Device model for intermediate band materials

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***Abstract*—For twenty years, intermediate band (IB) materials have been developed with the goal of making high-efficiency photovoltaics, with limiting efficiencies equivalent to triple-junction devices but with simpler and potentially less expensive device designs. IB devices have yet to produce any high efficiencies. Existing devices did not optimize such parameters as their layer thicknesses, because there was no device model that could treat all the IB-specific effects, e.g., charge transport within the IB and IB-filling-dependent absorptivity and photofilling. We present Simudo, a finite element optoelectronic device model that implements these effects, in addition to treating standard semiconductors. Simudo models charge transport and generation in the conduction, valence, and a number of intermediate bands. It solves the coupled Poisson/drift-diffusion equations in two dimensions, along with self-consistent optics for IB-filling-dependent absorption. We validate this new software by benchmarking it against Synopsys Sentaurus on a pn-diode test problem, and we show excellent agreement. Simudo enables optimization of devices as well as understanding of experimental results, bringing the well-established value of device modeling semiconductors to IB systems.**

***Index Terms*—charge carrier lifetime, photovoltaic cells, mathematical model.**

I. Introduction

The new class of intermediate band (IB) materials holds great promise in improving solar cell efficiency, equivalent to triple-junction solar cells [1], [2]. An IB material is a semiconductor with an additional band of electronic states deep inside the band gap, which enables sub-gap absorption while the photovoltaic voltage is set by the large band gap, producing high efficiency. IB materials are also considered for IR photodetectors [3]. Quantum dot, highly-mismatched alloy, and heavily doped systems are the three known classes of IB materials [2].

Although IB devices have been demonstrated, none has shown an efficiency improvement over a standard semiconductor cell without the IB. While the nonradiative processes are clearly a major problem [2], [4], [5], none of these devices' geometries, junctions, or doping were optimized before their manufacture because there was no device model capable of effectively treating the IB material. Existing IB device models do not allow consideration of the important properties of IB devices [6]–[13]. IB device models should, in addition to treating the physics of a standard semiconductor with a conduction band (CB) and valence band (VB), also treat

- carrier transport within the IB,
- nonradiative processes from both CB and VB to IB,
- IB-filling-dependent subgap absorptivity,
- interfaces with standard metals or semiconductors.

We present Simudo, a 2D optoelectronic device model that fully meets these requirements. Simudo solves the Poisson/drift-diffusion (PDD) system of equations for charge transport in semiconductors. Simudo uses the FEniCS finite element library [14], is written in Python and exposes a well-documented and carefully designed API to the user.

We benchmark Simudo against the industry standard Synopsys Sentaurus using a standard pn-diode problem, and we demonstrate excellent agreement in extracted current densities.

Simudo will be publicly released under a free software license, and we hope it will be of great use to the intermediate band community.

II. Device model

The core of Simudo is a solver for the PDD problem. This problem treats the carrier transport and generation in any number of bands; typically a CB, a VB, and a number of IB's. Simudo works in the approximation that each band's carriers are at thermal equilibrium with each other, so each band i has a well-defined quasi-Fermi level w_i. For a non-degenerate band, the band's carrier density u_i is then related to the quasi-Fermi level by

$$u_i = N_i e^{\mp(\mathcal{E}_i - w_i - q\phi)}, \tag{1}$$

where the upper and lower signs are used for holes ($u_i = p$) and electrons ($u_i = n$), respectively, $\mathcal{E}_i$ is the band edge energy, N_i is the effective density of states, and ϕ is the electrostatic potential. We assume for this discussion that an IB has an energetic bandwidth narrower than kT, so that its electron density can be approximated as

$$u_I = N_I f_I = N_I\, f(\mathcal{E}_I - w_I - q\phi), \tag{2}$$

where $f(E) = (\exp(E/kT) + 1)^{-1}$ is the Fermi function, f_I is the IB filling fraction, N_I is the IB's density of states, and $\mathcal{E}_I$ is the IB energy level. Transport and generation in each band i are governed by the drift-diffusion equations,

$$\vec{j}_i = \mu_i u_i \vec{\nabla} w_i \tag{3a}$$

$$\frac{\partial u_i}{\partial t} = \mp\frac{1}{q}\vec{\nabla}\cdot\vec{j}_i + g_i, \tag{3b}$$

where $\vec{j}_i$ is the band's contribution to current density, μ_i is the mobility, and g_i is the local carrier generation. The carrier generation g_i is the sum of contributions from all generation and recombination processes involving band i.

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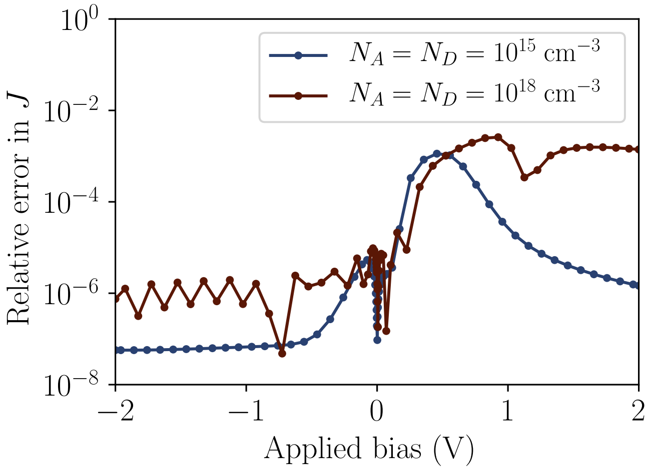

Fig. 1. Comparison between Simudo and Sentaurus on test pn-diode, showing the error in the integrated total current at the contacts.

Finally, the electrostatic potential ϕ is related to the local charge density ρ by Poisson's equation

$$\vec{\nabla} \cdot (\varepsilon \vec{\nabla} \phi) = -\rho \tag{4}$$

$$\rho = q\big(-n + p - N_I(f - f_0) + N_D - N_A \big) \tag{5}$$

where f_0 is the filling fraction of the IB at zero temperature, N_D and N_A are the donor and acceptor densities, respectively, assuming full ionization, and ε is the local dielectric constant.

Simudo solves the PDD problem on a 2D mesh, where material and band parameters (e.g., $\mathcal{E}_i, N_i, \mu_i, \varepsilon, N_A$) may be non-uniform and may depend upon other parameters. Carrier generation and recombination are also flexible; the user can implement their mechanisms with ease, and processes such as Shockley-Read trapping into the IB, Shockley-Read-Hall (SRH) recombination, radiative recombination, and optical carrier generation are provided by Simudo.

Simudo can also solve an auxiliary optical propagation problem, given by the Beer-Lambert law $\mathrm{d}I(\omega)/\mathrm{d}x = -\alpha(\omega, x)I$, where I is the optical intensity and α is the absorption coefficient. Self-consistent looping between the PDD and optical problem is necessary, as the optical absorption coefficient for IB processes depends on f_I [15],

$$\alpha_{IV}(\omega, x) = N_I(x)\, \sigma_{\mathrm{opt},IV}(\omega, x)\, [1 - f_I(x)] \tag{6}$$

$$\alpha_{CI}(\omega, x) = N_I(x)\, \sigma_{\mathrm{opt},CI}(\omega, x)\, f_I(x), \tag{7}$$

where $\sigma_{\mathrm{opt},fi}$ is the optical absorption cross section for the i to f process, with explicit spatial dependence. These optical processes can only occur to (from) empty (filled) IB states. Letting $g_{fi} = \int \alpha_{\mathrm{opt},fi}(\omega, x)\, I(\omega)\, \mathrm{d}\omega$, the optical carrier generations for each band in a three-band system are then $g_{\mathrm{opt},C} = g_{CI} + g_{CV}$, $g_{\mathrm{opt},V} = g_{IV} + g_{CV}$, and $g_{\mathrm{opt},I} = -g_{CI} + g_{IV}$.

III. Validation

We benchmark Simudo against Synopsys Sentaurus, which does not support IB's. We use a 1-dimensional silicon pn-diode as a common benchmark problem. We consider a set of symmetrically doped devices with doping $10^{15} - 10^{21}\,\mathrm{cm}^{-3}$ in p- and n-type regions each of length $83.35\,\mathrm{nm}$, with SRH lifetimes of $1\,\mathrm{ns}$ and $1\,\mu\mathrm{s}$, respectively. Figure 1 shows excellent agreement in the current for applied biases from -2 to 2 V. For the higher-doped devices (not shown), the maximum relative error is below 1%.

Simudo is a general-purpose device model for standard semiconductor and IB device problems, which brings the well-appreciated power of device modeling to IB devices for the first time. We expect it to be of great utility in the field.

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