Modeling of electronic properties of interfaces in solar cells

Annegret Glitzky and Alexander Mielke

Funding period 06/2010 - 05/2014
Requested funding: 1 position

DFG Research Center MATHEON
Mathematics for key technologies

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Aim / topic / background of project

In 2008, MATHEON has started activities in PhotoVoltaics

Technologies of Thin-Film Solar Cells
Org.: A. Münch, B. Wagner, V. Mehrmann, B. Rech (HZB)
Industry partners: Leybold Optics, Carl Zeiss AG, Schott AG, IBM.

Participation in PVcomB

Competence center for thin-film and nanotechnology for photovoltaics Berlin
• HZB, TUB, FHTW, MATHEON, IHP, U Potsdam, FZ Jülich
• V. Mehrmann, A. Mielke, F. Schmidt, B. Wagner
• Exp. budget: 18 M € for five years, including
• 3 positions for Mathematical Methods in Photovoltaics

Present proposal:
Improve mathematical modeling in cooperation with HZB
Technological aims in photovoltaics:
- maximize efficiency of the solar cells
- minimize production costs, ...

Principle of solar cells:
- Photons generate electron-hole pairs
- electrons/holes move to contacts
  → minimize recombination losses
**Aim / topic / background of project**

**Technological aims in photovoltaics:**
- maximize efficiency of the *solar cells*
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**Principle of solar cells:**
- Photons generate electron-hole pairs
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  ⇝ minimize recombination losses

At *heterointerfaces* new electrical effects may occur:
- electrons, holes are transmitted/reflected
- technological treatment of interfaces leads to defect distributions
- special recombination at defects
- quantum mechanical tunneling effects

⇝ new mathematical models required!
Contributions of the principal investigator

RG 1 of WIAS:

Analytical treatment of semiconductor models
Numerical simulation of semiconductor devices
Multiscale modeling, homogenization, dimension reduction

A. Mielke:

Multiscale modelling for evolutionary problems
Abstract existence results for geometric gradient flows
Γ convergence applied to evolutionary problems

A. Glitzky:

Analysis and numerical analysis for
Spin-polarized drift-diffusion models
Electro-reaction-diffusion systems
Energy models for semiconductor devices
WIAS-TeSCA simulations of semiconductor lasers

Modeling of electronic properties of interfaces in solar cells
(1) Modeling and analysis of nontrivial interface conditions

**Equations in the bulk** for \( n, p, \varphi, \eta = \text{defect-occupation probability} \)

\[
\frac{\partial}{\partial t} n - \text{div} \left( c_n (\nabla n - n \nabla \varphi) \right) = G_{\text{phot}}(t, x) - \langle \rho_n(\ldots, n, \eta) \rangle - R(n, p),
\]

\[
\frac{\partial}{\partial t} p - \text{div} \left( c_p (\nabla p + p \nabla \varphi) \right) = G_{\text{phot}}(t, x) - \langle \rho_p(\ldots, p, \eta) \rangle - R(n, p),
\]

\[-\text{div}(\varepsilon(x) \nabla \varphi) = d_{\text{dop}}(x) + p - n - \langle \eta \rangle \quad \text{where} \quad \langle g \rangle := \int_{E_V}^{E_C} g(E) N(x, E) \, dE\]

\[
\frac{\partial}{\partial t} \eta(t, x, E) = \rho_n(x, E, n, \eta) - \rho_p(x, E, p, \eta).
\]
(1) Modeling and analysis of nontrivial interface conditions

Equations in the bulk for \( n, p, \varphi, \eta = \text{defect-occupation probability} \)

\[
\begin{align*}
\frac{\partial}{\partial t} n - \text{div} \left( c_n (\nabla n - n \nabla \varphi) \right) &= G_{\text{phot}}(t, x) - \langle \rho_n(\ldots, n, \eta) \rangle - R(n, p), \\
\frac{\partial}{\partial t} p - \text{div} \left( c_p (\nabla p + p \nabla \varphi) \right) &= G_{\text{phot}}(t, x) - \langle \rho_p(\ldots, p, \eta) \rangle - R(n, p), \\
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\end{align*}
\]

\[
\frac{\partial}{\partial t} \eta(t, x, E) = \rho_n(x, E, n, \eta) - \rho_p(x, E, p, \eta).
\]

Interface conditions at \( x^I = x = x^{II} \)

- extra defect dynamics (\( \hat{\eta} \) localized at interface \( x \))
  \[
  \frac{\partial}{\partial t} \hat{\eta}(t, x, E) = \rho_n(x^I, E, n^I, \hat{\eta}) + \rho_n(x^{II}, E, n^{II}, \hat{\eta}) - \rho_p(x^I, E, p^I, \hat{\eta}) - \rho_p(x^{II}, E, p^{II}, \hat{\eta})
  \]

- current determined by thermionic emission and defect recombination
  \[
  c_n (\nabla n - n \nabla \varphi)^I \cdot \nu = \alpha_n^I n^I - \alpha_n^{II} n^{II} + \langle \rho_n(x^I, \cdot, n^I, \hat{\eta}) \rangle \quad \text{(plus 3 similar cond.)}
  \]
(1) Modeling and analysis of nontrivial interface conditions

Equations in the bulk for $n$, $p$, $\varphi$, $\eta = \text{defect-occupation probability}$

\[
\frac{\partial}{\partial t} n - \text{div} \left( c_n (\nabla n - n \nabla \varphi) \right) = G_{\text{phot}}(t, x) - \langle \rho_n(\cdot, n, \eta) \rangle - R(n, p),
\]

\[
\frac{\partial}{\partial t} p - \text{div} \left( c_p (\nabla p + p \nabla \varphi) \right) = G_{\text{phot}}(t, x) - \langle \rho_p(\cdot, p, \eta) \rangle - R(n, p),
\]

\[-\text{div}(\varepsilon(x) \nabla \varphi) = d_{\text{dop}}(x) + p - n - \langle \eta \rangle \quad \text{where} \ \langle g \rangle := \int_{E_V}^{E_C} g(E) N(x, E) \, dE\]

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  \]

Aims:

- thermodynamic wellposedness of resulting model equations
- existence theory for stationary/time-harmonic/instationary problems
  (starting from lower dimensional problems)
(2) Approximation by pseudo layers

For numerical implementations it is common practice to replace the interface conditions and the interface-trap kinetics by bulk kinetics on thin layer elements with suitably scaled properties.

(+++) classical interface conditions can be used
(−−−) the problem might become badly conditioned or even unstable
(2) Approximation by pseudo layers

For numerical implementations it is common practice to replace the interface conditions and the interface-trap kinetics by bulk kinetics on thin layer elements with suitably scaled properties.

(++) classical interface conditions can be used
(−−) the problem might become badly conditioned or even unstable

Aims:

- Investigate this approximation procedure in a rigorous fashion,
- Which nontrivial boundary conditions can be obtained by such limits? How much freedom do we have in such approximations?
- Approximate tunneling effects through interfacial potential barriers: Do pseudo-layers with fitted material data approximate the tunneling characteristics sufficiently well?
(3) Numerical approximation and simulation

1-dimensional software AFORS-HET of Helmholtz Zentrum Berlin (HZB) uses finite differences, no numerical analysis available

Aims:

- establish discretization schemes benefitting from analytical properties of the continuous problem
- implement such schemes or adapt WIAS-TeSCA
- predict characteristics of solar cells (band diagrams, recomb. rates, carrier densities, electrostatic pot., cv-characteristics, quantum efficiency)
- validation of the models by comparison with measurements of HZB
Cooperations within Application Area D
D23 (F. Schmidt) “Design of nanophotonic devices and materials” (interplay of material properties of interfaces with their optical and electronic properties)

Cooperations with other Application Areas of MATHEON
C10 (B. Wagner) “Modeling, asymptotic analysis and numerical simulation of interface dynamics on the nanoscale” (properties of surfaces, atomic layers)

External Cooperations:
Helmholtz Zentrum Berlin für Materialien und Energie, Group SE1 “Silizium-Photovoltaik”, Prof. Bernd Rech, Dr. Rolf Stangl, Dr. Lars Korte (discussion of models, experimental data to validate our models)

MATHEON projects C10, D22, and D23 supply basic research for PVcomB: Photovoltaics Competence Center Berlin (Head Prof. Bernd Rech)