left(\vec{r},\vec{k}'|\vec{k}\right) f\left(\vec{r},\vec{k},t\right) d^3k'$$

Integro-differential equation

Direct discretization of the 6D phase space is not possible

Spherical Harmonics Expansion solver (SHE) for the BTE
(Bologna group, Maryland group et al.)

Semiclassical Transport

Boltzmann Transport Equation

$$\frac{\partial f\left(\vec{r},\vec{k},t\right)}{\partial t} - \frac{q}{\hbar}\vec{E}(\vec{r})\cdot\nabla_{\vec{k}} f\left(\vec{r},\vec{k},t\right) + \vec{v}\left(\vec{k}\right)\cdot\nabla_{\vec{r}} f\left(\vec{r},\vec{k},t\right) =$$

$$\frac{\Omega_{\mathrm{sys}}}{(2\pi)^3}\int W\left(\vec{r},\vec{k}|\vec{k}'\right) f\left(\vec{r},\vec{k}',t\right) - W\left(\vec{r},\vec{k}'|\vec{k}\right) f\left(\vec{r},\vec{k},t\right) d^3k'$$

Integro-differential equation

Direct discretization of the 6D phase space is not possible

Spherical Harmonics Expansion solver (SHE) for the BTE
(Bologna group, Maryland group et al.)

Spherical Harmonics Expansion

Spherical coordinates for k-space

$$(k_x, k_y, k_z) \quad \rightarrow \quad (k, \vartheta, \varphi) \quad \rightarrow \quad (\varepsilon, \vartheta, \varphi)$$

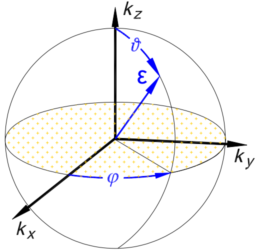
Dependence on angles is expanded with spherical harmonics $Y_{l,m}(\vartheta, \varphi)$

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,-1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \sin\varphi$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\vartheta$$

$$Y_{1,1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \cos\varphi$$



$$\oint Y_{l,m}(\vartheta, \varphi) Y_{l',m'}(\vartheta, \varphi) d\Omega = \delta_{l,l'} \delta_{m,m'} \ , \qquad d\Omega = \sin\vartheta d\vartheta d\varphi$$

Spherical Harmonics Expansion

Spherical coordinates for k-space

$$(k_x, k_y, k_z) \quad \rightarrow \quad (k, \vartheta, \varphi) \quad \rightarrow \quad (\varepsilon, \vartheta, \varphi)$$

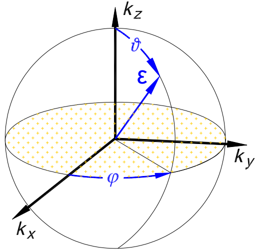
Dependence on angles is expanded with spherical harmonics $Y_{l,m}(\vartheta, \varphi)$

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,-1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \, \sin\varphi$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\vartheta$$

$$Y_{1,1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \, \cos\varphi$$



$$\oint Y_{l,m}(\vartheta, \varphi) Y_{l',m'}(\vartheta, \varphi) d\Omega = \delta_{l,l'} \delta_{m,m'} \;, \qquad d\Omega = \sin\vartheta d\vartheta d\varphi$$

Spherical Harmonics Expansion

Spherical coordinates for k-space

$$(k_x, k_y, k_z) \quad \rightarrow \quad (k, \vartheta, \varphi) \quad \rightarrow \quad (\varepsilon, \vartheta, \varphi)$$

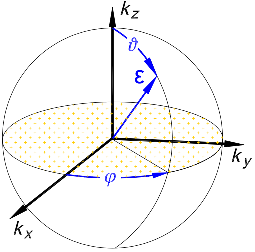
Dependence on angles is expanded with spherical harmonics $Y_{l,m}(\vartheta, \varphi)$

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,-1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \sin\varphi$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\vartheta$$

$$Y_{1,1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \cos\varphi$$



$$\oint Y_{l,m}(\vartheta, \varphi) Y_{l',m'}(\vartheta, \varphi) d\Omega = \delta_{l,l'} \delta_{m,m'} \ , \qquad d\Omega = \sin\vartheta d\vartheta d\varphi$$

Spherical Harmonics Expansion

Spherical coordinates for k-space

$$(k_x, k_y, k_z) \quad \rightarrow \quad (k, \vartheta, \varphi) \quad \rightarrow \quad (\varepsilon, \vartheta, \varphi)$$

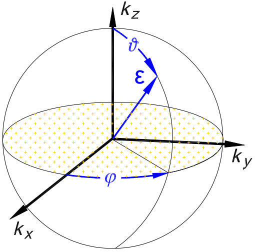
Dependence on angles is expanded with spherical harmonics $Y_{l,m}(\vartheta, \varphi)$

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,-1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \sin\varphi$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\vartheta$$

$$Y_{1,1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \cos\varphi$$



$$\oint Y_{l,m}(\vartheta, \varphi) Y_{l',m'}(\vartheta, \varphi) d\Omega = \delta_{l,l'} \delta_{m,m'} \;, \qquad d\Omega = \sin\vartheta d\vartheta d\varphi$$

Spherical Harmonics Expansion

Spherical coordinates for k-space

$$(k_x, k_y, k_z) \quad \rightarrow \quad (k, \vartheta, \varphi) \quad \rightarrow \quad (\varepsilon, \vartheta, \varphi)$$

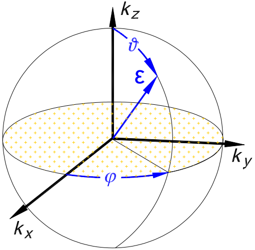
Dependence on angles is expanded with spherical harmonics $Y_{l,m}(\vartheta, \varphi)$

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,-1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \sin\varphi$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\vartheta$$

$$Y_{1,1} = \sqrt{\frac{3}{4\pi}} \sin\vartheta \cos\varphi$$



$$\oint Y_{l,m}(\vartheta, \varphi) Y_{l',m'}(\vartheta, \varphi) d\Omega = \delta_{l,l'} \delta_{m,m'} \ , \qquad d\Omega = \sin\vartheta d\vartheta d\varphi$$

Semiclassical transport

Spherical harmonics expansion of the distribution function

$$g_{l,m}(\vec{r},\varepsilon,t) = \frac{1}{(2\pi)^3} \int \delta\left(\varepsilon - \varepsilon(\vec{k})\right) Y_{l,m}(\vartheta,\varphi) f(\vec{r},\vec{k},t) d^3k$$

$$g(\vec{r},\vec{k},t) = g(\vec{r},\varepsilon,\vartheta,\varphi,t) \approx \sum_{l=0}^{l_{\max}} \sum_{m=-l}^{m=l} g_{l,m}(\vec{r},\varepsilon,t) Y_{l,m}(\vartheta,\varphi)$$

Electron density

$$n(\vec{r},t) = \frac{2}{(2\pi)^3} \int f(\vec{r},\vec{k},t) d^3k = 2\sqrt{4\pi} \int_0^\infty g_{0,0}(\vec{r},\varepsilon,t) d\varepsilon$$

Electron current density (spherical bands)

$$\vec{j}(\vec{r},t) = 2\sqrt{\frac{4\pi}{3}} \int_0^\infty v(\varepsilon) \begin{pmatrix} g_{1,1}(\vec{r},\varepsilon,t) \\ g_{1,-1}(\vec{r},\varepsilon,t) \\ g_{1,0}(\vec{r},\varepsilon,t) \end{pmatrix} d\varepsilon$$

Semiclassical transport

Spherical harmonics expansion of the distribution function

$$g_{l,m}(\vec{r},\varepsilon,t) = \frac{1}{(2\pi)^3}\int \delta\left(\varepsilon - \varepsilon(\vec{k})\right) Y_{l,m}(\vartheta,\varphi) f(\vec{r},\vec{k},t) d^3k$$

$$g(\vec{r},\vec{k},t) = g(\vec{r},\varepsilon,\vartheta,\varphi,t) \approx \sum_{l=0}^{l_{\max}} \sum_{m=-l}^{m=l} g_{l,m}(\vec{r},\varepsilon,t) Y_{l,m}(\vartheta,\varphi)$$

Electron density

$$n(\vec{r},t) = \frac{2}{(2\pi)^3}\int f(\vec{r},\vec{k},t) d^3k = 2\sqrt{4\pi}\int_0^\infty g_{0,0}(\vec{r},\varepsilon,t) d\varepsilon$$

Electron current density (spherical bands)

$$\vec{j}(\vec{r},t) = 2\sqrt{\frac{4\pi}{3}}\int_0^\infty v(\varepsilon) \begin{pmatrix} g_{1,1}(\vec{r},\varepsilon,t) \\ g_{1,-1}(\vec{r},\varepsilon,t) \\ g_{1,0}(\vec{r},\varepsilon,t) \end{pmatrix} d\varepsilon$$

Semiclassical transport

Spherical harmonics expansion of the distribution function

$$g_{l,m}(\vec{r},\varepsilon,t)=\frac{1}{(2\pi)^3}\int\delta\left(\varepsilon-\varepsilon(\vec{k})\right)Y_{l,m}(\vartheta,\varphi)f(\vec{r},\vec{k},t)d^3k$$

$$g(\vec{r},\vec{k},t)=g(\vec{r},\varepsilon,\vartheta,\varphi,t)\approx\sum_{l=0}^{l_{\max}}\sum_{m=-l}^{m=l}g_{l,m}(\vec{r},\varepsilon,t)Y_{l,m}(\vartheta,\varphi)$$

Electron density

$$n(\vec{r},t)=\frac{2}{(2\pi)^3}\int f(\vec{r},\vec{k},t)d^3k=2\sqrt{4\pi}\int_0^\infty g_{0,0}(\vec{r},\varepsilon,t)d\varepsilon$$

Electron current density (spherical bands)

$$\vec{j}(\vec{r},t)=2\sqrt{\frac{4\pi}{3}}\int_0^\infty v(\varepsilon)\begin{pmatrix}g_{1,1}(\vec{r},\varepsilon,t)\\ g_{1,-1}(\vec{r},\varepsilon,t)\\ g_{1,0}(\vec{r},\varepsilon,t)\end{pmatrix}d\varepsilon$$

Semiclassical transport

Spherical harmonics expansion of the distribution function

$$g_{l,m}(\vec{r},\varepsilon,t) = \frac{1}{(2\pi)^3}\int \delta\left(\varepsilon - \varepsilon(\vec{k})\right) Y_{l,m}(\vartheta,\varphi) f(\vec{r},\vec{k},t) d^3k$$

$$g(\vec{r},\vec{k},t) = g(\vec{r},\varepsilon,\vartheta,\varphi,t) \approx \sum_{l=0}^{l_{\mathrm{max}}} \sum_{m=-l}^{m=l} g_{l,m}(\vec{r},\varepsilon,t) Y_{l,m}(\vartheta,\varphi)$$

Electron density

$$n(\vec{r},t) = \frac{2}{(2\pi)^3}\int f(\vec{r},\vec{k},t) d^3k = 2\sqrt{4\pi}\int_0^\infty g_{0,0}(\vec{r},\varepsilon,t) d\varepsilon$$

Electron current density (spherical bands)

$$\vec{j}(\vec{r},t) = 2\sqrt{\frac{4\pi}{3}}\int_0^\infty v(\varepsilon)\begin{pmatrix} g_{1,1}(\vec{r},\varepsilon,t) \\ g_{1,-1}(\vec{r},\varepsilon,t) \\ g_{1,0}(\vec{r},\varepsilon,t)\end{pmatrix} d\varepsilon$$

Semiclassical transport

Spherical harmonics expansion of the Boltzmann equation

$$\frac{1}{(2\pi)^3} \int \delta\left(\varepsilon - \varepsilon(\vec{k})\right) Y_{l,m}(\vartheta,\varphi) \{\mathrm{BE}\}\, d^3k$$

yields balance equations over energy/real space

$$\frac{\partial g_{l,m}}{\partial t} - q\vec{E} \cdot \frac{\partial \vec{j}_{l,m}}{\partial \varepsilon} + \nabla_{\vec{r}} \cdot \vec{j}_{l,m} - \Gamma_{l,m} = W_{l,m}\{g\}$$

with

$$\vec{j}_{l,m}(\vec{r},\varepsilon,t) = v(\varepsilon) \sum_{l',m'} \vec{a}_{l,m,l',m'} g_{l'.m'}(\vec{r},\varepsilon,t)$$

The balance equations are coupled

Semiclassical transport

Spherical harmonics expansion of the Boltzmann equation

$$\frac{1}{(2\pi)^3}\int \delta\left(\varepsilon - \varepsilon(\vec{k})\right) Y_{l,m}(\vartheta,\varphi)\,\{\mathrm{BE}\}\,d^3k$$

yields balance equations over energy/real space

$$\frac{\partial g_{l,m}}{\partial t} - q\vec{E}\cdot\frac{\partial \vec{j}_{l,m}}{\partial \varepsilon} + \nabla_{\vec{r}}\cdot\vec{j}_{l,m} - \Gamma_{l,m} = W_{l,m}\{g\}$$

with

$$\vec{j}_{l,m}(\vec{r},\varepsilon,t) = v(\varepsilon)\sum_{l',m'}\vec{a}_{l,m,l',m'}\,g_{l'.m'}(\vec{r},\varepsilon,t)$$

The balance equations are coupled

Semiclassical transport

Spherical harmonics expansion of the Boltzmann equation

$$\frac{1}{(2\pi)^3} \int \delta\left(\varepsilon - \varepsilon(\vec{k})\right) Y_{l,m}(\vartheta, \varphi) \{\mathrm{BE}\}\, d^3 k$$

yields balance equations over energy/real space

$$\frac{\partial g_{l,m}}{\partial t} - q\vec{E} \cdot \frac{\partial \vec{j}_{l,m}}{\partial \varepsilon} + \nabla_{\vec{r}} \cdot \vec{j}_{l,m} - \Gamma_{l,m} = W_{l,m}\{g\}$$

with

$$\vec{j}_{l,m}(\vec{r}, \varepsilon, t) = v(\varepsilon) \sum_{l',m'} \vec{a}_{l,m,l',m'} g_{l'.m'}(\vec{r}, \varepsilon, t)$$

The balance equations are coupled

Semiclassical transport

Spherical harmonics expansion of the Boltzmann equation

$$\frac{1}{(2\pi)^3} \int \delta\left(\varepsilon - \varepsilon(\vec{k})\right) Y_{l,m}(\vartheta, \varphi) \{\mathrm{BE}\} \, d^3k$$

yields balance equations over energy/real space

$$\frac{\partial g_{l,m}}{\partial t} - q\vec{E} \cdot \frac{\partial \vec{j}_{l,m}}{\partial \varepsilon} + \nabla_{\vec{r}} \cdot \vec{j}_{l,m} - \Gamma_{l,m} = W_{l,m}\{g\}$$

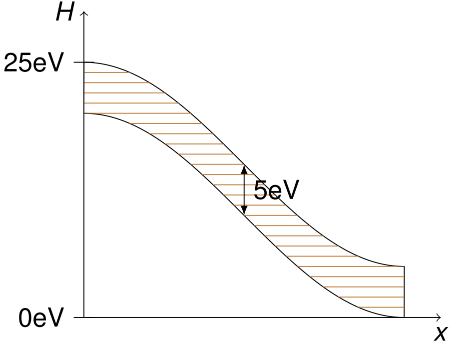
with

$$\vec{j}_{l,m}(\vec{r}, \varepsilon, t) = v(\varepsilon) \sum_{l',m'} \vec{a}_{l,m,l',m'} g_{l'.m'}(\vec{r}, \varepsilon, t)$$

The balance equations are coupled

Semiclassical transport

H-transform



$$H\left(\vec{r},\vec{k}\right)=\varepsilon\left(\vec{k}\right)-q\Psi\left(\vec{r}\right) \quad\Rightarrow\quad g'(\vec{r},H,t)=g(\vec{r},\varepsilon,t)$$

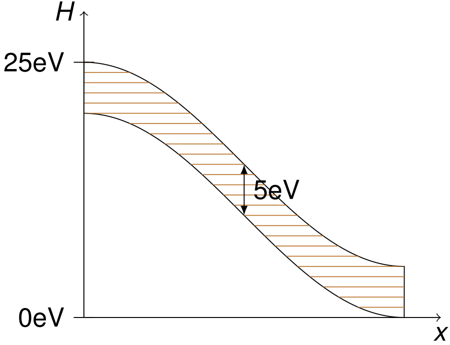
Cancels the energy derivative for the stationary state

$$\cancel{-q\vec{E}\cdot\frac{\partial\vec{j}'_{l,m}}{\partial\varepsilon}}+\nabla_{\vec{r}}\cdot\vec{j}'_{l,m}-\Gamma'_{l,m}=W_{l,m}\{g'\}$$

Captures ballistic transport

Semiclassical transport

H-transform



$$H\left(\vec{r},\vec{k}\right) = \varepsilon\left(\vec{k}\right) - q\Psi\left(\vec{r}\right) \quad \Rightarrow \quad g'(\vec{r},H,t) = g(\vec{r},\varepsilon,t)$$

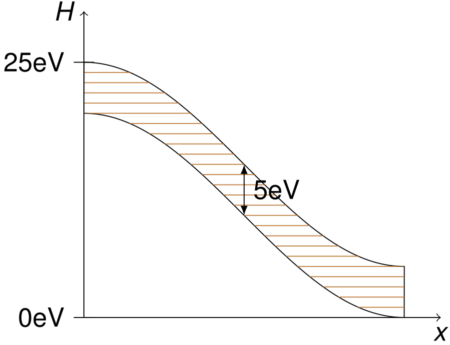
Cancels the energy derivative for the stationary state

$$\cancel{-q\vec{E}\cdot\frac{\partial \vec{j}'_{l,m}}{\partial\varepsilon}} + \nabla_{\vec{r}}\cdot\vec{j}'_{l,m} - \Gamma'_{l,m} = W_{l,m}\{g'\}$$

Captures ballistic transport

Semiclassical transport

H-transform



$$H\left(\vec{r},\vec{k}\right) = \varepsilon\left(\vec{k}\right) - q\Psi\left(\vec{r}\right) \quad \Rightarrow \quad g'(\vec{r},H,t) = g(\vec{r},\varepsilon,t)$$

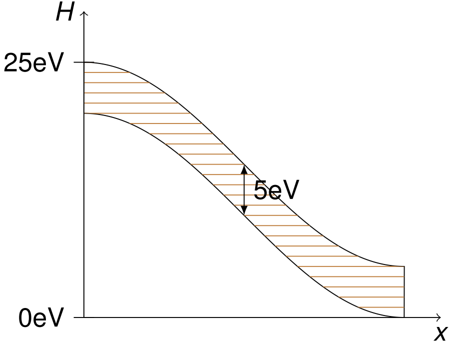
Cancels the energy derivative for the stationary state

$$\cancel{-q\vec{E}\cdot\frac{\partial \vec{j}'_{l,m}}{\partial\varepsilon}} + \nabla_{\vec{r}}\cdot\vec{j}'_{l,m} - \Gamma'_{l,m} = W_{l,m}\{g'\}$$

Captures ballistic transport

Semiclassical transport

H-transform



$$H\left(\vec{r},\vec{k}\right) = \varepsilon\left(\vec{k}\right) - q\Psi\left(\vec{r}\right) \quad \Rightarrow \quad g'(\vec{r},H,t) = g(\vec{r},\varepsilon,t)$$

Cancels the energy derivative for the stationary state

$$\cancel{-q\vec{E}\cdot\frac{\partial \vec{j'}_{l,m}}{\partial \varepsilon}} + \nabla_{\vec{r}}\cdot\vec{j'}_{l,m} - \Gamma'_{l,m} = W_{l,m}\{g'\}$$

Captures ballistic transport

Semiclassical transport

Numerics

- H-transform
- Maximum Entropy Dissipation Scheme
- Dimensional splitting
- Box Integration (exact particle number conservation)
- First order expansion has property M
- Newton-Raphson method to solve BE and PE self-consistently

Semiclassical transport

Numerics

- H-transform
- Maximum Entropy Dissipation Scheme
- Dimensional splitting
- Box Integration (exact particle number conservation)
- First order expansion has property M
- Newton-Raphson method to solve BE and PE self-consistently

Semiclassical transport

Numerics

- H-transform
- Maximum Entropy Dissipation Scheme
- Dimensional splitting
- Box Integration (exact particle number conservation)
- First order expansion has property M
- Newton-Raphson method to solve BE and PE self-consistently

Semiclassical transport

Numerics

- H-transform
- Maximum Entropy Dissipation Scheme
- Dimensional splitting
- Box Integration (exact particle number conservation)
- First order expansion has property M
- Newton-Raphson method to solve BE and PE self-consistently

Semiclassical transport

Numerics

- H-transform
- Maximum Entropy Dissipation Scheme
- Dimensional splitting
- Box Integration (exact particle number conservation)
- First order expansion has property M
- Newton-Raphson method to solve BE and PE self-consistently

Semiclassical transport

Numerics

- H-transform
- Maximum Entropy Dissipation Scheme
- Dimensional splitting
- Box Integration (exact particle number conservation)
- First order expansion has property M
- Newton-Raphson method to solve BE and PE self-consistently

Semiclassical transport

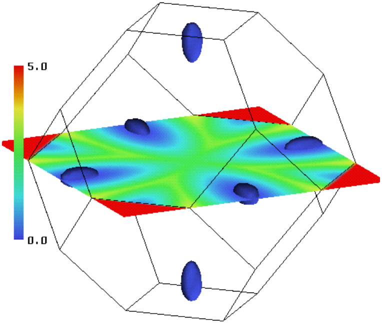
Numerics

- H-transform
- Maximum Entropy Dissipation Scheme
- Dimensional splitting
- Box Integration (exact particle number conservation)
- First order expansion has property M
- Newton-Raphson method to solve BE and PE self-consistently

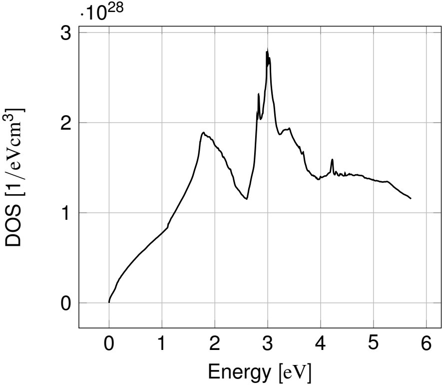
Semiclassical transport

Complex band structure effects

First conduction band of Si



Density of states of Si



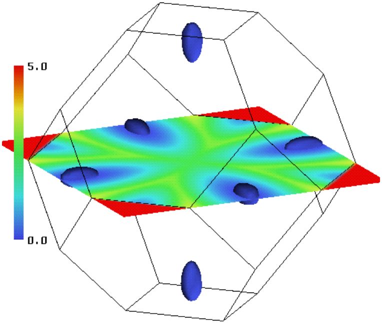
Calculated by the nonlocal empirical pseudopotential method

Only DOS and v^2 are required for SHE

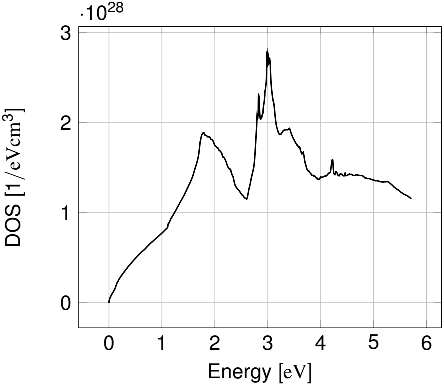
Semiclassical transport

Complex band structure effects

First conduction band of Si



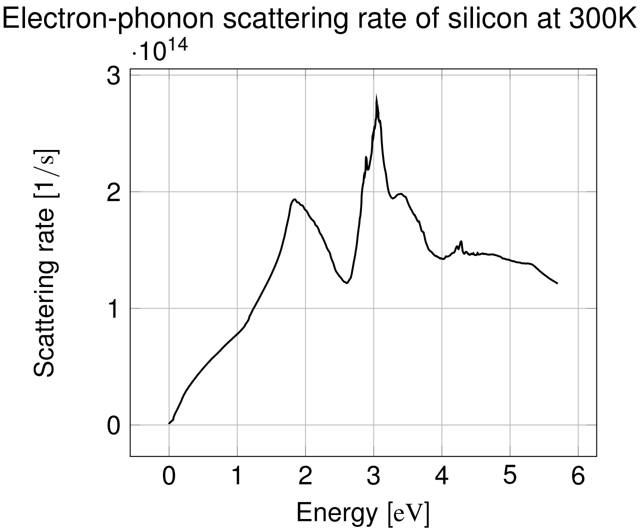
Density of states of Si



Calculated by the nonlocal empirical pseudopotential method

Only DOS and v^2 are required for SHE

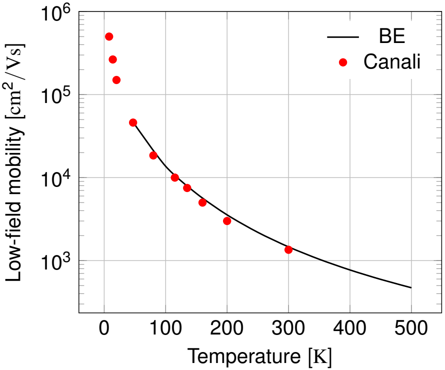
Semiclassical transport



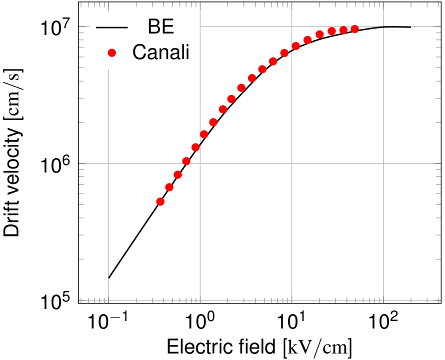
All parameters determined by theory or basic experiments

Semiclassical transport

Electron mobility



Electron velocity at 300K in $<111>$ direction

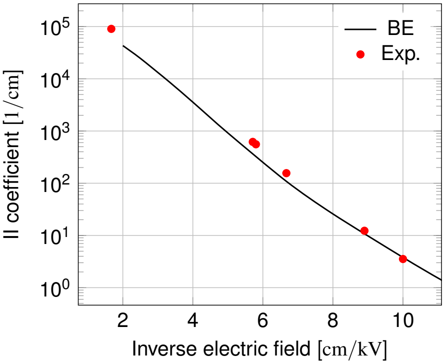


Good agreement between simulation and experiment for silicon

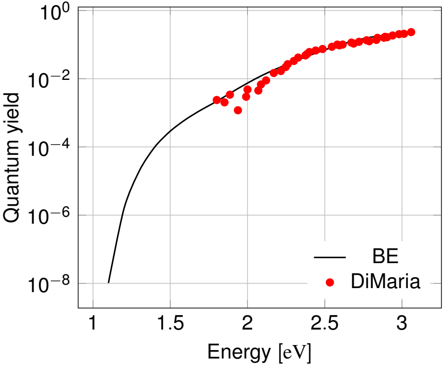
Semiclassical transport

Impact ionization

Ionization coefficient



Quantum yield



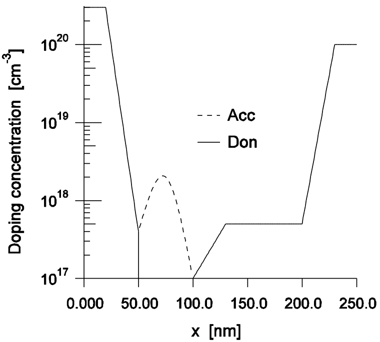
Good agreement between simulation and experiment for silicon

Results

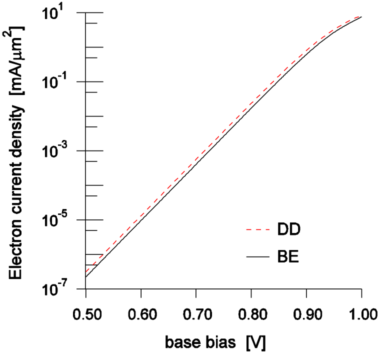
Bipolar transistor

Bipolar transistor

Doping profile



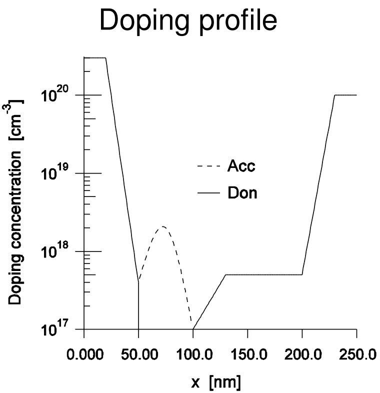
Collector current

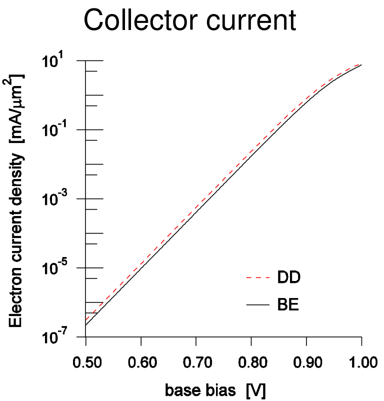


SHE can handle high doping concentrations without problems

SHE can handle small currents without problems

Bipolar transistor



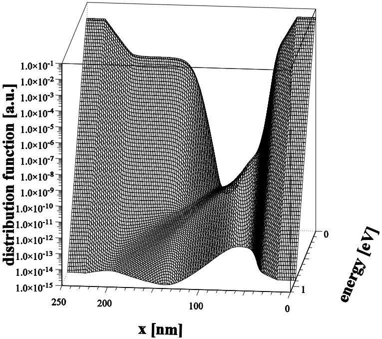


SHE can handle high doping concentrations without problems

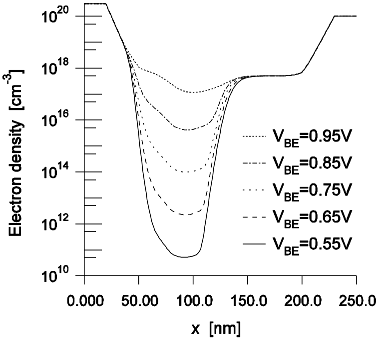
SHE can handle small currents without problems

Bipolar transistor

$V_{BE} = 0.55V,\ V_{CE} = 0.5V$
Energy distribution function



$V_{CE} = 0.5V$
Electron density



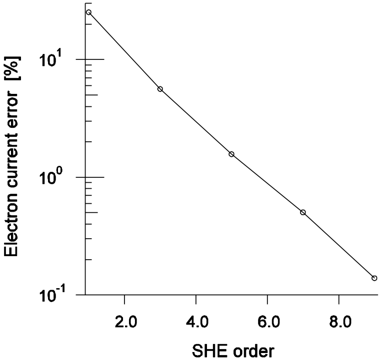
SHE can handle huge variations in the density without problems

Bipolar transistor

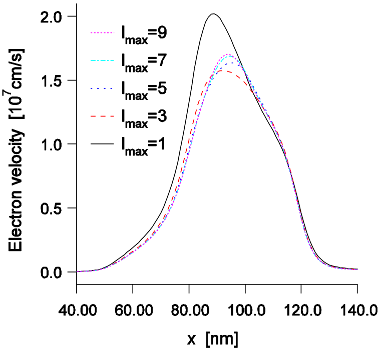
Dependence on the maximum order of SHE

$V_{BE} = 0.85\,V,\ V_{CE} = 0.5\,V$

Error in current



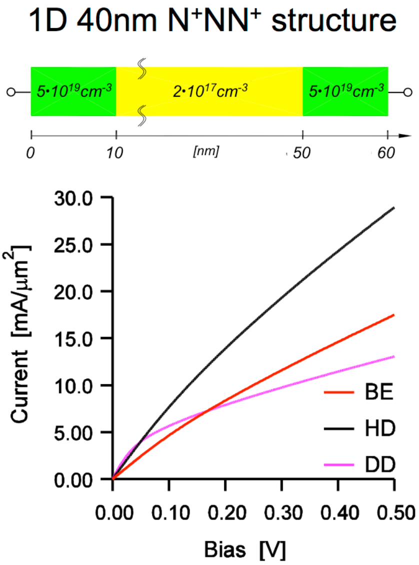
Electron velocity



Transport in nanometric devices requires at least 5th order SHE

N^+NN^+ structure

N^+NN^+ structure



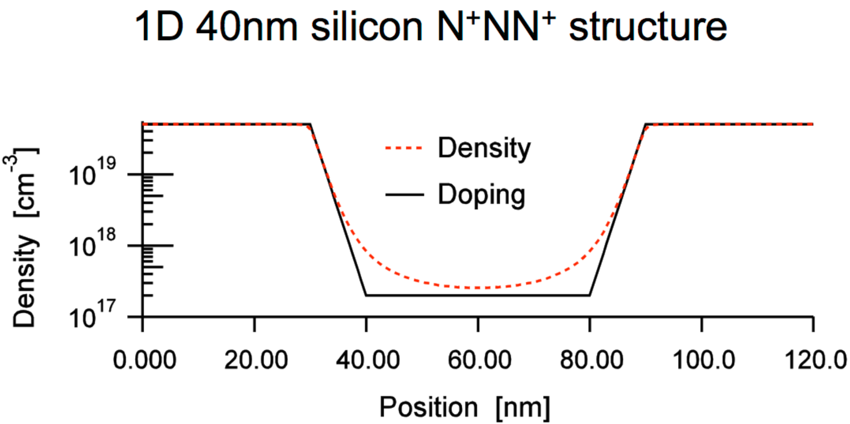
- Macroscopic models (DD, HD) fail for strong nonequilibrium due to

Ballistic transport!

- Macroscopic models also fail **near** equilibrium in nanometric devices!

Why?

N^+NN^+ structure



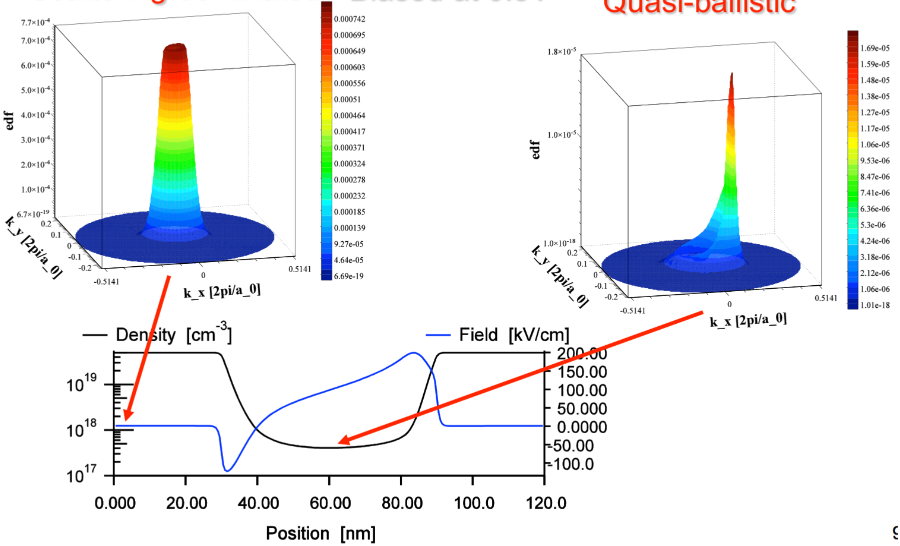
Transport is in x-direction

N^+NN^+ structure

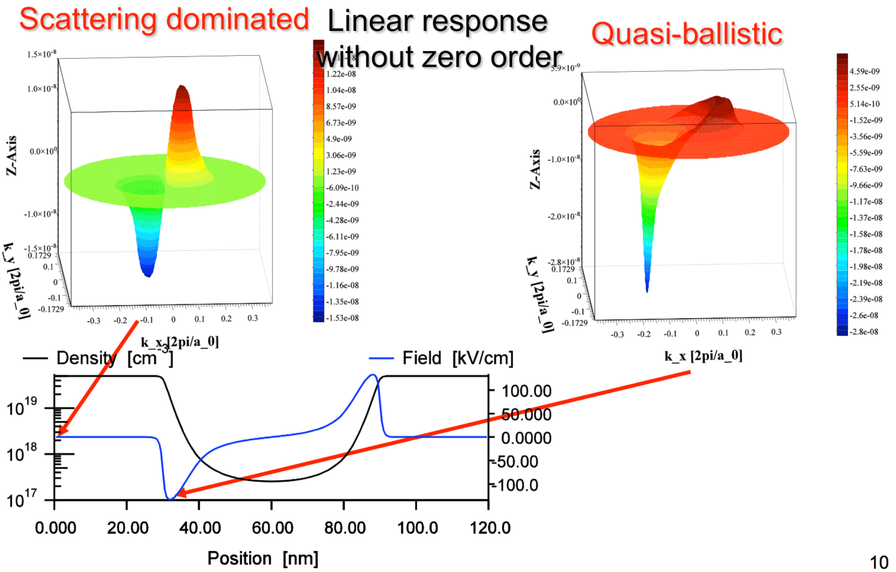
Scattering dominated

Biased at 0.5V

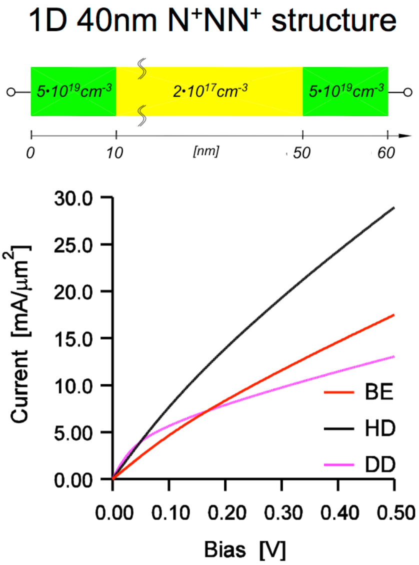
Quasi-ballistic



N^+NN^+ structure



N^+NN^+ structure

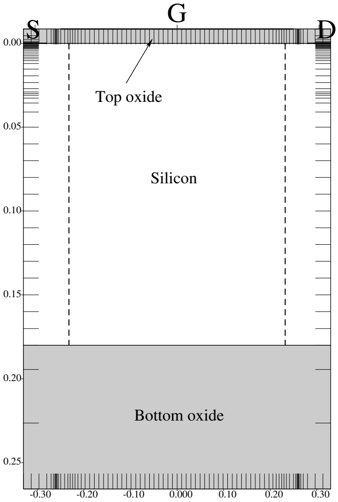


- Macroscopic models (DD, HD) fail for strong nonequilibrium due to

Ballistic transport!

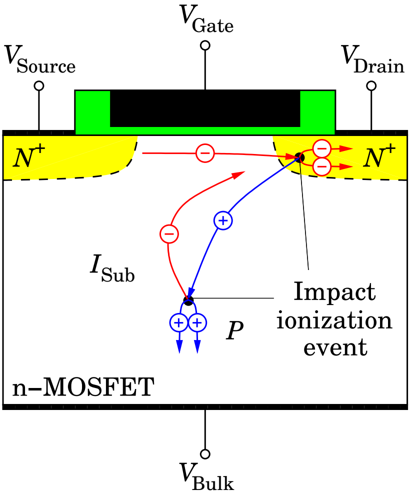
- Macroscopic models also fail **near** equilibrium in nanometric devices!

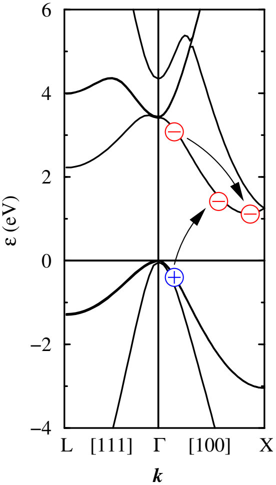
Why?



Partially depleted SOI NMOSFET

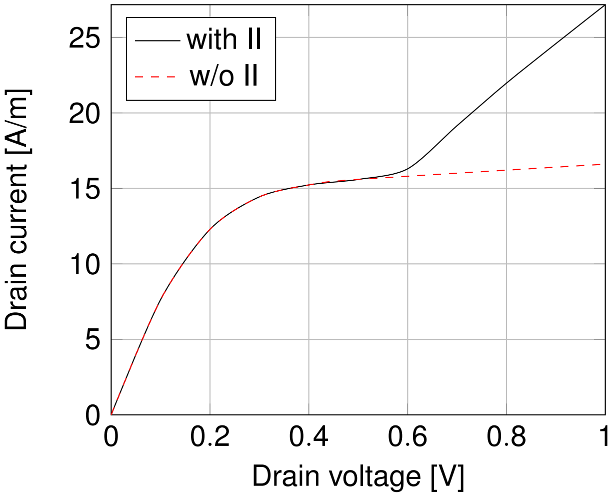
PDSOI NMOSFET





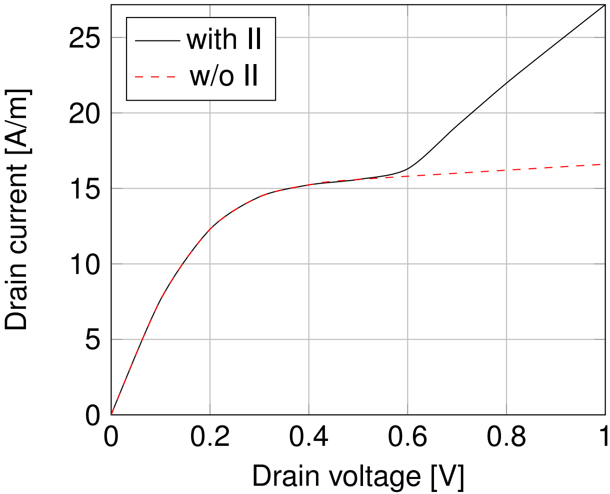
Every impact ionization event generates a secondary electron/hole pair

PDSOI NMOSFET



Kink effect due to impact ionization (II) ($V_{\text{gate}} = 1.0\,V$)

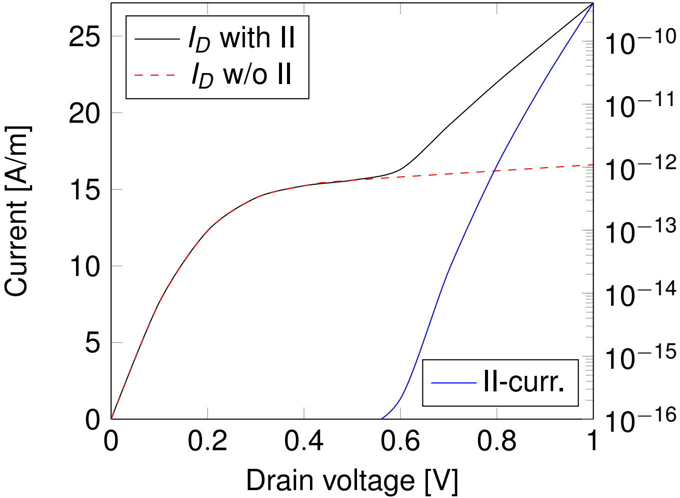
PDSOI NMOSFET



Kink effect due to impact ionization (II) ($V_{\text{gate}} = 1.0\,V$)

Exact stationary solutions

PDSOI NMOSFET

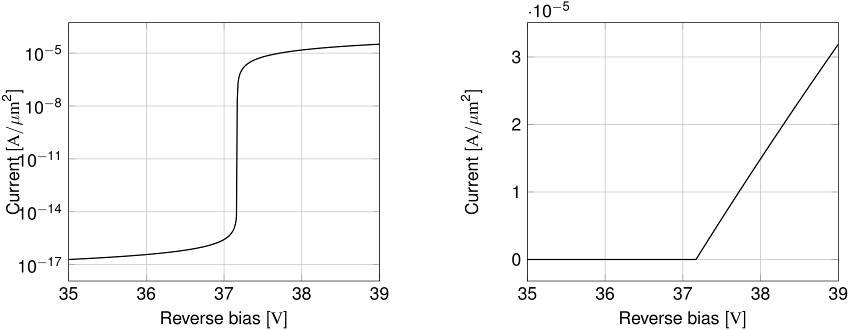


About 17 orders of magnitude difference in currents at kink

pn Junction

pn Junction

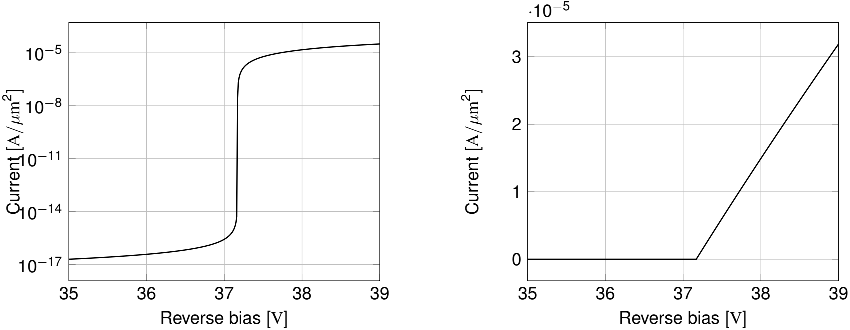
Simulation of avalanche breakdown



Extremely steep increase of current with voltage (20μV/dec)

pn Junction

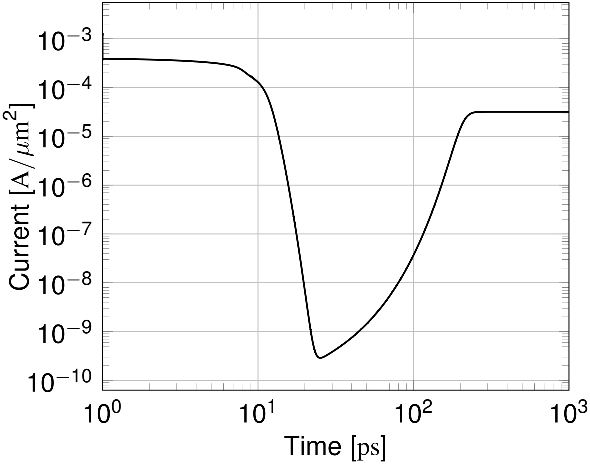
Simulation of avalanche breakdown



Extremely steep increase of current with voltage (20μV/dec)

pn Junction

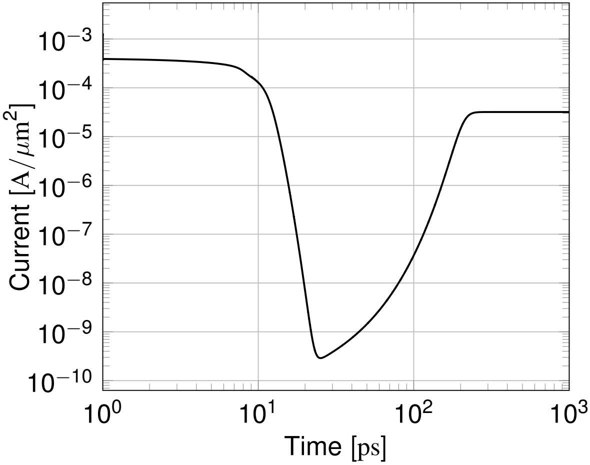
Transient DD simulation of switching a silicon pn-diode from 0 to -39V



Avalanche breakdown is slow!

pn Junction

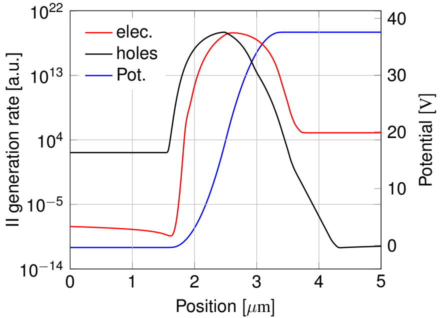
Transient DD simulation of switching a silicon pn-diode from 0 to -39V

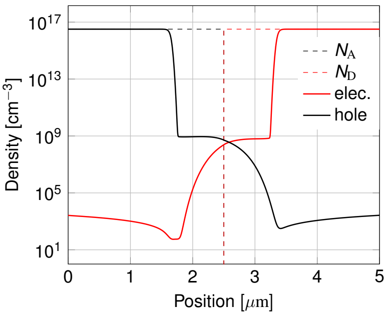


Avalanche breakdown is slow!

pn Junction

Simulation for 37.172V and 10pA/μm^2

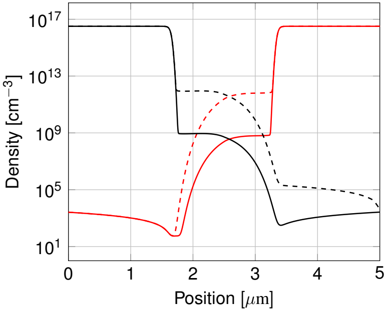


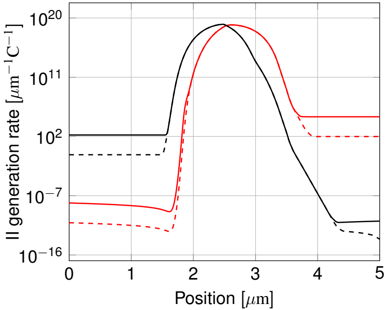


II generation increases number of particles in the space charge region

pn Junction

Increase of current by a factor of 1000 (dashed lines)





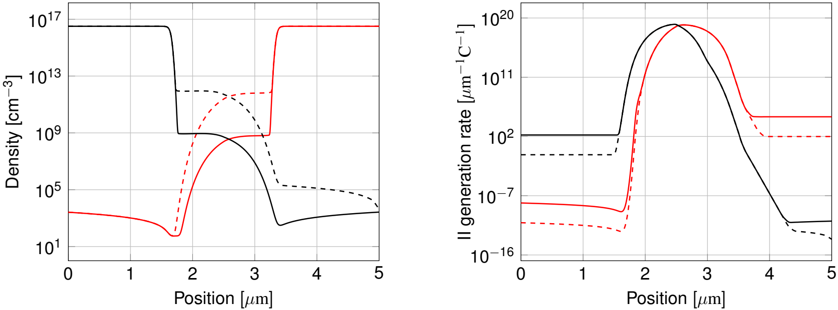
Particle density in the space charge region increases 1000 times

Relevant II generation rate scales with current

Hot electron/hole effects scale with current

pn Junction

Increase of current by a factor of 1000 (dashed lines)



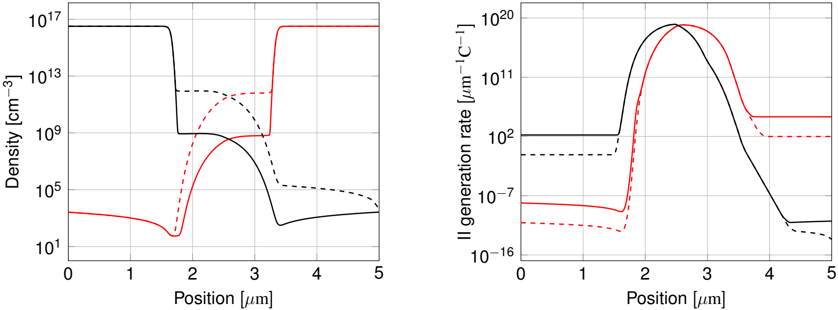
Particle density in the space charge region increases 1000 times

Relevant II generation rate scales with current

Hot electron/hole effects scale with current

pn Junction

Increase of current by a factor of 1000 (dashed lines)



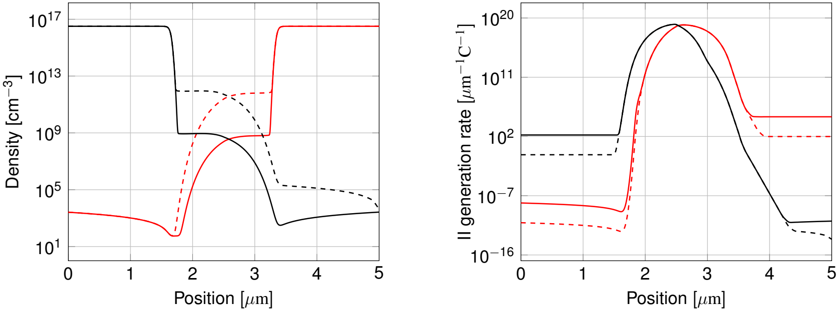
Particle density in the space charge region increases 1000 times

Relevant II generation rate scales with current

Hot electron/hole effects scale with current

pn Junction

Increase of current by a factor of 1000 (dashed lines)



Particle density in the space charge region increases 1000 times

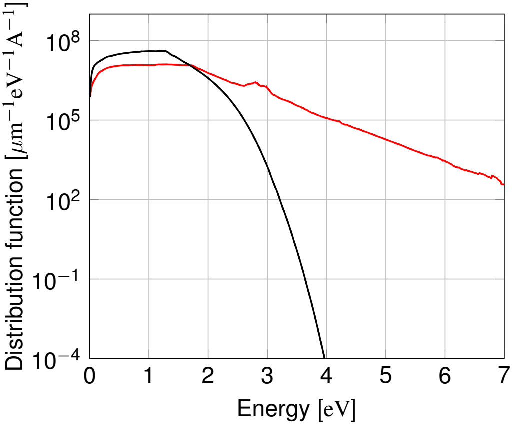
Relevant II generation rate scales with current

Hot electron/hole effects scale with current

pn Junction

Increase of current by a factor of 1000 (dashed lines)

Scaled electron/hole distribution function in the middle of the pn junction

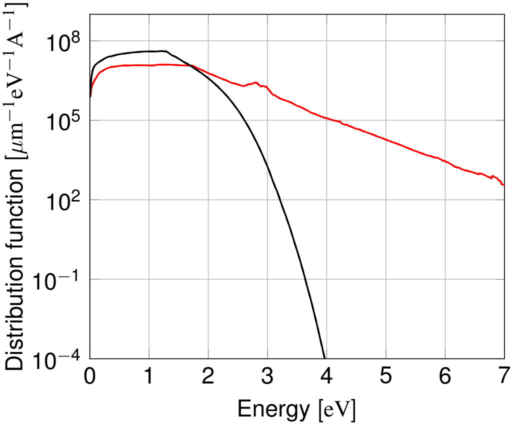


Hot electron/hole effects scale with current

pn Junction

Increase of current by a factor of 1000 (dashed lines)

Scaled electron/hole distribution function in the middle of the pn junction



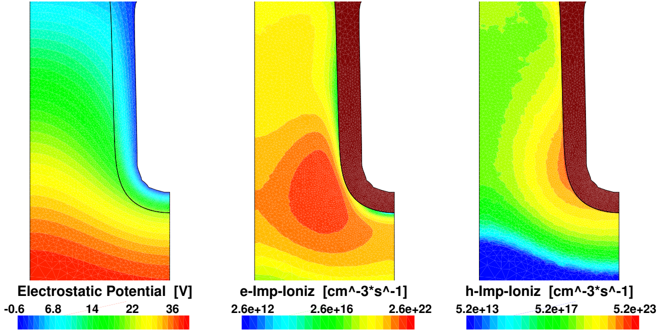
Hot electron/hole effects scale with current

Vertical power transistor

Power MOSFET

Avalanche breakdown of a power transistor

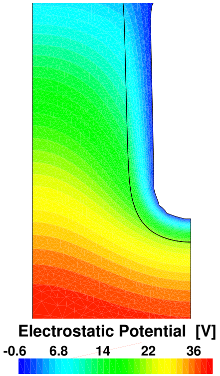
BE simulation for 35.83V and 10pA/μm^2

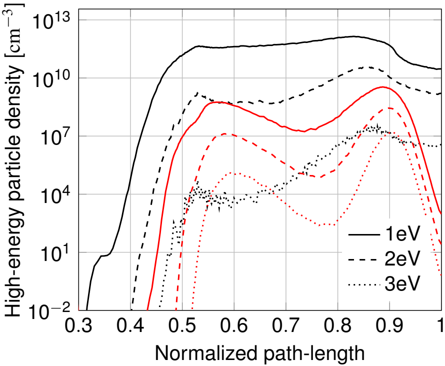


$45 \cdot 10^6$ variables, 2 CPU hours

Power MOSFET

BE simulation for 35.83V and 10pA/μm^2





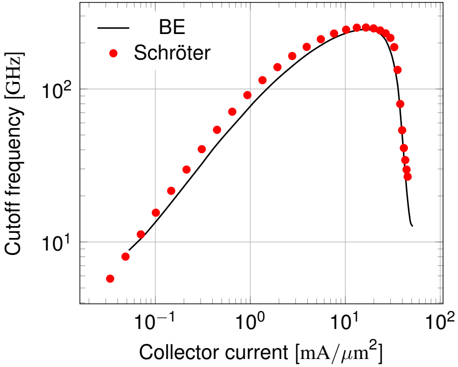
Injection of electrons and holes into the oxide can be calculated

Structure, DC and AC behavior of the npn THz SiGe HBT

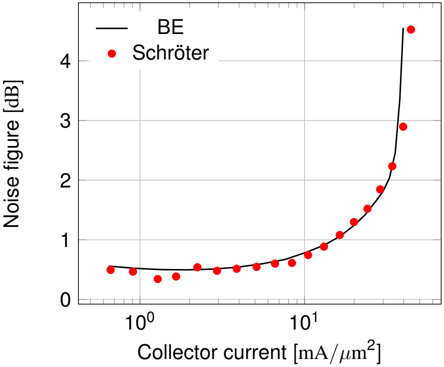
Comparison with experiments

Comparison for an ST-Microelectronics SiGe HBT
at 10GHz and $V_{\mathrm{CE}} = 1.2\mathrm{V}$

Cutoff frequency

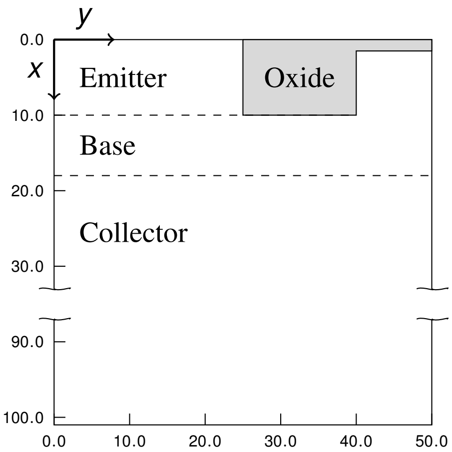


Minimum noise figure



Good agreement between simulation and measurement

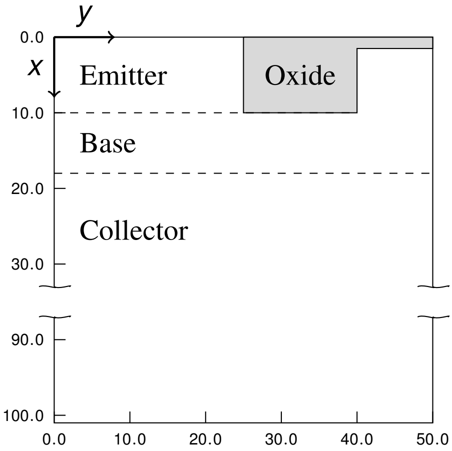
Device structure



Emitter-window width: 2 $\times$ 25nm

- 149 nodes in *x*-direction
- 20 nodes in *y*-direction
- 5th order SHE expansion (21 spherical harmonics)
- Up to $1.42 \cdot 10^8$ unknown variables (spacing in energy is 5.17meV and number of energy grid points depends on bias)
- Over 200 GB of memory required (for AC)
- Up to 10^5 CPU-seconds for a DC point

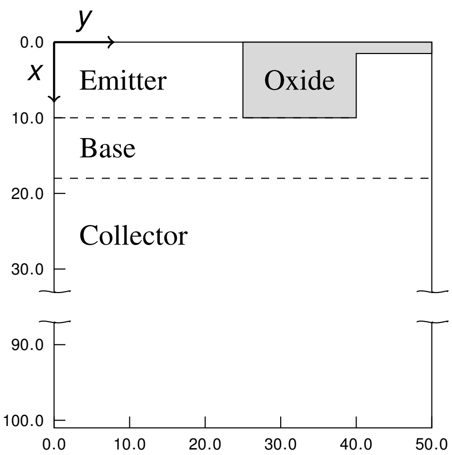
Device structure



Emitter-window width: 2 × 25nm

- 149 nodes in x-direction
- 20 nodes in y-direction
- 5th order SHE expansion (21 spherical harmonics)
- Up to $1.42 \cdot 10^8$ unknown variables (spacing in energy is 5.17meV and number of energy grid points depends on bias)
- Over 200 GB of memory required (for AC)
- Up to 10^5 CPU-seconds for a DC point

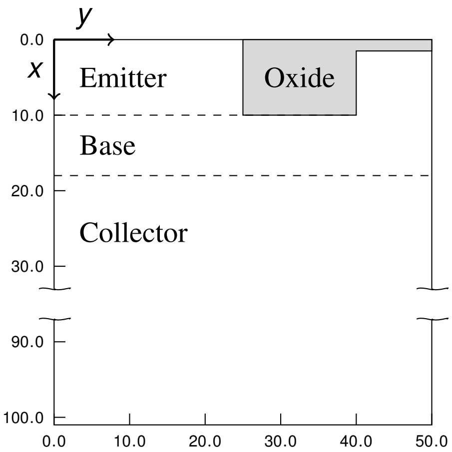
Device structure



Emitter-window width: 2×25nm

- 149 nodes in x-direction
- 20 nodes in y-direction
- 5th order SHE expansion (21 spherical harmonics)
- Up to $1.42 \cdot 10^8$ unknown variables (spacing in energy is 5.17meV and number of energy grid points depends on bias)
- Over 200 GB of memory required (for AC)
- Up to 10^5 CPU-seconds for a DC point

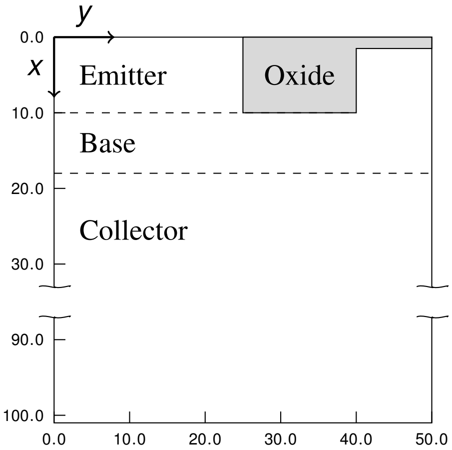
Device structure



Emitter-window width: 2×25nm

- 149 nodes in x-direction
- 20 nodes in y-direction
- 5th order SHE expansion (21 spherical harmonics)
- Up to $1.42 \cdot 10^8$ unknown variables (spacing in energy is 5.17meV and number of energy grid points depends on bias)
- Over 200 GB of memory required (for AC)
- Up to 10^5 CPU-seconds for a DC point

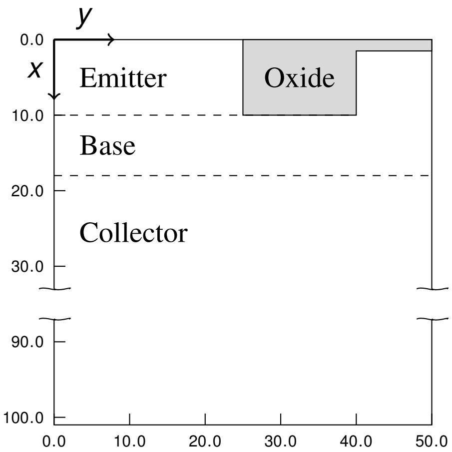
Device structure



Emitter-window width: 2 × 25nm

- 149 nodes in x-direction
- 20 nodes in y-direction
- 5th order SHE expansion (21 spherical harmonics)
- Up to $1.42 \cdot 10^8$ unknown variables (spacing in energy is 5.17meV and number of energy grid points depends on bias)
- Over 200 GB of memory required (for AC)
- Up to 10^5 CPU-seconds for a DC point

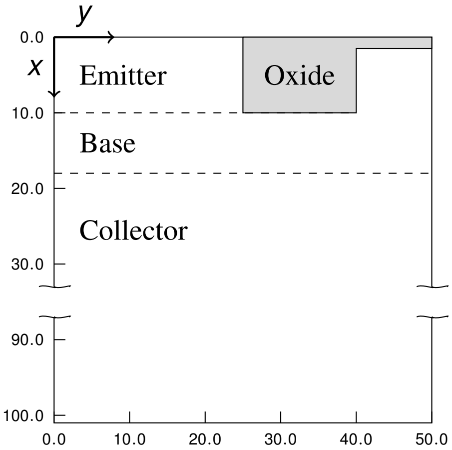
Device structure



Emitter-window width: 2×25nm

- 149 nodes in x-direction
- 20 nodes in y-direction
- 5th order SHE expansion (21 spherical harmonics)
- Up to $1.42 \cdot 10^8$ unknown variables (spacing in energy is 5.17meV and number of energy grid points depends on bias)
- Over 200 GB of memory required (for AC)
- Up to 10^5 CPU-seconds for a DC point

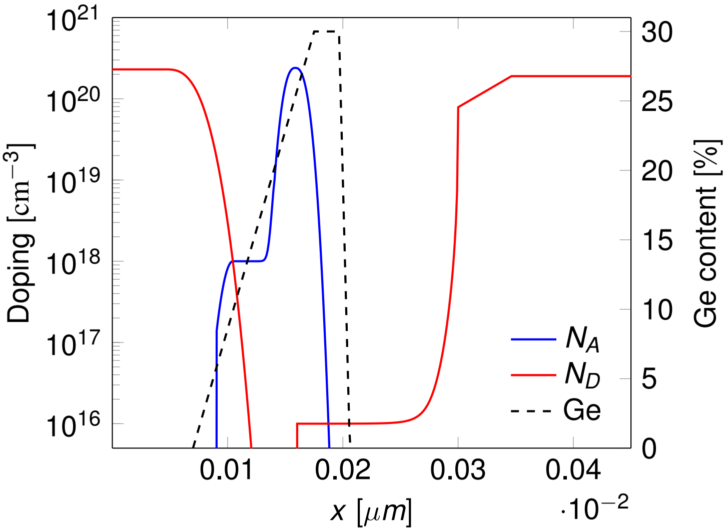
Device structure



Emitter-window width: 2×25nm

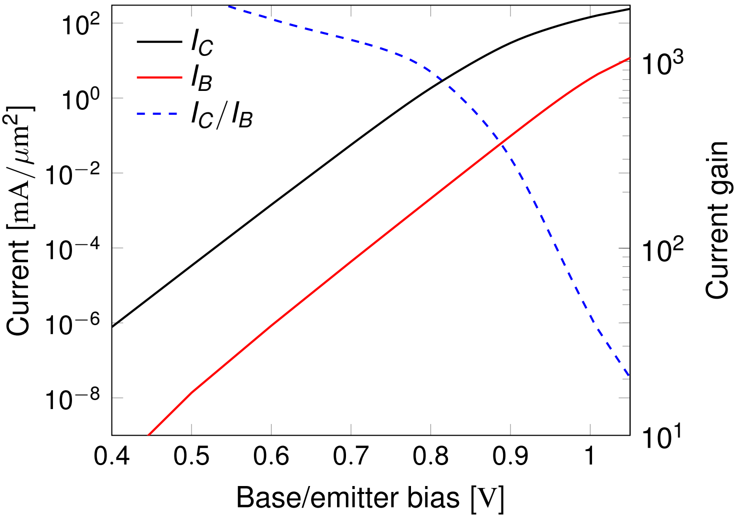
- 149 nodes in x-direction
- 20 nodes in y-direction
- 5th order SHE expansion (21 spherical harmonics)
- Up to $1.42 \cdot 10^8$ unknown variables (spacing in energy is 5.17meV and number of energy grid points depends on bias)
- Over 200 GB of memory required (for AC)
- Up to 10^5 CPU-seconds for a DC point

Doping and germanium profile



Base thickness: 7nm

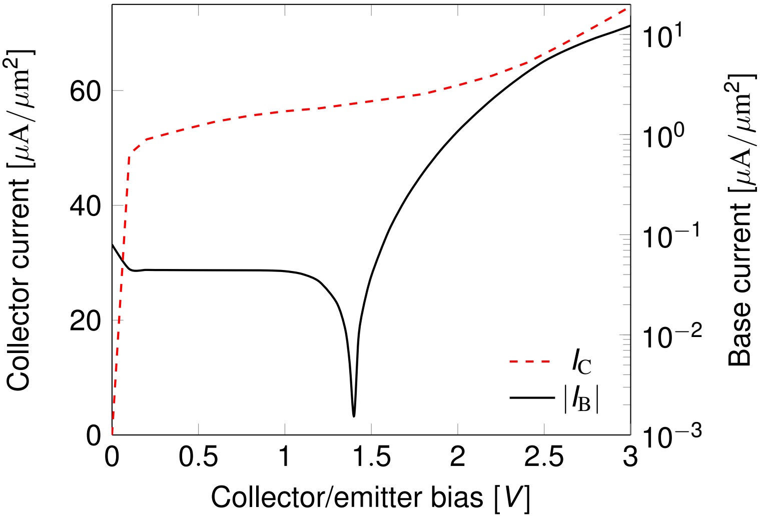
Input characteristic



$V_{\mathrm{CE}} = 1.0\mathrm{V}$

No SRH recombination

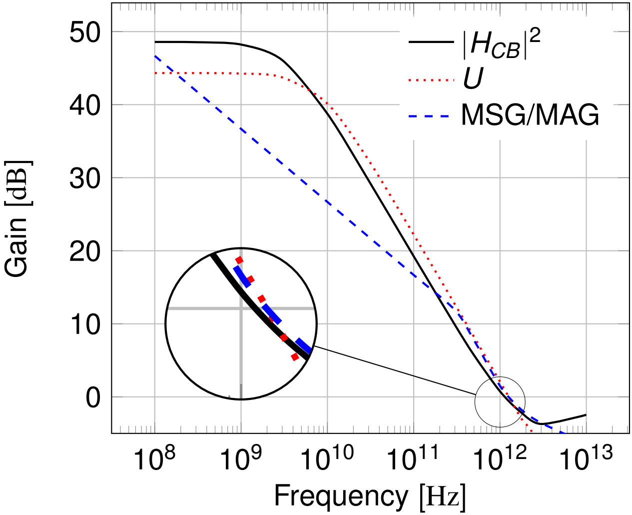
Output characteristic



$$V_{BE} = 0.7V$$

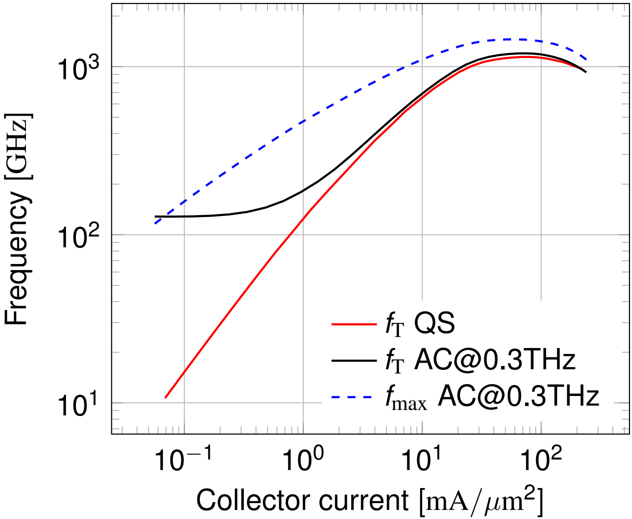
$$BV_{CE0} = 1.4V$$

Gains



$V_{BE} = 0.88\text{V}$, $V_{CE} = 1.0\text{V}$, $I_C = 18.2\text{mA}/\mu\text{m}^2$

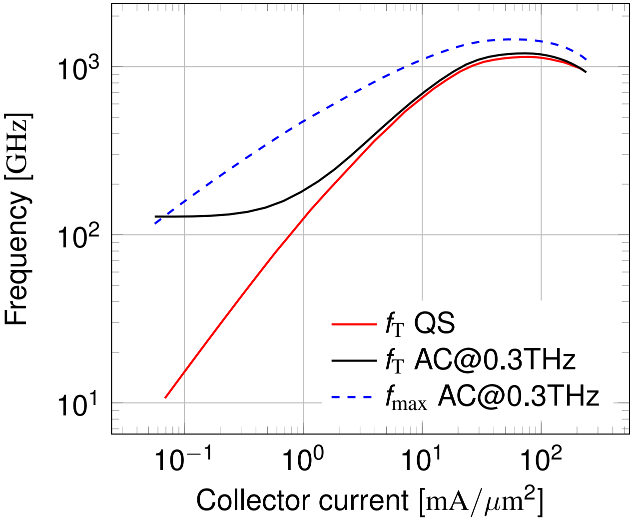
Cutoff and max. oscil. frequencies



$V_{CE} = 1.0V$, f_{max} by extrapolation of U

peak $f_T = 1.2$THz, peak $f_{max} = 1.45$THz

Cutoff and max. oscil. frequencies

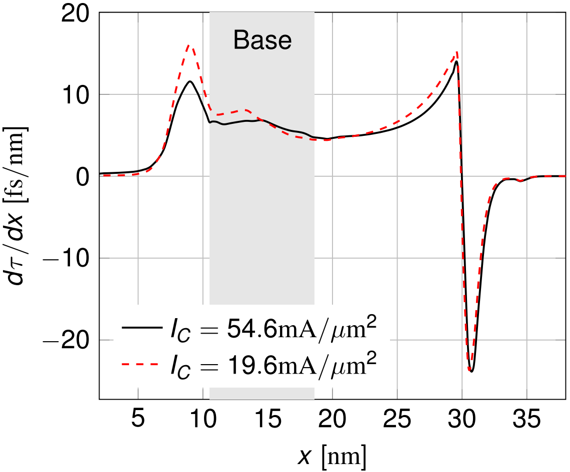


$V_{CE} = 1.0\mathrm{V}$, f_{max} by extrapolation of U

peak $f_T = 1.2$THz, peak $f_{max} = 1.45$THz

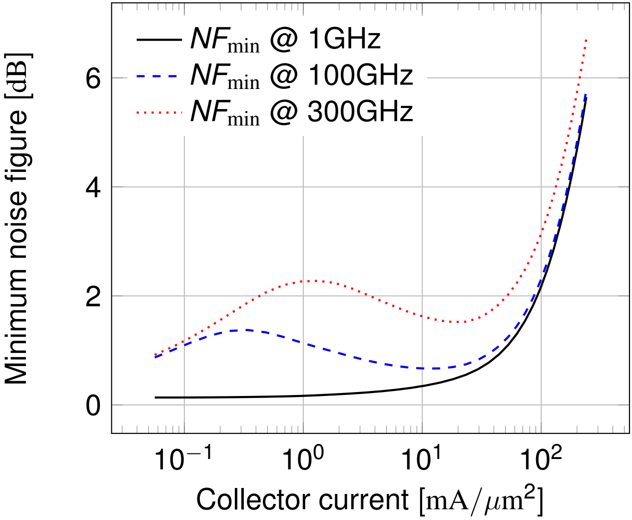
Local contribution to the transit time

$$f_{\mathrm{T}} = \frac{1}{2\pi\tau}\ , \quad \tau = \int \frac{d\tau}{dx} dx$$



$V_{\mathrm{CE}} = 1.0\mathrm{V}$

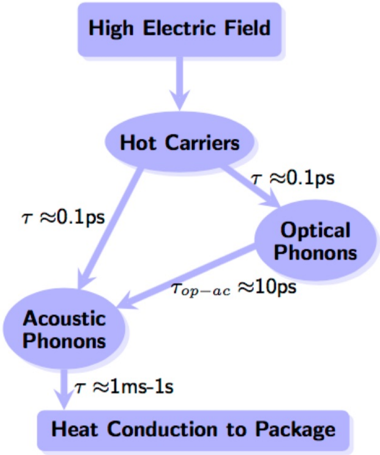
Minimum noise figure

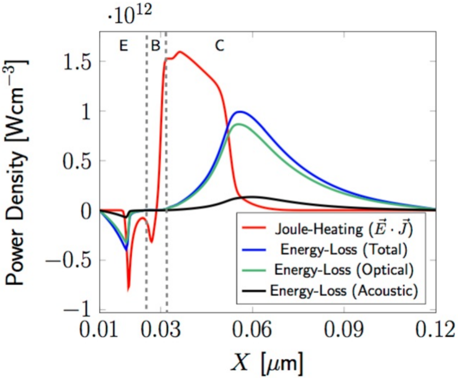


$V_{\mathrm{CE}} = 1.0\mathrm{V}$

Electrothermal Transport

High power densities lead to self-heating



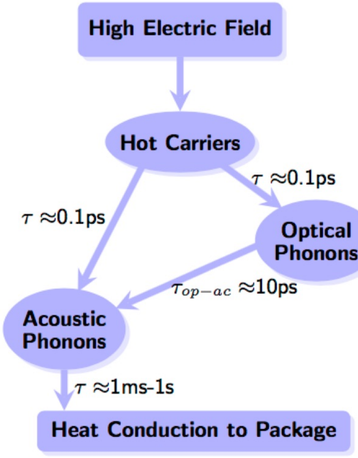


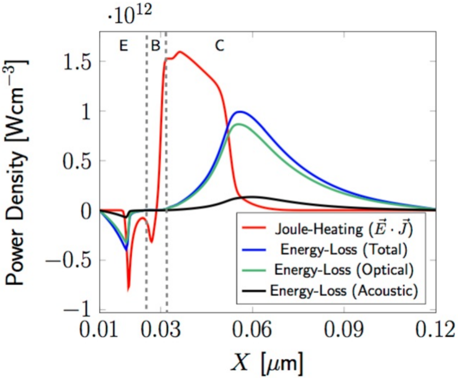
Spatial distribution of power density for V_{CB}=0.6V, and V_{BE}=0.9V.

Heating is non-local!

Electrothermal Transport

High power densities lead to self-heating

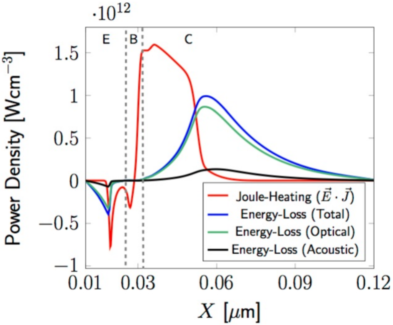




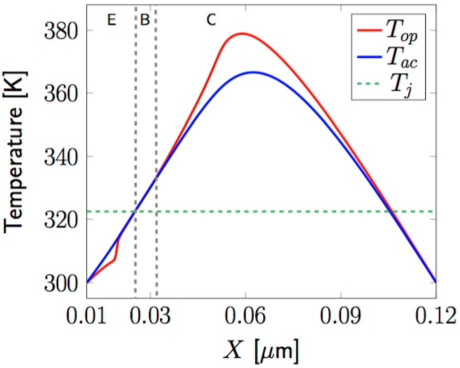
Spatial distribution of power density for V_{CB}=0.6V, and V_{BE}=0.9V.

Heating is non-local!

Electrothermal Transport



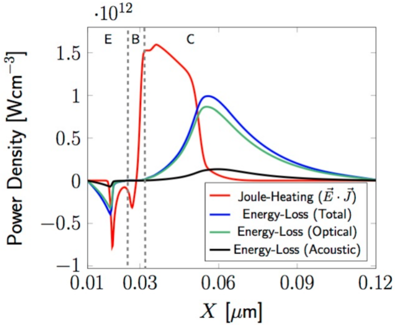
Spatial distribution of power density for V_{CB}=0.6V, and V_{BE}=0.9V.



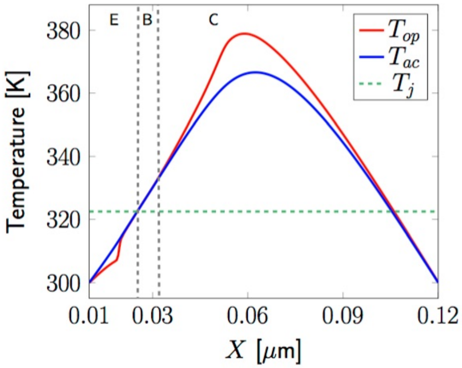
Dirichlet boundary conditions

Scattering between optical and acoustic phonons goes both ways

Electrothermal Transport



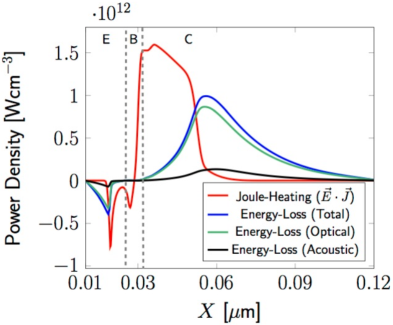
Spatial distribution of power density for V_{CB}=0.6V, and V_{BE}=0.9V.



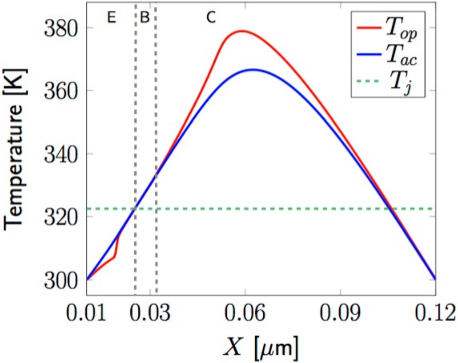
Dirichlet boundary conditions

Scattering between optical and acoustic phonons goes both ways

Electrothermal Transport



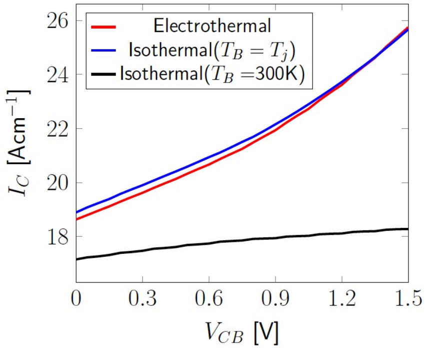
Spatial distribution of power density for V_{CB}=0.6V, and V_{BE}=0.9V.



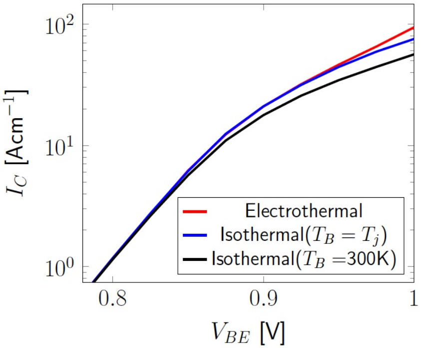
Dirichlet boundary conditions

Scattering between optical and acoustic phonons goes both ways

Electrothermal Transport



I_C-V_{CB} characteristic for V_{BE}=0.9V.

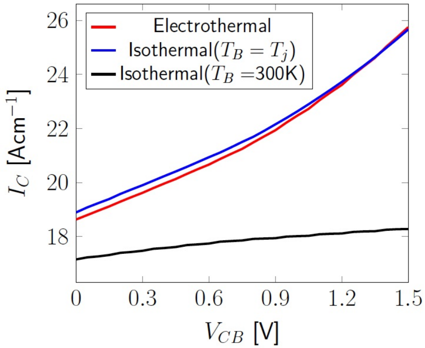


I_C-V_{BE} characteristic for V_{CB}=0.6V.

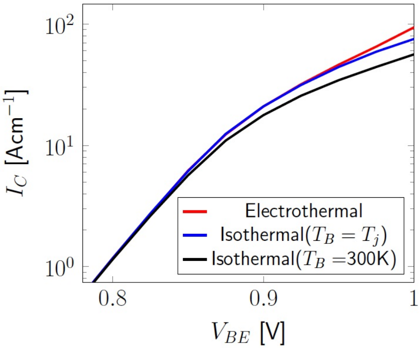
Junction temperature determines the current

Self-heating can lead to thermal runaway

Electrothermal Transport



I_C-V_{CB} characteristic for V_{BE}=0.9V.

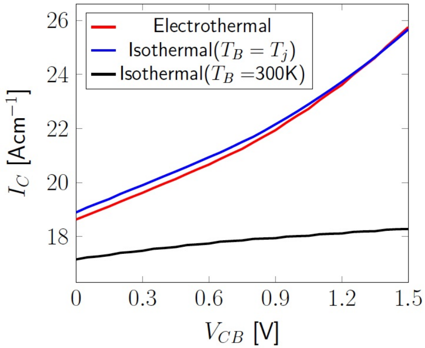


I_C-V_{BE} characteristic for V_{CB}=0.6V.

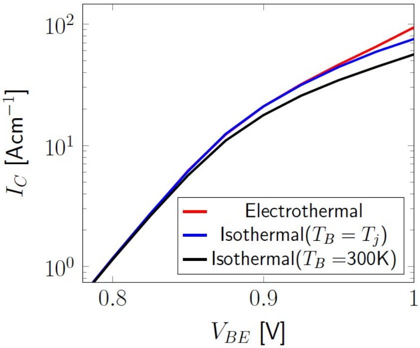
Junction temperature determines the current

Self-heating can lead to thermal runaway

Electrothermal Transport



I_C-V_{CB} characteristic for V_{BE}=0.9V.



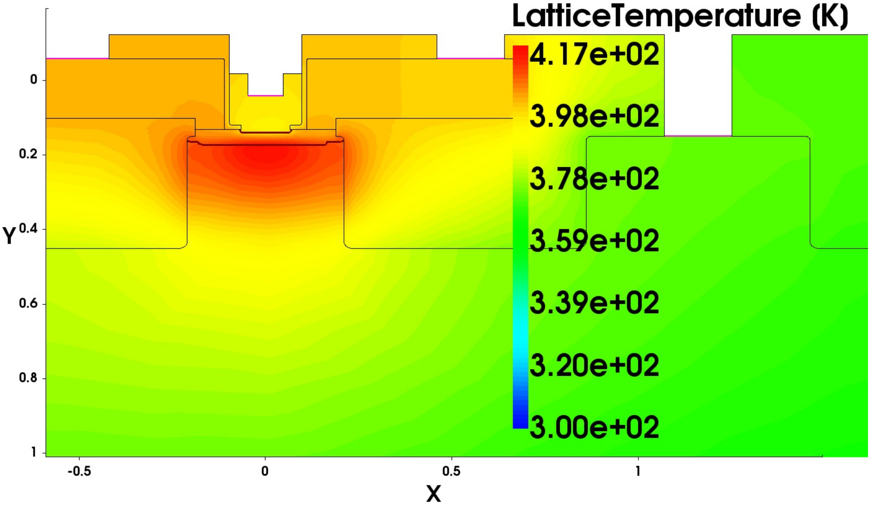
I_C-V_{BE} characteristic for V_{CB}=0.6V.

Junction temperature determines the current

Self-heating can lead to thermal runaway

Electrothermal Transport

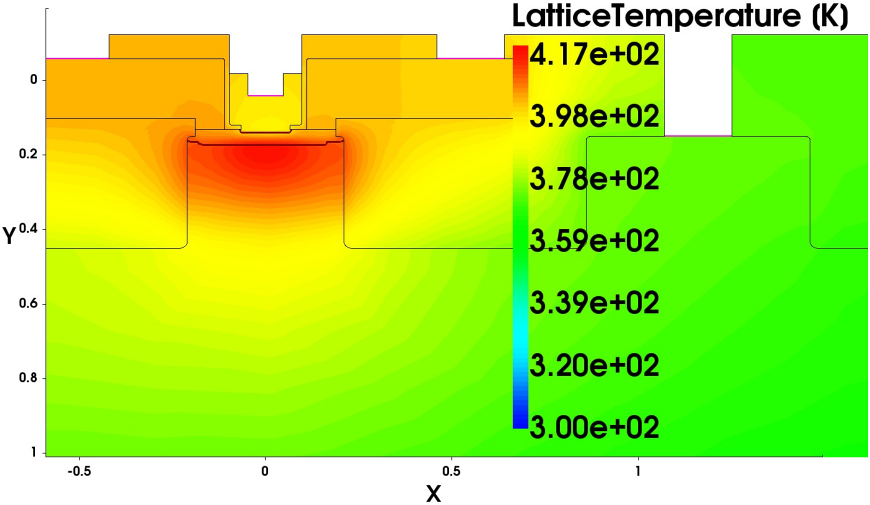
2D electrothermal simulation with SHE



Exact thermal simulation requires 3D simulation including metalization

Electrothermal Transport

2D electrothermal simulation with SHE



Exact thermal simulation requires 3D simulation including metalization

Conclusions

Conclusions

- Semiclassical simulations give detailed physics at the price of high CPU times and a 2D real space
- Various effects can be included at a microscopic level
- DC, AC and noise analysis
- Device degradation, self-heating, mechanical strain, ...
- Transport at the nanoscale is very complex

Conclusions

- Semiclassical simulations give detailed physics at the price of high CPU times and a 2D real space
- Various effects can be included at a microscopic level
- DC, AC and noise analysis
- Device degradation, self-heating, mechanical strain, ...
- Transport at the nanoscale is very complex

Conclusions

- Semiclassical simulations give detailed physics at the price of high CPU times and a 2D real space
- Various effects can be included at a microscopic level
- DC, AC and noise analysis
- Device degradation, self-heating, mechanical strain, ...
- Transport at the nanoscale is very complex

Conclusions

- Semiclassical simulations give detailed physics at the price of high CPU times and a 2D real space
- Various effects can be included at a microscopic level
- DC, AC and noise analysis
- Device degradation, self-heating, mechanical strain, ...
- Transport at the nanoscale is very complex

Conclusions

- Semiclassical simulations give detailed physics at the price of high CPU times and a 2D real space
- Various effects can be included at a microscopic level
- DC, AC and noise analysis
- Device degradation, self-heating, mechanical strain, ...
- Transport at the nanoscale is very complex

Conclusions

- Semiclassical simulations give detailed physics at the price of high CPU times and a 2D real space
- Various effects can be included at a microscopic level
- DC, AC and noise analysis
- Device degradation, self-heating, mechanical strain, ...
- Transport at the nanoscale is very complex