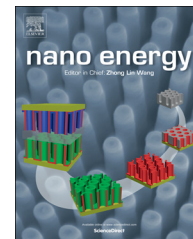




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RAPID COMMUNICATION

Oxygen passivation of silicon nanocrystals: Influences on trap states, electron mobility, and hybrid solar cell performance



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Abstract

Surface quality of nanostructures has a significant influence on related device performance. In this study, a large number of dangling bonds are detected on the silicon nanocrystal (Si NC) surface after surface modification. These dangling bonds work as carrier traps and degrade particle electrical properties. Therefore, controlled particle oxidization is proposed as a substitution method for surface passivation, which can reduce carrier traps easily and effectively. Electron mobility is improved dramatically after a 12-hour controlled oxidation, and as a result, Si NC/PTB7 hybrid solar cells (HSC) achieves an efficiency of 3.6%; this is more than twice the efficiency of devices fabricated with fresh Si NCs (without passivation), and the highest efficiency for Si NC-based HSCs reported to date. However, excessive oxidation should be avoided because it introduces an oxygen rich layer on the particle surface, which blocks carrier transport and deteriorates electrical properties inversely.

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Introduction

As the attractive candidates of acceptor materials, inorganic semiconductor nanocrystals (NCs) are being increasingly introduced into organic-based bulk heterojunction solar cells [1,2]. Compared to the organic counterparts, normally fullerene derivatives, NCs have promising potential in more efficient

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light-harvesting [3,4]; whilst keeping the superiorities which organic materials possess such as lightweight, flexible and solution-processable. In addition, NCs have several unique advantages. First, the shape can be tailored through synthesis methods; this has been proven useful for light trapping, exciton dissociation, as well as carrier transportation [5,6]. Also, when the size is comparable or smaller than its Bohr radius, the quantum effect makes NC work totally different with its bulk material. Indirect bandgap increases with decreasing size; this fact changes light absorption properties and provides the possibility of choosing the spectral window of the complementary absorption profile [7-9]. Meanwhile, continuous energy bands start to separate into discrete states [10,11]. This limits the energy loss through thermal relaxation, and facilitates multiple exciton generation (MEG) process [12,13], an effective strategy expected to promote solar cell power conversion efficiency (PCE) [14,15].

Recently, remarkable accomplishments have been achieved in NC/polymer hybrid solar cells (HSCs). Among them, CdS and PbS-based HSCs with PCE of 4.1% and 7% have been achieved, respectively [16-18]. However, toxicity prohibits their vast applications. Even so, from a scientific view, it is still a worthwhile endeavor to gain a deeper understanding of HSCs. Employing wide bandgap metal-oxide NCs such as TiO₂ and ZnO has achieved a PCE as high as 2% [19-21]. Nevertheless, further promotion would be a big challenge due to the wide bandgap, which assists a little in light-harvesting.

In addition to those mentioned above, silicon nanocrystal (Si NC) has been extensively studied and shown feasibility as a proper acceptor material in HSCs [22-25]. Silicon is environmentally benign and has strong absorption especially in the UV region [26,27]. Furthermore, instead of the complicated solution process commonly employed for NC synthesis (e.g., ZnO, PbS, and CdS.), mass production can be realized conveniently by means of a nonthermal plasma [28-32]. Devices with PCE at about 2% have already been achieved [33,34]. It is well known that surface quality of nanostructures has a significant influence on related device performance. Several pioneer works on Si NC-based device have shown that the performance can be further improved through proper Si NCs surface treatment [35-38]. In this work, we demonstrate that controlled particle oxidation can be employed as an easy and effective way for surface passivation. It plays a critical role in reducing particle dangling bonds, enhancing electron mobility, and lastly PCE of Si NC-based HSCs. Nevertheless, excessive oxidation should be avoided as electron mobility deteriorates reversely. Device PCE as high as 3.6% has been achieved after an optimized oxidation, which is the best value for Si NC-based HSCs until now, and indicates that it is competitive with other types of HSCs.

Experimental section

Si NC synthesis

Si NCs were synthesized from silicon tetrachloride (SiCl₄) by using a nonthermal plasma as previously reported elsewhere [25,30]. A quartz tube with inner diameter of 45 mm was employed as the reactor. Very high frequency (VHF) at 70 MHz was supplied on two copper electrodes surrounding the quartz tube. Particle properties such as crystallinity and size can be

well controlled through changing synthesis parameters. Here, Si NCs were synthesized with 8 standard cubic centimeters per minute (sccm) of SiCl₄, 80 sccm of H₂, and 240 sccm of Ar at a pressure of 400 Pa with an applied power of 65 W. Si NCs synthesized in the plasma were collected downstream of the plasma on a stainless steel mesh. All of the synthesis and handling of Si NCs were conducted without exposure to air. Synthesized Si NCs are highly crystallized as illustrated in Figure S1 (Supporting Information), where a typical transmission electron microscope (TEM) image and Raman spectrum of particles are shown. And particles have a mean diameter of 6 nm, which is achieved by statistical size measurement from atomic force microscopy (AFM) image of freestanding Si NCs as discussed elsewhere [25,34].

Si NC surface modification

However, as-produced particles are terminated by a large number of chlorine atoms because SiCl₄ is employed as the precursor [25,28]. The chlorine terminated surface is highly reactive and has been proven to be detrimental to device performance [25,34,39]. Hence, before use, chlorine was completely replaced by hydrogen through surface modification [34]. Firstly, as-produced, chlorine terminated Si NCs were intentionally exposed to open air for 30 minutes. During air exposure, chlorine atoms will be removed completely and particles were oxidized quickly. After this, HF vapor etching was employed to obtain hydrogen terminated particles. Specifically, oxidized particles were transferred on a Teflon supporting mesh, and put it above 50% HF acid in a sealed container. HF vapor etching was conducted at room temperature for 24 hours providing a sufficient reaction. Surface oxide will be etched completely during this process, and the particle surface will be mainly terminated by hydrogen, which is denoted as fresh Si NCs in the following. The resulting fresh Si NCs were immediately collected and returned back to a nitrogen-purged glovebox (<1 ppm water and oxygen) for further use.

Si NC surface oxygen passivation and solution preparation

Fresh Si NCs were oxidized carefully in air with controlled humidity of 30% and a temperature of 25 °C for 0, 1, 12, 24, and 48 hours, respectively. The resulting Si NCs were returned back to glovebox immediately. 30 mg/mL Si NC solutions were prepared by dispersing particles in chlorobenzene (CB, anhydrous, Sigma Aldrich) with homogenizer. Dense Si NC solutions can be diluted to desirable concentrations for specific experiments. For solar cells fabrication, Si NC and poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b']dithiophene-2,6-diyl][3-fluoro-2-[(2-ethylhexyl)carbonyl]-thieno[3,4-b]thiophenediyl]] (PTB7, Sigma Aldrich) solutions with the same concentration of 15 mg/mL in CB were blended together with a 1:1 volume ratio; blend solutions were stirred for 24 hours prior to use.

TFT fabrication and testing

Fabrication, handling, and measurement of TFTs were performed in a glovebox without exposure to air. A p⁺-type silicon wafer (resistivity ≤ 0.02 Ω · cm) with a 150 nm thermal

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