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DOMAIN DECOMPOSITION FOR HETEROJUNCTION PROBLEMS IN SEMICONDUCTORS

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Our work presents a multiscale approach for heterojunction interfaces in semiconductors. This research is part of a larger interdisciplinary effort between computational mathematicians, physicists, and material scientists who are interested in such structures for the purpose of building more efficient solar cells. Phenomena at the heterojunction must be resolved at the angstrom scale while the size of the device is that of microns. The challenge is therefore to account for correct physics and keep the model computationally tractable. Thus we use an approach from [5] in which the physics at the interface is approximated at the device scale, which is handled by traditional drift diffusion equations, by unusual jump conditions, called the thermionic emission equations. In this model the heterojunction region is approximated by an abrupt interface, resulting in a loss of continuity in the primary variables. The thermionic emission equations consist of a nonhomogeneous jump in the electrostatic potential, and unusual Robin-like conditions for carrier transport. We determine the data for these jumps from an angstrom scale first principles calculation in the true heterojunction region using Density Functional Theory.

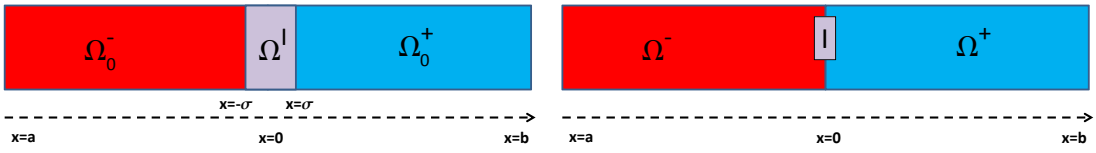

Figure 1: Illustration of approximation of the heterojunction region by abrupt interface

This model lends itself well to a domain decomposition approach. In 1D the problem is amenable to a monolithic approach where the transmission conditions are treated explicitly in the algebraic system resulting from a discretization of the drift diffusion equations in each semiconductor material. However, this approach may be intractable in 2 and 3 dimensions where more complicated interface geometries may arise.

We present domain decomposition methods that allow for the use of "black box" drift diffusion solvers in subdomains by enforcing the thermionic emission transmission conditions at the level of the domain decomposition driver. These domain decomposition methods are iterative substructuring methods, designed as Richardson schemes for equations posed on the idealized abrupt interface. The interface equations are similar to the Steklov-Poincaré equation for a problem with homogeneous transmission conditions. The relaxation parameter, θ, for these methods depends on material parameters which vary by many orders of magnitude across the heterojunctions. Finding appropriate values for θ thus relies on analysis of these interface equations.

In the talk we present results of various simulations. For example in Figure 2 we simulate two heterojunction semiconductor structures.

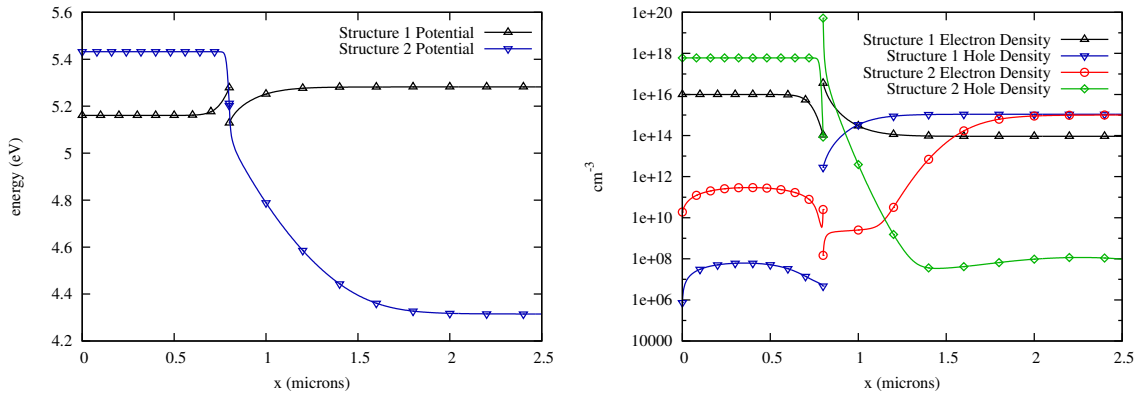

Figure 2: Simulation of potential (left) and carrier densities (right) for two heterojunction structures. Structure 1 has the design principle of a solar cell, and Structure 2 is a Cu_3PSe_4-Si interface.

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