

Simulation of Charge-Carrier Transport in Cadmium Sulfide Nanowires

We simulated electrically contacted CdS nanowires (drift-diffusion with photoexcitation) in COMSOL Multiphysics® and validated the results against photocurrent and Kelvin probe experiments, using the model to identify transport parameters and sensitivities along the wire.

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Abstract

A combination of scanning-force microscopy, transport measurements, and numerical simulations was utilized to study the charge transport properties of contacted CdS nanowires. A two-step routine was used to fit a two-dimensional, axis symmetric, drift-diffusion/Poisson model to surface-potential data obtained by Kelvin probe force microscopy (KPFM) and current-voltage (IV) data measured under local illumination of a nanowire. The fitting yielded unique values for a whole set of material

parameters that are not accessible by either experiment or simulation alone. We found a low doping concentration, suggesting strong electron surface trapping. Furthermore, the high electron mobility hints to an efficient transport inside the NW. The very low hole mobility can be explained by trap-assisted carrier hopping at the nanowire surface. Finally, the small recombination factor indicates a weak electron-hole overlap. A Sobol sensitivity analysis confirmed parameter sensitivity across regions.

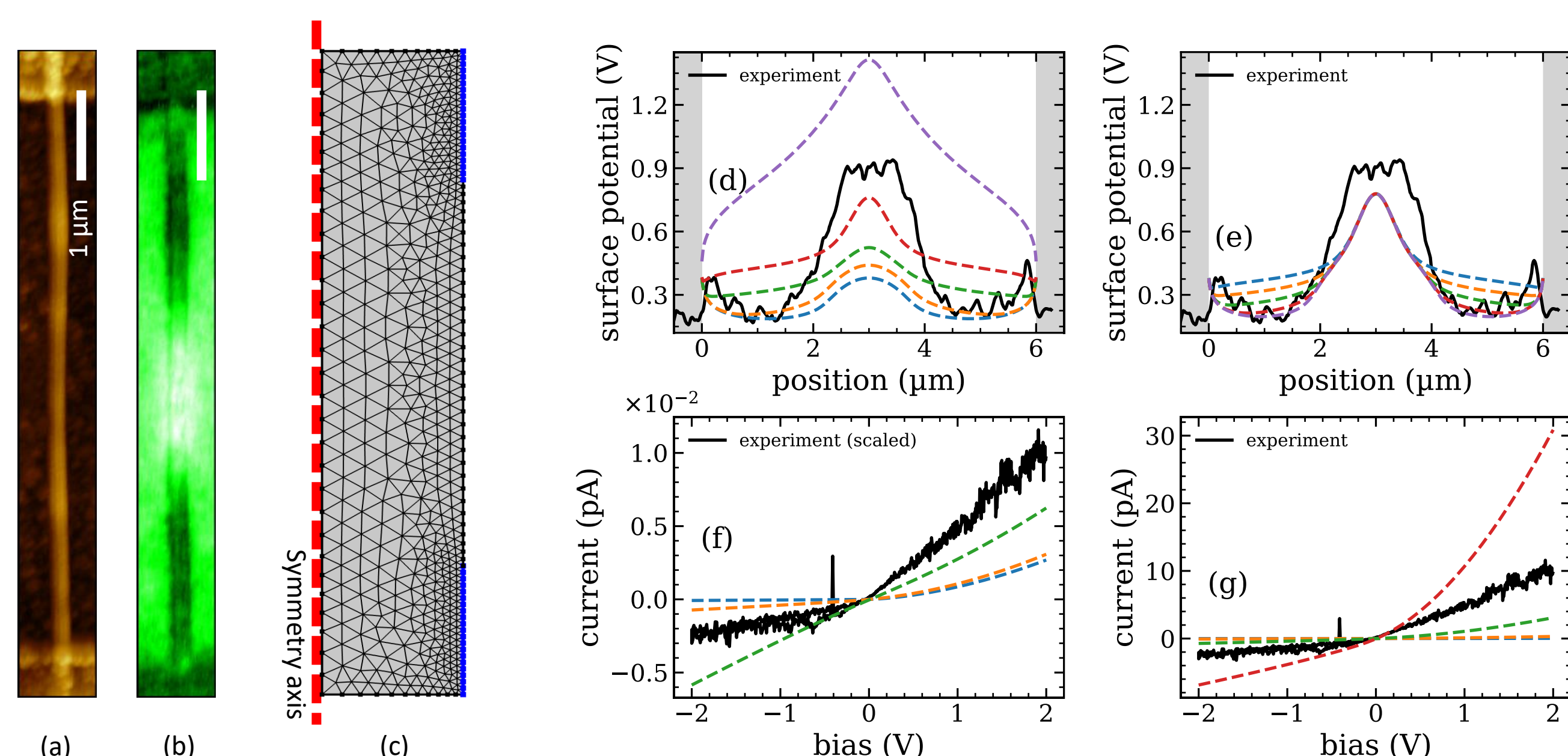


FIGURE 1. (a) AFM scan, (b) KPFM scan, (c) meshed NW mode, (d-g) parameter variation.

Methodology

A contacted nanowire was modeled in a 2d-axisymmetric approach based on AFM measured topography data. For transport physics, the Semiconductor Module was used and solved for a stationary solution, based on a drift-diffusion model coupled with Poisson's equation.

The material parameters were then fitted in a two-step fitting routine on two individual datasets. In addition we performed a Sobol sensitivity analysis for the fitted material parameters, computing main (S1) and total (ST) effects.

Results

By combining experiment and simulation, we extracted key transport parameters for the CdS nanowires. The effective doping concentration is only about 10^{13} cm^{-3} , far below typical literature values, indicating that most donor electrons are trapped at the nanowire surface and do not contribute to conduction. The electron mobility is relatively high, suggesting efficient transport of photogenerated electrons away from surface traps. In contrast, the hole mobility is extremely low, consistent with slow trap-assisted hopping on the surface. The recombination factor is exceptionally small, likely due to weak overlap between electrons in the nanowire core and holes localized at surface traps.

Sobol analysis showed that each parameter contributes differently across regions, and multiparameter fitting across datasets yielded a unique parameter set.

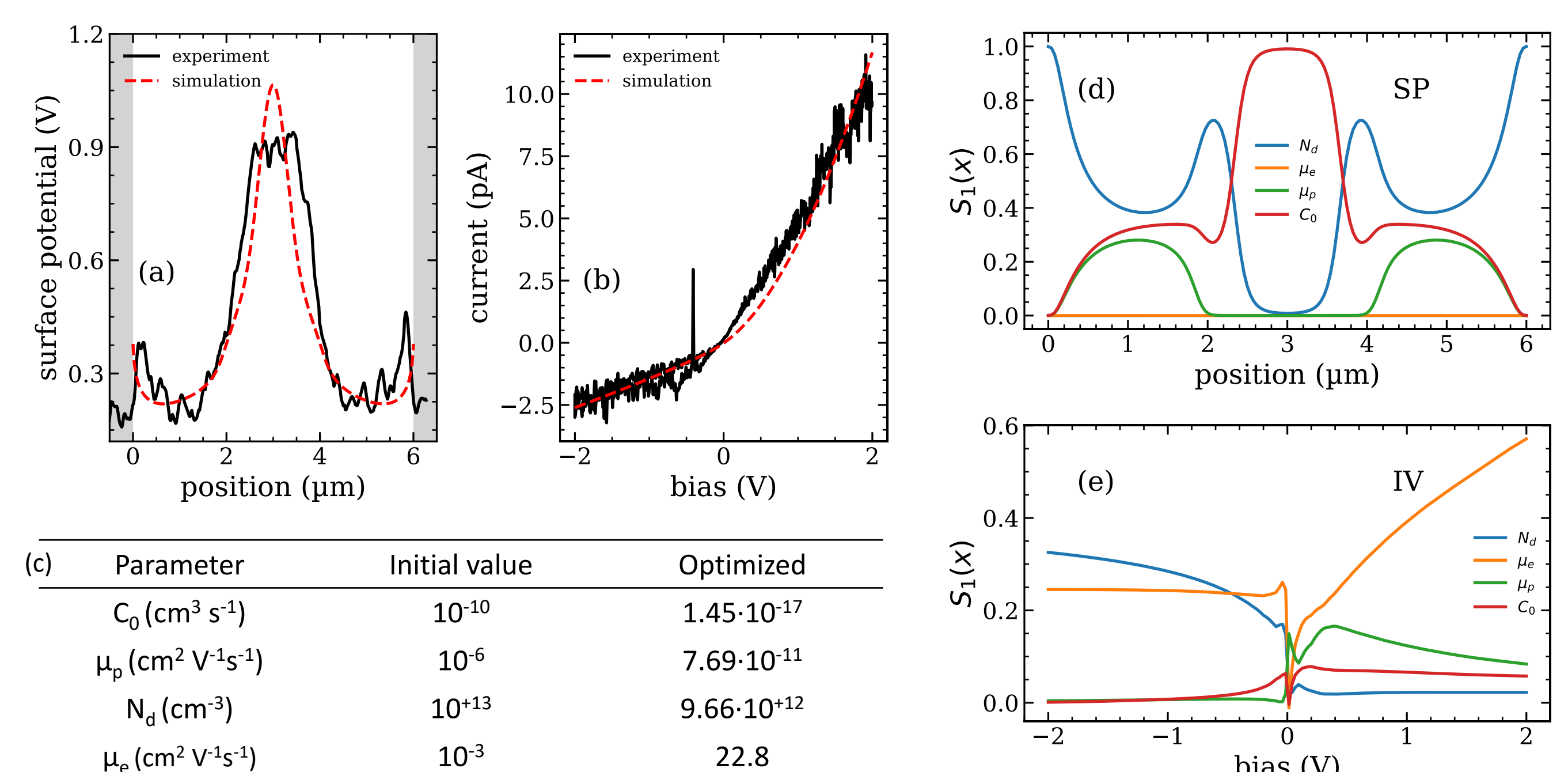


FIGURE 2. (a+b) final fits, (c) model parameters, (d+e) sobol analysis.

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