A new strategy to enhance the performance of silicon heterojunction solar cells

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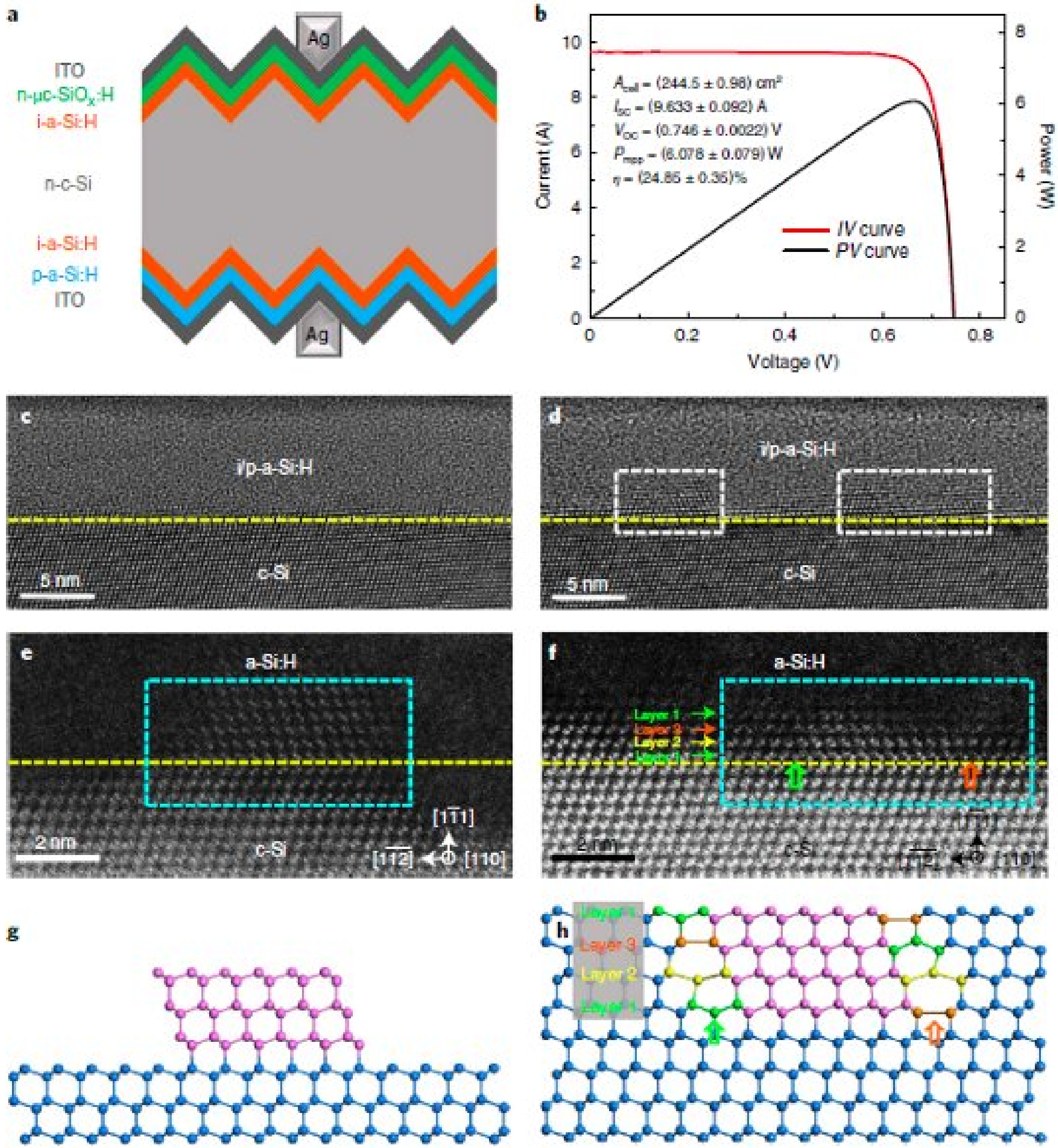

c-Si/a-Si:H interface structure characteristics of a SHJ solar cell. a, Cross-section schematic image of the SHJ solar cell. b, Current–voltage (IV) curve and power–voltage (PV) curve of the SHJ cell with conversion efficiency of 24.85%. c and d, HRTEM images of c-Si/a-Si:H interface viewed from orientation showing the slight normal epitaxial layer and defected epitaxial structures, respectively. e and f, Atomic-resolution HAADF-STEM images of two types of defects, which are free nanotwin and embedded nanotwin, respectively. g and h, Geometrical atomic structure models derived from green dashed rectangle areas in 1e and 1f, respectively. Credit: Qu et al.

Crystalline silicon (c-Si) solar cells are among the most promising solar technologies on the market. These solar cells have numerous advantageous properties, including a nearly optimum bandgap, high efficiency and stability. Notably, they can also be fabricated using raw materials that are widely available and easy to attain.

In recent years, many companies and engineers specifically focused their research efforts on Si heterojunction (SHJ) solar cells. These solar cells, which consist of amorphous silicon layers deposited on crystalline silicon surfaces, have been found to achieve remarkable power conversion efficiencies (PCE).

Researchers at Beijing University of Technology, the Hanergy Chengdu Research and Development Center, and Jiangsu University in China recently carried out a study aimed at closely examining the structure of the c-Si/a-Si:H interface in high-efficiency SHJ solar cells. Their paper, published in *Nature Energy*, offers valuable insight that could help to improve the performance of SHJ solar cells further, by allowing engineers greater control over the c-Si/a-Si:H interface.

"With continuous manufacturing improvements, Kaneka has realized SHJ solar cells with 24.5% PCE (total area, 239 cm^2) and 25.1% PCE (aperture area, 151.9 cm^2)," Yongzhe Zhang, one of the researchers who carried out the study, told TechXplore. "However, further efficiency enhancements of single-junction SHJ solar cells seem to have stalled in the last three years. Therefore, it is urgent that we discover new breakthroughs to solve the bottlenecks and obtain higher SHJ solar cell PCEs."

The interface between c-Si and a-Si:H in SHJ solar cells is of key importance in ensuring that the cells achieve a high PCE. To identify strategies that could improve the PCE of these cells, many researchers have thus closely examined the c-Si/a-Si:H interface using a technique known as transmission electron microscopy (TEM). These examinations, however, were often limited by the poor spatial resolution of traditional TEM techniques or by the sensitivity of high-resolution TEM (HRTEM) imaging to the thickness of interface samples.

Due to these limitations, so far, TEM-based studies were merely able to gather information about the thickness or abruptness of the SHJ cells' epitaxial layer. The structural characteristics of the c-Si/a-Si:H interface at the atomic scale, however, have not yet been identified.

To improve the efficiency of SHJ cells further, researchers need to examine the c-Si/a-Si:H interface in depth and identify strategies to control it at the atomic scale. In their study, Zhang and his colleagues used HRTEM imaging techniques and theory-based simulations to represent the atomic and electronic structure of c-Si/a-Si:H interfaces. They examined the atomic structure of the c-Si/a-Si:H interface in high-efficiency SHJ solar cells using an alternative TEM technique known as spherical aberration-corrected transmission electron microscopy (C_S-corrected TEM).

"To acquire best atomic contrast for accurately interpreting HR-(S)TEM images, we used two techniques called focused ion beam (FIB) and nanomill to prepare carefully cross-sectional samples of SHJ solar cells," the authors said. "The theoretical evaluation of c-Si/a-si:H interface structures was also crucial in this work, as it helped us to draw a physical connection between HRTEM images and device performance, in consideration of embedded nanotwins as the deep defects level of recombination center resulting in a short carrier lifetime, based on first-principles calculations."

The results gathered by Zhang and his colleagues were fairly unexpected and surprising. In addition to the cells' normal epitaxial structure, the researchers observed high-density nanotwins in the thin epitaxial layer between c-Si and a-Si:H, which exist in two different forms, as free nanotwins and as embedded nanotwins. Their calculations also showed that embedded nanotwins in this layer impair the performance of the SHJ solar cells.

After they identified high-density nanotwins in the thin epitaxial layer between c-Si and a-Si:H and determined that they impaired the performance of SHJ solar cells, the researchers tried to determine their origin and how they evolved over time. To do this, they examined c-Si/a-Si:H interface structures at different stages of the cell fabrication process using HRTEM techniques.

To illustrate the evolution of the c-Si/a-Si:H interface's structure, the researchers performed additional in situ annealing experiments using a microelectromechanical systems (MEMs)-based heating system, combined with C_S-corrected TEM. Their findings revealed that the nanotwins nucleate during the deposition of the i-a-Si:H layer and form during the subsequent annealing process.

"From our analysis, we conclude that suppressing twin nucleation in the initial stages is the critical step in reducing embedded nanotwins," the authors said. "We thus fabricated SHJ solar cells with low-density nanotwins by introducing an extra ultra-thin i-a-Si:H buffer layer and these cells exhibited better performance."

Zhang and his colleagues found that their strategy to restrain embedded nanotwins in c-Si/a-Si:H interfaces further enhanced the PCE of SHJ solar cells. As part of their study, they explored the potential of this strategy further, using it to change the initial surface of the c-Si wafer to ensure that it deviates from the {111} plane.

"The key objective of our work is the realization of a high-efficiency SHJ solar cell with a conversion efficiency of 24.85% prepared by an industry-compatible process," the authors said. "The discovery of embedded twins and the revelation that they hinder the improvement of cell conversion efficiency broke the traditional understanding: the dangling bonds at the c-Si/a-Si:H interface are the main stumbling block that affects the carrier interface."

The study by Zhang and his colleagues introduces a new strategy that could help to improve the efficiency of SHJ solar cells. In addition, it offers new insight about the structure of the c-Si/a-Si:H interface in high-efficiency SHJ solar cells at the atomic scale, showing that high-density embedded nanotwins are detrimental to these cells' performance.

"Employing first-principle calculations, our theoretical simulations revealed the nature of nano-twin, which is inevitable defect structure during the industrialized passivation process," the authors said. "Considering extra-deep levels of embedded nano-twin, it acts as recombination centers and impacting the performance strongly, we therefore proposed strategies to avoid from its generation, an ultrathin passivation layer. Following those process, our in-situ TEM measurements observed the density reducing of embedded nanotwins and we provided a novel approach to improve the performance of silicon solar cells."

So far, the recombination of c-Si/a-Si:H interfaces was considered the primary cause for energy loss in SHJ solar cells. Zhang and his colleagues investigated efficiency losses in their highest performing solar cells and found that high-density embedded nanotwins, detrimental to the device performance, typically formed in the thin epitaxial layer between c-Si and a-Si:H layers. They also found that adding an ultra-thin a-Si buffer layer significantly reduced the presence of embedded nanotwins and improved the cells' efficiency.

"Our findings imply that the PCE of SHJ solar cells can be improved when embedded nanotwins are restrained," the authors added. In fact, in our study we achieved an obvious performance improvement by reducing the density of embedded nanotwins. We will now focus on how to reduce/eliminate the nanotwins furtherly by adjusting their evolution process on c-Si and a-Si:H interface."

More information: Xianlin Qu et al. Identification of embedded nanotwins at c-Si/a-Si:H interface limiting the performance of high-efficiency silicon heterojunction solar cells, *Nature Energy* (2021). DOI: 10.1038/s41560-020-00768-4

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