

# Opto-electro-thermal simulation technology of solar cells\*

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**Citation:** Y D An, Y Zhao, T S Ma, and X F Li, Opto-electro-thermal simulation technology of solar cells[J]. *J. Semicond.*, 2019, 40(5), 050403. <http://doi.org/10.1088/1674-4926/40/5/050403>

The solar cells (SCs) are the most typical devices used to convert the solar energy into electricity to help relieving the energy shortage crisis. In the photovoltaic (PV) communities, improving the power-conversion efficiency (PCE) of SC keeps to be a long-term objective. In the past decades, enormous efforts have been paid on exploring various new structural scenarios or PV mechanisms (e.g., near-field thermophotovoltaic and hot-carrier SCs) in order to approach or even break the Shockley-Queisser (SQ) efficiency limits of various SCs<sup>[1]</sup>. However, besides the perovskite SCs<sup>[2]</sup>, the rate of efficiency improvement is extremely slow in the past decade, especially for the traditional semiconductor-based SCs. In practice, for a high-performance SC, a comprehensive optimization should simultaneously consider increasing the optical absorption, improving the electrical collection efficiency, and controlling the thermodynamic effect<sup>[3, 4]</sup>. The challenge lies in that managing the SC operation is accompanied by the coupled photo-electric, photo-thermal and thermoelectric processes, which have to be managed from the perspectives of operation basics, material systems, structural designs and fabrication feasibility.

Such a multi-domain and multi-physical behavior can hardly be estimated conveniently in experiments (even in theoretical calculations or simulations), so that the performance improvement by balancing the optical, electrical, and thermal effects is very challenging. For instance, the transportation of photocurrent is not just regulated by the temperature, but also accompanied by the emission of photons and the generation of heat that affect the temperature of SC. Therefore, in order to further enhance the SC efficiency, it is necessary to thoroughly investigate the coupled multiphysical effect from the complete opto-electro-thermal (OET) domains.

The recent research proposes the full-coupled OET simulation technology of SC<sup>[5]</sup>, which reveals the fundamental physical mechanisms in SCs by addressing the coupled optical, electrical and thermal effects simultaneously<sup>[5, 6]</sup>. The OET simulation technology interprets the energy conversion and dissipation paths inside the SC system from both macroscopic and microscopic perspectives, as plotted in the Fig. 1. For the photovoltaic system, the energy losses and conversion processes can attribute to three channels (i.e., optical, electrical and

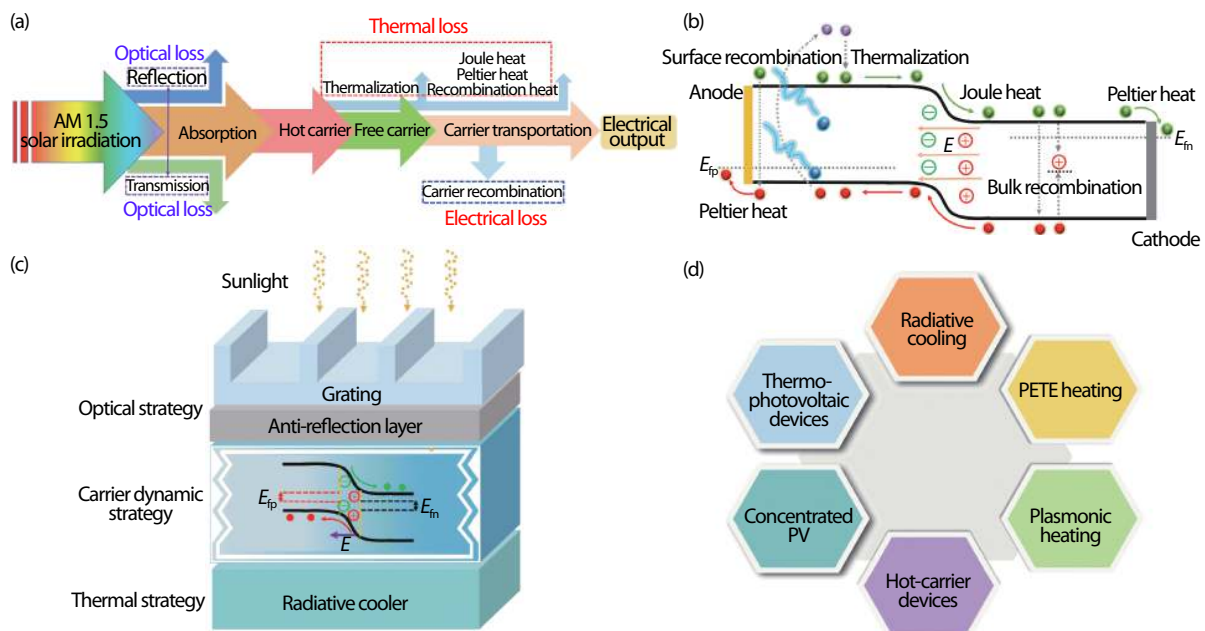


Fig. 1. (Color online) (a) Schematic diagrams of energy flow distribution in SCs under sunlight illumination. (b) The carrier thermodynamic physics in SCs. (c) The schematic diagrams of optical, electrical and thermal optimization strategy applied in the SC. (d) The possible applications of the OET simulation technology<sup>[5]</sup>.

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thermal ways), as shown in Fig. 1(a). Based on the OET model of SC, firstly, the energy loss flows by optical effects can be estimated by examining the reflection, absorption, and transmission characteristics of the SC. Then, with quantifying the carrier electrodynamic behaviors (i.e., generation, transportation, recombination, and collection processes), the electrical losses can be estimated. Finally, addressing the carrier thermodynamic behaviors (e.g., thermalization, recombination heat, Joule and Peltier heat) in the SC, the thermal effect and the operation temperature of SC can be predicted, as shown in Fig. 1(b). All these energy losses via various channels can be readily obtained under the OET simulation technology.

With quantitatively analyzing the energy losses in SCs by the OET simulation, the optimization can be achieved very conveniently, as shown in the Fig. 1(c). From the optical perspective, introducing an anti-reflection layer or back-reflection mirror is the basic optimization strategy. Besides, with the development of the photonic crystal, the optical absorption can be greatly enhanced by designing various light-trapping structures (e.g., gratings or pyramids)<sup>[7]</sup>. From the electrical perspective, the photogenerated electron-hole pairs suffer from the serious recombinations<sup>[8]</sup>. Thus, by tailoring the doping concentration and engineering the energy band alignment, the electrical performance of SC can be effectively managed<sup>[9]</sup>. From the thermodynamic perspective, the temperature dependence of the performance of SC can be examined so that thermal controlling strategies can be introduced, e.g., the radiative cooler<sup>[10]</sup>.

In summary, the coupled OET simulation technology provides a feasible way for comprehensively exploring the fundamental physics and light-matter interactions in photovoltaic devices so that high-performance SCs can be achieved. Besides, more extensive optoelectronic devices (e.g., photodetect-

ors, light-emitting diodes) as being exemplified in Fig. 1(d) can be studied by extending the current OET model with introducing the corresponding physics<sup>[11]</sup>, enabling a device-level and accurate design of the various optoelectronic devices.

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