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Project D22

Modeling of electronic properties of interfaces in solar cells

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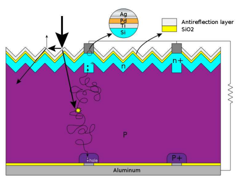
Domain of Expertise: Electronic devices

Background

Photovoltaic cells are semiconductor heterostructures
Effects of rough interfaces in thin-film cells:
- used for light trapping, have strong impact on the functionality of the device
- nanoscale-treatment of interfaces to tune electronic properties

Helmholtz-Zentrum Berlin für Materialien und Energie investigates thin-film a-Si:H/c-Si solar cells built from layers of amorphous and crystalline silicon
Issues:
- reduction of recombination losses at the a-Si:H/c-Si interface
- improvement of the charge-carrier transport over the heterointerface

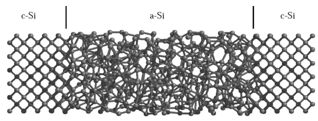


Technological aims in photovoltaics:
- maximize efficiency of the solar cells
- minimize production costs, . . .

Principle of solar cells:
- photons generate electron-hole pairs
- electrons/holes move to contacts

$\rightsquigarrow$ 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



$\rightsquigarrow$ **new mathematical models required!**

Equations in the bulk

$$\frac{\partial}{\partial t}n - \mathrm{div}\big(c_n(\nabla n - n\nabla\varphi)\big) = G_{\mathrm{phot}}(t,x) - \langle\langle \rho_n(..,n,\eta)\rangle\rangle - R(n,p),$$
$$\frac{\partial}{\partial t}p - \mathrm{div}\big(c_p(\nabla p + p\nabla\varphi)\big) = G_{\mathrm{phot}}(t,x) - \langle\langle \rho_p(..,p,\eta)\rangle\rangle - R(n,p),$$
$$-\mathrm{div}(\varepsilon(x)\nabla\varphi) = d_{\mathrm{dop}}(x) + p - n - \langle\langle \eta\rangle\rangle$$
$$\frac{\partial}{\partial t}\eta(t,x,E) = \rho_n(x,E,n,\eta) - \rho_p(x,E,p,\eta)$$

$n,\ p$	densities of electrons and holes
$\varphi,\ \eta$	electrostatic potential, defect-occupation probability
$R(n,p),\ G_{\mathrm{phot}}$	recombination rate, optical generation rate
$\rho_n,\ \rho_p$	ionization rates of defects

$$\langle\langle g\rangle\rangle := \int_{E_V}^{E_C} g(E)N(x,E)\,\mathrm{d}E, \qquad E \text{ energy levels}$$

Research plan for the project

(1) Nontrivial interface conditions

Conditions at interfaces $x^{\mathrm{I}} = x = x^{\mathrm{II}}$
- extra defect dynamics ($\widehat{\eta}$ localized at interface x)

$$\frac{\partial}{\partial t}\widehat{\eta}(t,x,E) = \rho_n(x^{\mathrm{I}},E,n^{\mathrm{I}},\widehat{\eta}) + \rho_n(x^{\mathrm{II}},E,n^{\mathrm{II}},\widehat{\eta}) - \rho_p(x^{\mathrm{I}},E,p^{\mathrm{I}},\widehat{\eta}) - \rho_p(x^{\mathrm{II}},E,p^{\mathrm{II}},\widehat{\eta})$$

- current determined by thermionic emission and defect recombination

$$c_n(\nabla n - n\nabla\varphi)^{\mathrm{I}}\cdot\nu = \alpha_n^{\mathrm{I}} n^{\mathrm{I}} - \alpha_n^{\mathrm{II}} n^{\mathrm{II}} + \langle\langle \rho_n(x^{\mathrm{I}},\cdot,n^{\mathrm{I}},\widehat{\eta})\rangle\rangle$$

(plus 3 similar conditions)

Aims:
- thermodynamic wellposedness of resulting model equations
- existence theory for stationary/instationary problems (starting from lower dimensional problems)

(2) Approximation by pseudo layers

Numerical implementations replace the interface conditions and the interface-trap kinetics by bulk kinetics on thin layer elements with suitably scaled properties

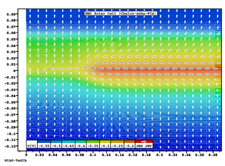
(++)	classical interface conditions can be used
(−−)	the problem might become badly conditioned or even unstable

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, cv-characteristics, quantum efficiency)
- validation/comparison with measurements (HZB)



WIAS-TeSCA Simulation (R. Nürnberg): Electron current through a structured passivation layer and electrostatic potential in a thin-film solar cell.

Cooperation

Helmholtz Zentrum Berlin für Materialien und Energie, Group SE1 “Silizium-Photovoltaik” (discussion of models, experimental data to validate our models)
PVcomB: Photovoltaics Competence Center Berlin (Head Prof. Bernd Rech)
ODERSUN AG Berlin · Frankfurt (Oder) · London (modeling and simulation)

References

A. Glitzky and K. Gärtner, Energy estimates for continuous and discretized electro-reaction-diffusion systems, *Nonlinear Analysis*, 70:788–805, 2009.
A. Glitzky and K. Gärtner, Existence of bounded steady state solutions to spin-polarized drift-diffusion systems, *SIAM J. Math. Anal.* 41:2489–2513, 2010.
A. Mielke, Weak-convergence methods for Hamiltonian multiscale problems. *Discr. Cont. Dynam. Systems Series A*, 20(1):53–79, 2008.