doi:10.1017/S1431927614003705
Microsc. Microanal. 20 (Suppl 3), 2014

STEM-EELS Studies of the Local Structure and Coordination of Al_2O_3/Si interfaces in Si Solar Cells

Wei Zhang,[1] Kristopher O. Davis,[2] Winston V. Schoenfeld,[2] Pat Looney[1] and Feng Wang[1]

[1.]Sustainable Energy Technologies Department, Brookhaven National Lab, Upton, New York, 11973
[2]CREOL, The College of Optics and Photonics, and The Florida Solar Energy Center (FSEC), University of Central Florida, 4000 Central Florida Blvd, Orlando, FL

The efficiency of the Si solar cells may be significantly improved by coating of aluminum oxide (Al_2O_3) on Si surfaces for surface passivation[1]. Recent studies show that the efficiency is largely governed by the nature of the interface between Al_2O_3 and Si layer, which can be changed *via* post-annealing process[2]. Due to the limited thickness of Al_2O_3/Si interface, of only one or two nanometers, measurements by general methods such as x-ray photoelectron spectroscopy[3] and secondary ion mass spectrometry[4], can hardly provide detailed information on this interface. In the present work, the microstructure and chemical bonding of interfaces in Si/$Al_2O_3$and their change with annealing were investigated by high-resolution scanning transmission electron microscopy (STEM) imaging and electron energy-loss spectroscopy (EELS), at sub-nm resolution. The local coordination of Al and Si at the interface was determined by energy-loss near-edge structure (ELNES) of EELS spectra.

Amorphous Al_2O_3 passivation on Si (001) film was fabricated *via* a novel atmospheric pressure chemical vapor deposition (APCVD) process and activated by annealing at different temperatures. Annular dark-field (ADF), atomic Z-contrast images and EELS spectra were recorded from as-deposited and annealed samples in a JEOL 2100F microscope operated at 200 KV. A focused probe with full-width at half-maxima (FWHM) of 0.26 nm was used to obtain ADF, atomic z-contract images and Si Ledge and Al L-edge EELS spectra across the Al_2O_3/Si interface. The energy resolution of EELS spectra is about 1.2 eV. The background in EELS spectra was subtracted by using the power-law model[5].

Figure 1 shows the cross-sectional annular dark-field (ADF) images of the as-deposited and annealed (at 500 ℃) Al_2O_3/Si samples. An interfacial layer exists at the Al_2O_3/Si interface in both samples. The thicknesses of Al_2O_3 and interfacial layers were measured to be 21.8±0.4 nm and 1.5±0.2 nm for as-deposited sample. After post-annealing, the thickness Al_2O_3 of film decreased slightly (19.5±0.7 nm), and interfacial layer becomes thicker (2.3±0.4 nm). Beyond the crystalline Si layer, no lattice structure is visible, indicating that the interfacial and Al_2O_3 layers are amorphous before and after annealing.

EELS spectra of Si and Al L-edges acquired from the two samples, across the Al_2O_3/Si interfaces are given in Fig. 2. Clear differences of the spectra were observed in the interfacial regions (red curves). In the as-deposited samples, Si is in the elemental state, as evidenced by Si L_{23} edge located at 100 eV. And only octahedral peak from AlO_6 exists in the amorphous alumina layer (marked as octahedral peak O). However, after annealing at 500C , in addition to the octahedral peak at 80 eV, there is a new peak at 78eV (labeled as T), indicating the formation of tetrahedra Al_2O_4 in the Al_2O_3 layer. Also the tetrahedral configuration of SiO_4 emerges across the whole interface, as evidenced by intense Si L_{23} edge at about 105 eV.

Bulk properties of the samples, such as surface defect density (D_{it}) and fixed negative charge (Qf), were also measured from the same samples. The results from detailed STEM-EELS studies, with a correlation with bulk measurements will be presented. The impact of post-annealing on structural properties of the Al_2O_3/Si interface and efficiency of the Si solar cell will be discussed.

References:

[1] L.E. Black, K.R. McIntosh, Applied Physics Letters **100** (2012), p 202107.
[2] J. Benick, et al., Photovoltaic Specialists Conference (PVSC) (2010) p. 000891.
[3] V. Naumann, et al., Journal of Vacuum Science & Technology A **30** (2012), p 04D106.
[4] L. Gosset, et al., Journal of non-crystalline solids **303** (2002), p 17.
[5] R.F. Egerton in "Electron energy-loss spectroscopy in the electron microscope", ed. R.F. Egerton, (Springer, New York) p.269.

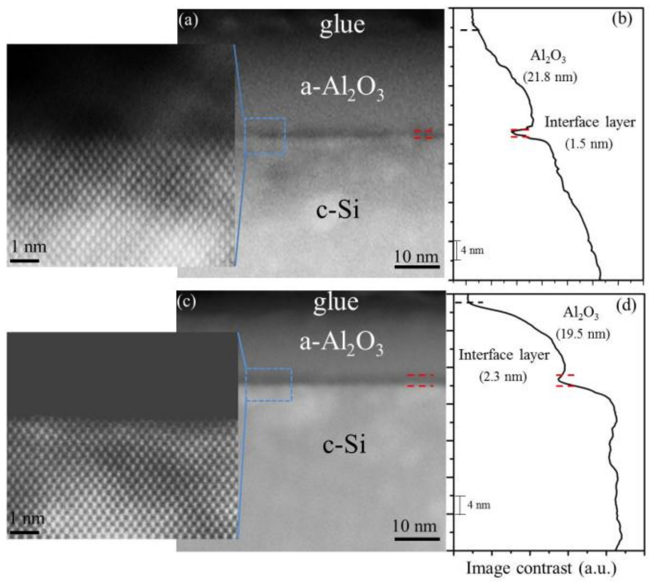

Figure 1. (a, c) Cross sectional ADF images of as-deposited samples (upper) and the sample annealed at 500 **°C** (lower) along the [011] direction and STEM images from the interface area (inset), (b, d) the profiles of the image contrast.

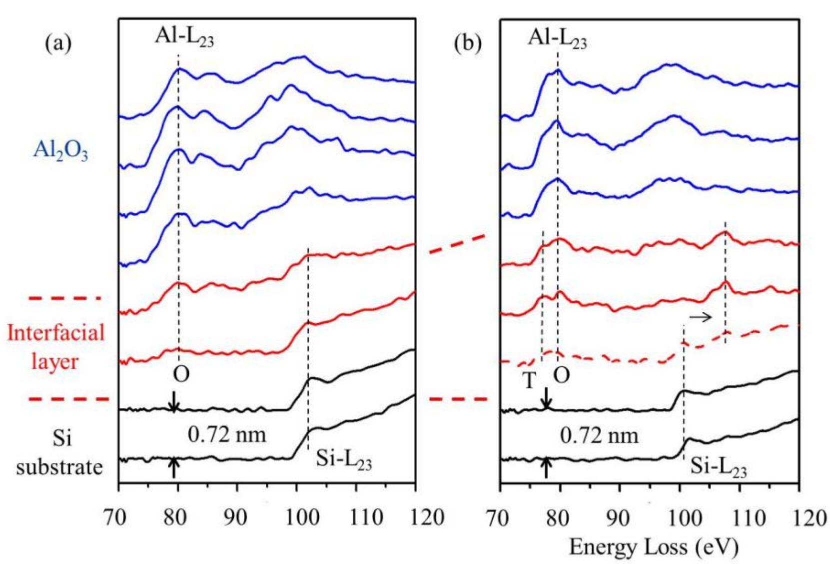

Figure 2. EELS spectra before (a) and after annealing at 500 ^{0}**C (b)**.

https://doi.org/10.1017/S1431927614003705 Published online by Cambridge University Press