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ABSTRACT

The atomic structure and electronic properties of crystalline silicon/hydrogenated amorphous silicon (c-Si/a-Si:H) interfaces in silicon heterojunction (SHJ) solar cells are investigated by high-resolution transmission electron microscopy, atomic-resolution Z-contrast imaging, and electron energy loss spectroscopy. We find that all high-performance SHJ solar cells exhibit atomically abrupt and flat c-Si/a-Si:H interfaces and high disorder of the a-Si:H layers. These atomically abrupt and flat c-Si/a-Si:H interfaces can be realized by direct deposition of a-Si:H on c-Si substrates at a substrate temperature below 150°C by hot-wire chemical vapor deposition from pure silane.

1. Objectives

The silicon heterojunction (SHJ) solar cell is one of the most attractive device structures for fabrication of high-efficiency silicon solar cells at low temperatures (< 250°C) with simple processing. The superior performance of the SHJ structure is believed to be the result of the excellent passivation of the crystalline silicon (c-Si) surface by the hydrogenated amorphous silicon (a-Si:H) layer, which is used as both the front junction emitter and as a full contact back-surface-field (BSF). The outstanding performance of the c-Si/a-Si:H SHJ solar cells has been demonstrated successfully by the Sanyo HIT cells employing plasma-enhanced chemical vapor deposition to deposit p/i- and n/i-a-Si:H thin layers.¹ Recently, with an a-Si:H emitter only, NREL has achieved SHJ solar cells with an efficiency of 17% and an open-circuit voltage of 652 mV on planar p-type float-zone (FZ) silicon with a screen-printed aluminum BSF. Employing a-Si:H as both the front emitter and the back collector, NREL has achieved an open-circuit voltage of 691 mV on planar n-type FZ-Si and 660 mV on textured p-type FZ-Si.²

Our objectives are to investigate the atomic structure and electronic properties of the c-Si/a-Si:H interfaces using advanced electron microscopy techniques such as high-resolution transmission electron microscopy (HRTEM), Z-contrast imaging, and electron energy loss spectroscopy (EELS). We correlate our observations with the solar cell performance to provide critical information for further device improvement.

2. Technical Approach

We investigated the atomic structure and electronic properties of the c-Si/a-Si:H interfaces using our newly purchased transmission electron microscope (TEM), the Tecnai TF20-UT. Cross-sectional TEM samples were prepared by cleaving the SHJ devices without

further ion milling, so that no sample preparation-related damage or contamination were introduced to the samples. The microscope, equipped with a Gatan Image Filtering system, was operated at 200 kV. The Z-contrast images were formed by scanning a 1.4-Å probe across a specimen and recording the transmitted high-angle scattering with an annular detector (inner angle ~45 mrad). EELS data were taken with an energy resolution of 1.2 eV

3. Results and Accomplishments

The a-Si:H layers were grown by the hot-wire chemical vapor deposition technique from pure silane at a substrate temperature below 150°C. The details were described elsewhere.² Because the undoped intrinsic a-Si:H layers normally have a far lower density of defects and a slightly larger energy gap than doped a-Si:H layers, the undoped intrinsic a-Si:H is believed to provide better passivation effects than doped a-Si:H. Therefore, the NREL SHJ solar cells contain a thin (~5 nm) intrinsic a-Si:H layer.

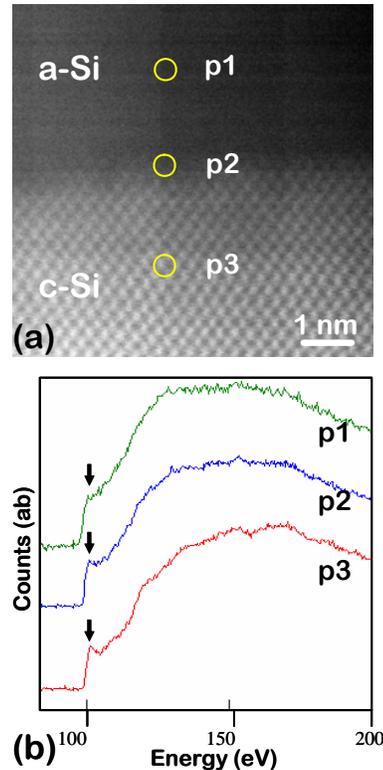


Fig. 1. (a) Z-contrast image of the front c-Si/a-Si:H interface in a double-heterojunction SHJ solar cell, and (b) Si-L edges spectra taken from different points around the c-Si/a-Si:H interface.

Figure 1(a) shows a Z-contrast image of the front (100) c-Si/a-Si:H interface in a double-heterojunction SHJ solar cell with a high V_{oc} of 680 mV. The electron beam is along the [110] zone axis. The intrinsic and doped a-Si layers are not distinguishable in the images. On the c-Si side, the elongated bright spots directly represent the two closely spaced (110) silicon columns, or silicon “dumbbells.” The dumbbells are not well resolved because the electron-probe of our microscope is slightly larger than the distance between the silicon columns. The amorphous feature is shown as continuous background in the Z-contrast image. Combining this Z-contrast image with other HRTEM images, we conclude that the interface is atomically abrupt and flat. To understand the electronic structure change across the interface, EELS spectra were taken at different points around the interface.

Figure 1(b) shows the Si-L edges spectra taken from three points indicated as p1, p2, and p3 in Fig. 1(a). Point 1 is inside the a-Si:H layer, point 2 is at the interface, and point 3 is inside the c-Si. It is seen that the intensity of the first peak (as indicated by black arrows) is reduced as the electron beam is moved from the c-Si area to the interface. It is further reduced when the electron beam is moved into the a-Si:H layer. The Si-L edges spectra represent the transition from the silicon $2p$ band to the conduction band. The intensity reduction of the first peak indicates that the density of states is reduced around the minimum of the conduction band. The reduction at the interface and in the a-Si is likely caused by the disorder. Thus, the intensity of this peak tells us the quality of the a-Si:H layer, i.e., the lower the intensity, the more disorder, i.e., the better a-Si. The EELS spectra in Fig. 1(b) indicate a high-quality a-Si:H layer is achieved.

Figure 2(a) shows a Z-contrast of the back c-Si/a-Si:H interface in a double-heterojunction SHJ solar cell. The electron beam is along the [110] zone axis. The intrinsic and doped a-Si layers are not distinguishable in the Z-contrast images. Combining our Z-contrast images and HRTEM images, we found that the c-Si/a-Si:H interface at the back side is also abrupt and flat. To understand the electronic structure change across the interface at the back side, we also obtained EELS spectra at different points around the interface. Figure 2(b) shows the Si-L edges spectra taken at three different points around the interface. Point 1 is inside the a-Si:H layer, point 2 is at the interface, and point 3 is inside the c-Si. It is seen again that the intensity of the first peak, as indicated by black arrows, is reduced as the electron beam is moved from the c-Si area to the interface. However, the intensity reduction in the a-Si:H area is not as great as that in Fig. 1(b). This might suggest that the quality of the a-Si:H layer in the back side is not as good as in the front side. This residual ordering in the a-Si:H layer should be removed to improve the quality of this a-Si:H layer.

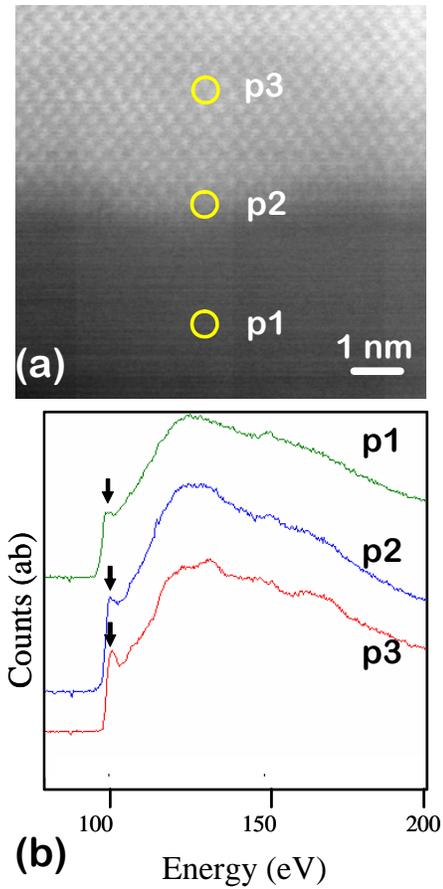


Fig. 2. (a) Z-contrast image of the back c-Si/a-Si:H interface in a double-heterojunction SHJ solar cell and (b) Si-L edges spectra taken at three different points around the interface.

4. Conclusions

The atomic structure and electronic properties of c-Si/a-Si:H interfaces in SHJ solar cells are investigated by HRTEM, atomic-resolution Z-contrast imaging, and EELS. Our results suggest that a high-performance SHJ solar cell should have an atomically abrupt and flat c-Si/a-Si:H interface and high degree of disorder in the a-Si:H layer.

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