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Impact of built-in fields and contact configuration on the characteristics of ultra-thin GaAs solar cells

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We discuss the effects of built-in fields and contact configuration on the photovoltaic characteristics of ultra-thin GaAs solar cells. The investigation is based on advanced quantum-kinetic simulations reaching beyond the standard semi-classical bulk picture concerning the consideration of charge carrier states and dynamics in complex potential profiles. The thickness dependence of dark and photocurrent in the ultra-scaled regime is related to the corresponding variation of both, the built-in electric fields and associated modification of the density of states, and the optical intensity in the films. Losses in open-circuit voltage and short-circuit current due to the leakage of electronically and optically injected carriers at minority carrier contacts are investigated for different contact configurations including electron and hole blocking barrier layers. The microscopic picture of leakage currents is connected to the effect of finite surface recombination velocities in the semi-classical description, and the impact of these non-classical contact regions on carrier generation and extraction is analyzed. Published by AIP Publishing. [http://dx.doi.org/10.1063/1.4959244]

Solar cells based on high-quality crystalline materials with strong optical absorption, such as GaAs, are known to provide very high single junction efficiencies. However, the fabrication of ordinary solar cells based on such materials is expensive and limits the commercial viability of the technology. Recently, ultra-thin high-efficiency absorber architectures were proposed as one way to mitigate the problem of high material and fabrication costs. To compensate for the reduced absorber thickness, the absorption in these solar cells is enhanced by nanophotonic light-trapping structures. In this way, almost complete absorption of the solar spectrum could be achieved over a wide range of photon frequencies with absorber thicknesses below 100 nm.

For the conventional single-junction $p-i-n$ architectures exhibiting a doping-induced built-in potential of the order of the band gap energy at short-circuit conditions, such ultra-scaled absorber dimensions amount to very strong built-in fields even at the operating point of the solar cell. Hence, the validity of the assumption of bias-independent flat-band bulk (FBB) material properties conventionally used in semiclassical solar cell simulation models becomes increasingly questionable for these devices. A further aspect of ultra-thin absorber architectures where the conventional treatment is likely to miss the physical picture concerns the electron and hole blocking layers (EBL/HBL) introduced to increase the carrier selectivity by reducing leakage of minority carriers. The doped barrier layers introduce interfacial regions where charge carriers experience the effects of quantum confinement and can thus not be described properly within a classical picture. These non-classical contact regions become increasingly relevant as the bulk absorber volume decreases.

In order to assess the validity of the semiclassical bulk picture in ultra-scaled photovoltaic architectures, one needs to resort to a theoretical framework where the simplifying assumptions of the conventional approach are relaxed. A theoretical framework that is suitable for this purpose is the quantum-kinetic non-equilibrium Green’s function formalism (NEGF), which can be used to describe the non-equilibrium quantum statistical mechanics of open electronic systems even if featuring complex nanoscale potentials and in the presence of inelastic scattering mechanisms such as the electron-photon and electron-phonon interactions relevant for photovoltaic device operation at room temperature. In contrast to the conventional semiclassical models, this approach is able to capture any deviation from bulk-like behavior induced in the electronic properties by strong fields or heterostructure potentials and in the optical properties by nanophotonic structures. Recently, the NEGF picture was implemented for ultra-thin GaAs solar cell devices at the radiative limit and revealed substantial deviations from the bulk behavior provided by the semiclassical description.

In this letter, we investigate the thickness dependence of the photovoltaic characteristics due to the variation of absorption and emission with built-in fields and optical intensity. We further consider the effects of non-classical regions induced by the barrier potentials of electron and hole blocking layers mediating enhanced carrier selectivity of contacts.

For the semiclassical simulation of generation, transport, and recombination of charge carriers in ultra-thin absorber devices, the conventional 1D drift-diffusion-Poisson solver ASA (Advanced Semiconductor Analysis, TU Delft) is used. The generation rate is computed locally from the differential absorbance as a function of the density of the transverse electromagnetic field as given by the built-in transfer matrix method (TMM) and of the local absorption coefficient. The coherent wave approach of the TMM enables the consideration of optical resonator modes at sub-wavelength absorber thicknesses. Recombination is restricted to the fundamental radiative process as described by the detailed-balance approach in terms of the local absorption coefficient and the black body radiation flux.
The quantum-kinetic simulations are performed with an in-house developed NEGF-Poisson solver devised for the simulation of nanostructure-based solar cell devices. For the electronic structure of the bulk absorber materials, two decoupled single orbital tight-binding bands are used, with parameters obtained via the analogy to the effective mass approximation (EMA). The photogeneration is described in terms of coupling to the classical transverse field as obtained again from the TMM, while for the spontaneous emission, coupling to the photon density of states of the absorber as encoded in the slab photon Green’s function is considered.

In order to maximize the comparability of the macroscopic semiclassical approach with the microscopic quantum formalism, in addition to relying on the same optical model (TMM), the material parameters in the semi-classical approach were extracted from the two band EMA model of the bulk electronic structure used in the microscopic picture. The numerical values of the parameters used can be found in Ref. 11. Since this simple band structure deviates considerably from the experimental data at energies far from the band edges, the investigation is focused on the device behavior at excitation energies close to the band gap.

In a recent publication, the qualitative and quantitative discrepancies between the drift-diffusion picture assuming flat band bulk material and the NEGF simulations of photovoltaic device characteristics were investigated for a simple p-i-n structure as shown in Fig. 1, with \( N_{AD} = 10^{18} \text{ cm}^{-3} \), \( d_{np} = 20 \text{ nm} \), \( d_l = 60 \text{ nm} \) and perfectly selective contacts (\( \Delta E_{C,V} \rightarrow \infty \)). It was found that the differences originate mostly in the effects of the strong built-in fields on absorption and emission (Franz-Keldysh effect). With further thickness reduction, the discrepancies between semiclassical flat-band bulk (FBB) and quantum-kinetic (NEGF) descriptions that are related to field effects—absent in the FBB—increase due to the growing built-in potentials, as displayed in Fig. 2. In subfigures (a) and (b), the current-voltage characteristics are shown for the dark and under illumination with monochromatic light of photon energy \( E_p = 1.44 \text{ eV} \) and intensity \( I_p = 0.1 \text{ kW/m}^2 \) for the same devices and simulation approaches as in (a). The effect of increasing fields on the absorption is partially masked by the strong fluctuation of the optical intensity with thickness variation.

![FIG. 1. Model system used in the simulations, corresponding to an ultrathin p-i-n photodiode. The chemical potentials \( \mu_{L,R} \) at left and right contacts are split by the applied bias voltage \( V_{bias} \). The electron (hole) blocking layer EBL (HBL) prevents carrier leakage via band offset \( \Delta E_C (\Delta E_V) \). The gold reflector is only used for the optical simulation.](image)

![FIG. 2. (a) Dark current-voltage characteristics for absorber thicknesses of 100 nm, 50 nm, and 20 nm, computed using the quantum-kinetic approach (NEGF, filled symbols) and the semiclassical flat-band bulk model (FBB, open symbols). The increase of the built-in potential with reduced absorber thickness leads to a strong enhancement of dark current due to the recombination between field-induced tail states. (b) Characteristics under monochromatic illumination \( (E_p = 1.44 \text{ eV}, I_p = 0.1 \text{ kW/cm}^2) \) for the same devices and simulation approaches as in (a). The effect of increasing fields on the absorption is partially masked by the strong fluctuation of the optical intensity with thickness variation.](image)
The effect of the contacts is mainly related to their behavior with respect to absorption, reflection, and injection of charge carriers. In an ideal solar cell, the contacts are perfectly carrier selective, i.e., they are ideally transmissive for majority carriers, while reflecting all minority carriers, thereby acting as the “semipermeable membrane” that is essential for photovoltaic device operation. In the NEGF picture, the contacts are described by corresponding boundary self-energies that relate the absorber states to the extended states of the electrodes. At vanishing contact barriers ($\Delta E_{CV} \to 0$, “open”), there are photovoltaic performance losses due to the leakage of both electrically and optically injected carriers. As shown in Fig. 5(a), the leakage component of the dark current—i.e., the intraband component—results in severe reduction of $V_{OC}$. In the semiclassical picture, this behavior can be reproduced by increasing the value of the surface recombination velocity $S$.

FIG. 3. Absorption coefficient and spectral emission rate of the $p$-$i$-$n$ diode at $V_{bias} = 0.8$ V, for absorber thicknesses of 100 nm, 50 nm, and 20 nm, respectively. While the value of the absorption coefficient is almost constant for the photon energy $E_\gamma = 1.44$ eV of the monochromatic illumination, the emission rate exhibits a pronounced red shift and broadening with shrinking absorber thickness owing to the field-induced tailing of the joint density of states.

FIG. 4. Absorptance of the $p$-$i$-$n$ structure at $V_{bias} = 0.8$ V for the different absorber thicknesses, exhibiting a strongly non-monotonous behavior reflected in the short-circuit current of the characteristics in Fig. 2(b), which originates in the strong variation of the optical intensity for the different configurations.

FIG. 5. (a) $J$-$V$-characteristics for open and selective contacts for a 100 nm $p$-$i$-$n$ diode under monochromatic illumination with $E_\gamma = 1.44$ eV at an intensity of 0.1 kW/cm$^2$, as obtained using the NEGF formalism. The open contacts lead to severe $V_{OC}$-reduction due to dark leakage currents. The corresponding dark current-voltage characteristics are displayed in the inset (log scale). (b) Semiclassical $J$-$V$-characteristics under consideration of leakage loss via a corresponding surface recombination term characterized by the surface recombination velocity $S$. The inset displays again the dark current for the different values of $S$.

FIG. 6. NEGF-based $J$-$V$-characteristics for a 50 nm $p$-$i$-$n$ structure with open contacts (“open”), carrier selective contacts (“selective”), and with electron/hole blocking layers (“barriers”). The inset shows the ratio of extracted to generated photocurrent at short circuit conditions, which depends on the photon energy: the farther away from the band edge the carriers are generated, the higher the probability of photocurrent leakage.
S at minority carrier contacts [Fig. 5(b)]: for increasing S, $V_{OC}$ is gradually reduced, and at very large surface recombination, also $J_{SC}$ is degraded. In the NEGF picture, the reduction of $J_{SC}$ additionally depends on photon energy: the larger the distance to the band edge, the more likely is the extraction of photogenerated carriers to the “wrong”—i.e., minority carrier—contact, especially for carriers generated far away from the contact.\(^{18}\) This behavior is displayed in the inset of Fig. 6 showing the ratio $J/J_{gen}$ of extracted to generated charge current for the 50 nm thick absorber.

The leakage losses can be partially mitigated by introducing electron and hole blocking layers (EBL/HBL), as displayed in Fig. 6. In the present case, $d_{EBL} = 5$ nm of Al\(_{40}\)Ga\(_{60}\)As is chosen for the EBL, and the HBL is composed of $d_{HBL} = 5$ nm of In\(_{49}\)Ga\(_{51}\)P. While dark leakage current is successfully reduced, there is also a reduction in photogeneration due to the impact of barriers on the electronic states inside the absorber, especially in close proximity to the interfaces, as can be verified in Figs. 7(a) and 7(b) displaying the spectral current of electrons in the two architectures. For comparison, the band profile of the open contact cell (a) is also indicated (dashed lines) in subfigure (b) showing the situation for the system with barrier layers. Obviously, the small variation in built-in field cannot explain the observed photocurrent reduction. Indeed, the comparison of the absorption coefficients of the two structures, shown in Fig. 8(a), reveals sizable modifications induced by the presence of confining barriers, most pronounced in the vicinity of the blocking layers, which explains the difference in absorptance displayed in Fig. 8(b).

![FIG. 7. Spectral electron current for (a) the 50 nm p-i-n cell with open contacts at $V_{bias} = 0.87$ V, featuring significant leakage of electronically injected carriers and (b) the architecture with blocking layers, where leakage is prevented, but at the price of sizable reduction and modification of the photocurrent spectrum. The dashed line in (b) corresponds to the band profile from (a) and shows that the built-in field is only weakly modified by the presence of barriers.](image)

![FIG. 8. (a) Ratio $\alpha_{barr}/\alpha_{open}$ of the spatially resolved absorption coefficients for the structure with blocking layers and the diode with open contacts, revealing the strong reduction of absorption in close vicinity of the barriers. (b) Comparison of the overall absorptance of the two structures, which explains the large difference in photocurrent seen in Fig. 6.](image)
Thus, while a homogeneous 50 nm GaAs slab behaves essentially bulk-like from an electronic point of view, the modification of contact regions has sizeable impact on the electronic structure and, hence, on the optoelectronic response of the device. As a result, simulation approaches that take into account only optical confinement effects and neglect the electronic modification of the absorber due to built-in fields and contact regions become inappropriate and should be replaced by a more comprehensive and generally valid picture, such as the NEGF framework used here.

In conclusion, the computational investigation of ultrathin GaAs solar cells based on a rigorous approach that is valid beyond the limits of the semi-classical bulk picture reveals significant discrepancies with respect to the latter due to the non-classical effects that strong built-in fields and contact barriers have on absorption, emission, and charge carrier extraction. The NEGF approach presented here will therefore provide a valuable tool for the investigation, design, and optimization of solar cell device structures in the ultra-scaled regime, where the exact device geometry and configuration starts to affect not only the optical modes but also the relevant electronic states of the absorber.

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