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Silicon Quantum Dots in Photovoltaic Devices: Device Fabrication, Characterization and Comparison of Materials

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Short introductive summary

The realization of crystalline silicon tandem solar cells relies on silicon nanocrystal (Si NC) quantum dots as the absorber of the top solar cell. Quantum confinement of charge carriers within the nanocrystals permits to achieve a band gap up to 2 eV which can be adjusted according to the size of the nanocrystals. This enables the construction of all-crystalline Si tandem solar cells, and increases the theoretical efficiency limit from 33 % to 42.5 % due to the addition of a second band gap[1]. In this work, the electrical and photovoltaic properties of Si NC films are assessed and the most prominent material systems (SiO_2, Si_3N_4, SiC) are compared. *P-i-n* solar cells are presented which feature Si NC as the intrinsic absorber layer and permit to characterize quantum confinement electrically on device level. *P-i-n* solar cells with Si NC in SiC in the *i*-region have yielded open circuit voltages of up to 370mV.

Purpose of the work

Quantum confinement in Si nanocrystals has been shown optically with photoluminescence [2], and absorption, and theoretical studies have yielded much insight into the band structure and the role of the nanocrystal chemical environment [3]. However, electrical evidence for quantum confined carriers, i.e. a quasi Fermi level splitting higher than in bulk Si, still has to be given. This requires a device with a contacting scheme that permits to extract the implied photovoltage to the contacts [4]. In order to reach not only a high voltage but also a reasonable current and fill factor, electrical transport through the nanocrystal network has to be achieved.

Approach

Several test structures have been developed for the characterization of the photovoltage and the current transport properties of Si NC films. As the superlattice structure introduces an anisotropy which might favour transport either parallel or perpendicular to the layers, test structures for both cases are being realized. One of the main obstacles here is that the Si NC superlattice has to be crystallized at high temperature (>1000°C) on an insulating substrate before establishing the selective contacts for electrons and holes. To meet this requirement, we present in this paper a device which enables to characterize silicon quantum dot layers on device level without substrate influence.

Scientific innovation and relevance

Unlike in devices presented so far, the device presented here separates Si NC crystallization from the formation of the selective contacts to collect electrons and holes. Therefore the built-in voltage is not affected by any high-temperature treatments. The device structure can be applied to the host matrices SiO_2, Si_3N_4 and SiC and allows a direct comparison of the different material systems.

Results

P-i-n diodes were fabricated with SiC containing Si nanocrystals as the absorber in its intrinsic region. Selective contacts for electrons and holes were realized with phosphorous- and boron-doped a-Si_xC_{1-x}:H, respectively. With the structure and method presented here we are conclusively able to demonstrate that the photovoltaic activity originates only from the Si NC membrane *p-i-n* diode, without any contribution from peripheral (bulk Si) parts of the device. First structures have yielded open circuit voltages of 300 mV to 370 mV. Successive SiC-based devices with optimized material and defect passivation are currently being realized. Furthermore, superlattices of Si NC embedded in SiO_2 are implemented into the device.

Conclusions

With the device presented here we were conclusively able to demonstrate that the photovoltaic activity originates only from the film of Si NC in SiC, which forms the intrinsic region of a *p-i-n* diode. This device structure paves the way for unambiguous characterization of Si quantum dot and other thin film materials. Open-circuit voltages of up to 370 mV were shown which is encouraging for future tandem solar cells.

1. Meillaud, F., et al., Solar Energy Materials & Solar Cells, 2006. **90**(18-19): p. 2952-9.
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3. Guerra, R., E. Degoli, and S. Ossicini, Physical Review B, 2009. **80**(155332): p. 1-5.
4. Pysch, D., et al., Journal of Applied Physics, 2011. **110**: p. 094516.

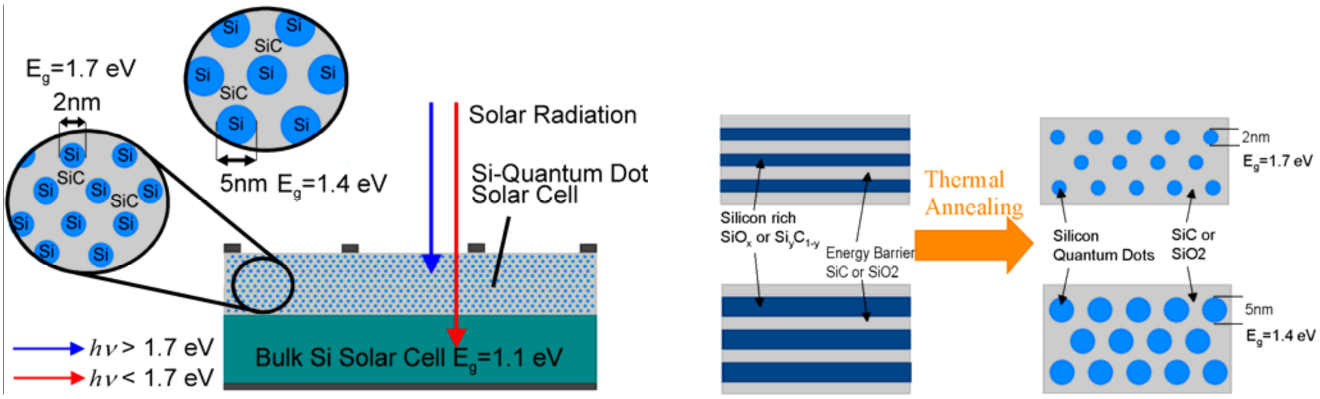

Figure 1: Principle of a crystalline Silicon tandem solar cell. The top solar cell consists of silicon nanocrystals in a silicon-based dielectric matrix such as SiO_2, Si_3N_4 or SiC. The bandgap of the nanocrystal solar cell can be controlled by the nanocrystal size due to quantum confinement effects. The high band gap silicon compounds SiO_2, SiC and Si_3N_4 are used as embedding matrices. All material systems are deposited as multilayers of alternating stoichiometric and Si rich layers. Si crystallites are formed in the Si rich layers by thermal annealing around 1100 °C. The stoichiometric layers act as diffusion barriers in the thermal annealing step and limit the size of the Si nanocrystals.

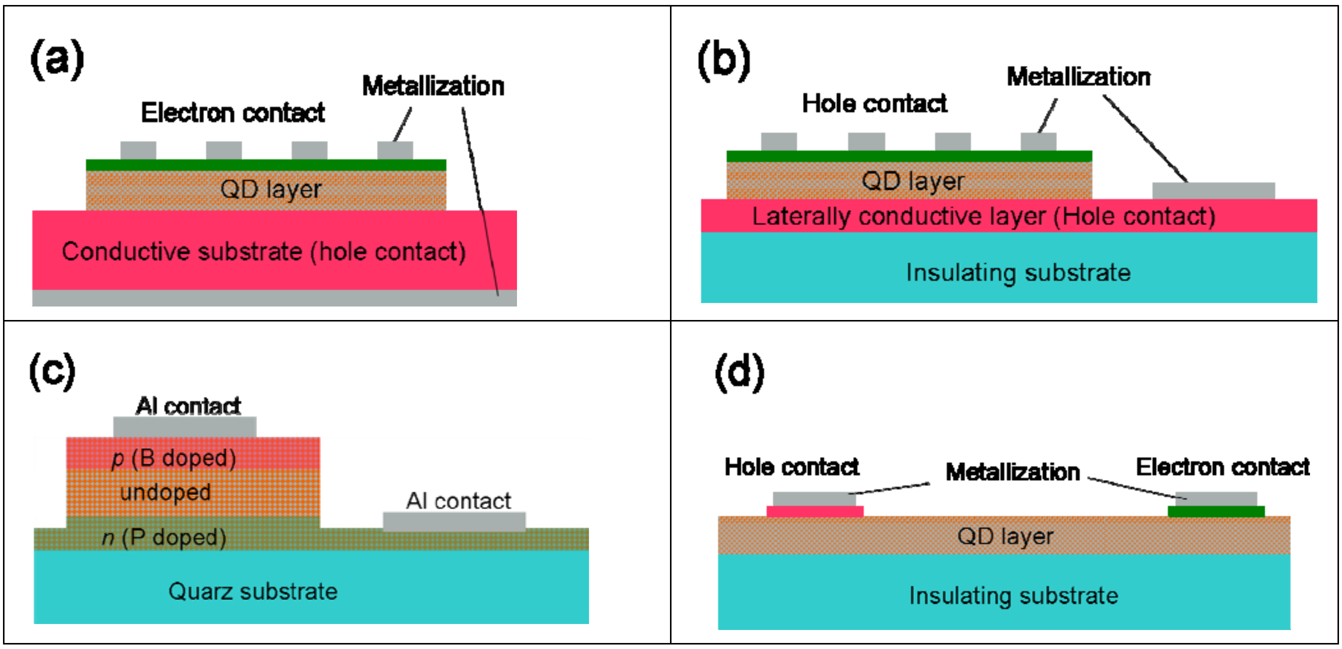

Figure 2: Contact possibilities for recrystallized layers. The contact can be established directly by a conductive substrate (a), or a doped layer on top of an insulating substrate (b). In a variant of (b), the Si nanocrystal layer itself is doped during its deposition, resulting in the structure shown in (c). For full flexibility in choosing the contact materials and processes, both contacts can be placed on top of the recrystallized layer (d). The structures (a) and (b) may be used to investigate the current transport through the Si nanocrystal superlattice. However, because the built-in voltage is heavily affected by the interdiffusion that occurs during thermal annealing, a device such as (d) is better suited to measure the photovoltage.

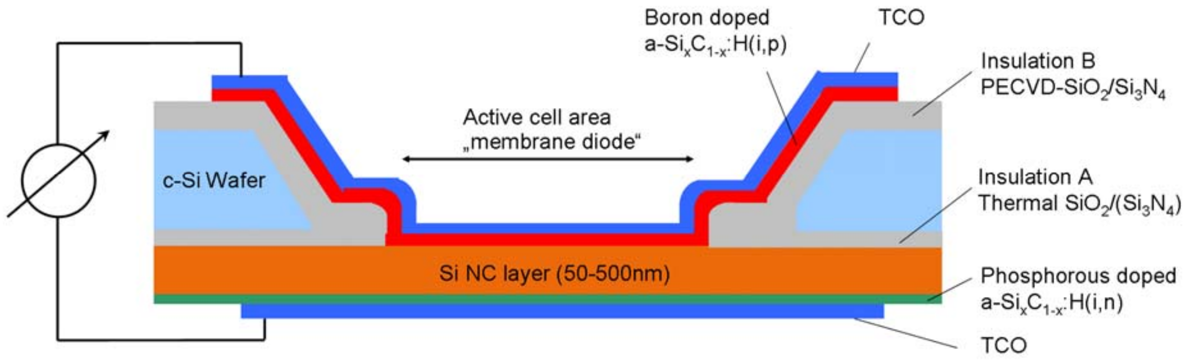

Figure 3. Structure for a vertical *p-i-n* solar cell with a Si nanocrystal thin film in the intrinsic region and selective electron and hole contacts by doped amorphous silicon carbide (a-Si_xC_{1-x}:H). The active cell is an entirely vertical device, i.e. no lateral conductivity is required and the device can be considered to be one dimensional.

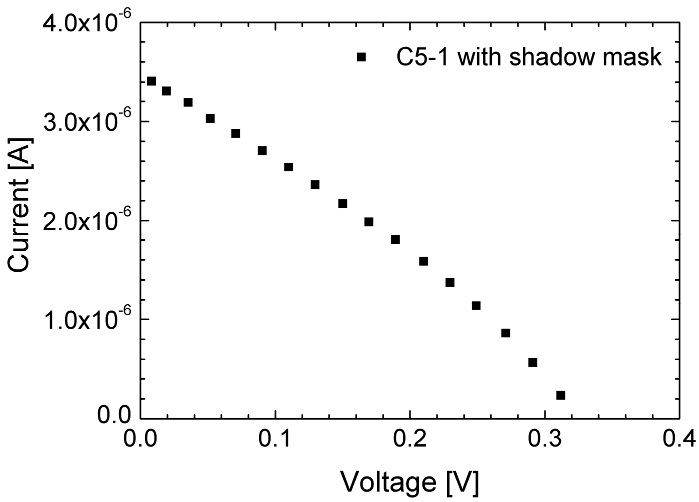

Figure 4: Current-voltage curve of a *p-i-n* solar cell with Si NC in SiC in the intrinsic region under illumination (sun simulator). An open-circuit voltage of 320 mV was achieved. The best cell yielded 370 mV open-circuit voltage.

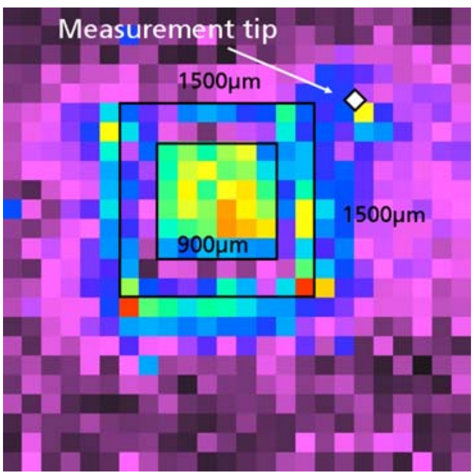

Figure 5: Light beam induced current (LBIC) map corresponding to the cell whose *IV*-curve is shown in Figure 4. The black boxes indicate the position of the cell itself (inner box) and reflected light into the cell (outer box). The light beam was reflected at the measurement tip. Therefore, also at the tip position a current is measured.