

Structural characterization of intrinsic a-Si:H thin films for silicon heterojunction solar cells

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We have utilized ex-situ spectroscopic ellipsometry and HRTEM to characterize the optical and structural properties of intrinsic a-Si:H thin layer that plays a key role for the improvement of the open circuit voltage in silicon heterojunction solar cells. Intrinsic a-Si:H films were deposited on (100) p-type CZ silicon wafers by using Plasma Enhanced Chemical Vapor Deposition (PECVD) technique at 225 °C substrate temperature and deposition time ranges from 15 s to 1800 s. Observed changes in the imaginary part of pseudo dielectric constant, ϵ_2 , of c-Si spectrum with two peaks centered in 3.4 eV and 4.2 eV to a-Si:H which has an intermediate spectrum with a soft peak at about 4.2 eV has been analyzed with using effective medium approximation model.

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1. Introduction

There is a continuing efforts that silicon epitaxy could be used to thicken the crystal silicon seed layers for the fabrication of low cost and high efficiency photovoltaics on glass substrates [1]. Epitaxial growth has been successfully achieved on hydrogen terminated silicon wafers using for example plasma enhanced chemical vapour deposition (PECVD) [2-4]. Growth of epitaxial silicon is critically controlled by deposition conditions and it is generally not homogeneous. Although, about 1 μ m thick epitaxial growth has been achieved, generally after a critical thickness, epitaxial growth breaks down into either amorphous silicon or polycrystalline silicon [5]. Epitaxial silicon growth on silicon is analyzed using various techniques such as transmission electron microscopy (TEM), Rutherford backscattering or spectroscopic ellipsometry (SE).

Despite continuing efforts for the growth of silicon epitaxy, this is not desirable for the fabrication of a-Si:H/c-Si heterojunction solar cells since surface passivation of a-Si:H is better [6]. Often, epitaxial growth is observed on <100> oriented p-type substrates and at high temperatures in n-type substrates and is avoided by appropriately controlling deposition conditions [7].

In the present work, we have investigated the change in structure of the deposited epitaxial silicon growth on <100> oriented, p-type crystalline silicon wafers using spectroscopic ellipsometer, HRTEM and Fourier transform infrared spectroscopy (FTIR). SE data is analyzed using Bruggeman effective medium approximation method and is sustained with FTIR and HRTEM data.

2. Experimental details

Films were deposited in multi chamber UHV-PECVD system operating at 13.56 MHz on p-type, <100> oriented, 1-20 ohm.cm, CZ crystalline silicon wafers. Prior to deposition the substrates were cleaned by RCA cleaning and dipped into HF acid before placing into deposition chamber. Substrate temperature was 225 °C and deposition time is varied from 15s to 1800s.

Spectroscopic ellipsometer data were acquired with a variable angle spectroscopic ellipsometer (SA Jobin Yvon-Horiba) of the rotating analyzer type. All measurements were performed in air at room temperature in the wavelength range of 245 to 1200 nm. Measurements were carried out at 70° angle of incidence. All data analyses were made using DeltaPsi II software. In order to obtain the optical constants for the samples, measured data was fitted with the Tauc-Lorentz formula. The analysis of SE data was performed using a multilayer model. The surface roughness layer was modeled as mixture of the bulk material and voids using the Bruggeman effective medium approximation.

In TEM (Transmission Electron Microscopy) studies HRTEM (High Resolution Transmission Electron Microscopy) techniques were used to investigate the deposited films with JEOL JEM 2100 at 200 kV. TEM samples were prepared with Gatan 691 Precision Ion Polishing System (PIPS). Fourier Transform Infrared Attenuated Total Reflection spectroscopy (FTIR-ATR) technique was applied to measure the vibrational response of the Si-H bonds in the frequency range of 400-4000 cm⁻¹ with a resolution of 4 cm⁻¹.

3. Results and discussion

Variation of surface roughness, bulk thickness and crystallinity of deposited film can be investigated using SE. Imaginary part of the dielectric function for c-Si has two peaks centered at 3.4 eV and 4.2 eV, while a broad peak is observed for a-Si:H at 3.5 eV [8]. Additionally, μ c-Si:H has an intermediate spectrum with a soft peak at about 4.2 eV and there is a bump with a shoulder in the dielectric constant at low photon energies.

Fig. 1(a) shows imaginary component of the dielectric function for c-Si wafer and a-Si:H film deposited for 120s on c-Si wafer. Micro-crystalline phase in the films is identified from a bump with a shoulder at low photon energies. Additionally, HRTEM image of 120s film is also presented in Fig. 1(b). From HRTEM and SE measurements we have observed the presence of epi layer and the amorphous layer together in the structure of the deposited film. In order to obtain the thickness and the optical parameters of the deposited layer, we have successfully applied a multilayer model which consists of a substrate, an epitaxial silicon layer, a graded breakdown layer for transition from crystal silicon at the bottom to amorphous silicon at the top, an amorphous layer itself and an effective medium of amorphous silicon and void layer, which yields a full history of the deposition.

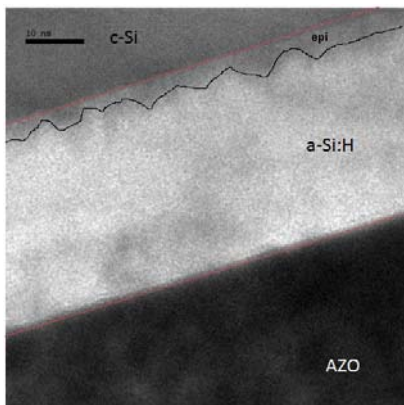
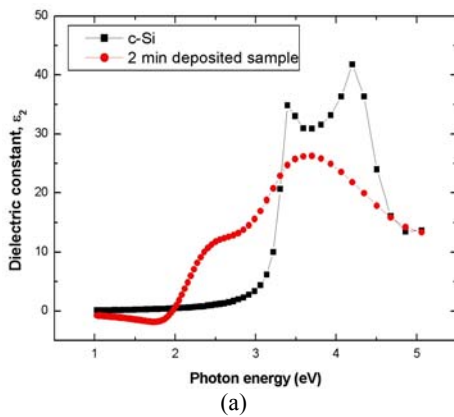


Fig. 1. (a) Photon energy versus ϵ_2 for c-Si and 120s a-Si:H film, (b) HRTEM image of 120 s a-Si:H film.

In order to study the structural variation of a-Si:H on c-Si surface with deposition time, series of films were grown at 225 °C and obtained dielectric function graph of these samples are given in Fig. 2. It is observed that the crystallinity in the films decreases with deposition time. While, a-Si:H layer deposited at $t = 15$ s and 30 s exhibit similar optical constants as crystalline silicon, which implies that the films are nearly completely epitaxial; a broad featureless spectra for $t=1800$ s suggests nearly a-Si:H structure.

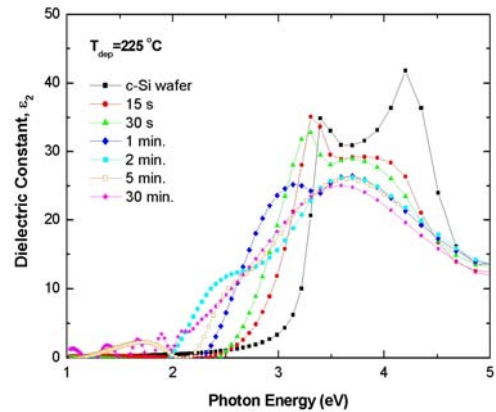


Fig. 2. Photon energy versus ϵ_2 graph of deposited a-Si:H thin films at different deposition time periods.

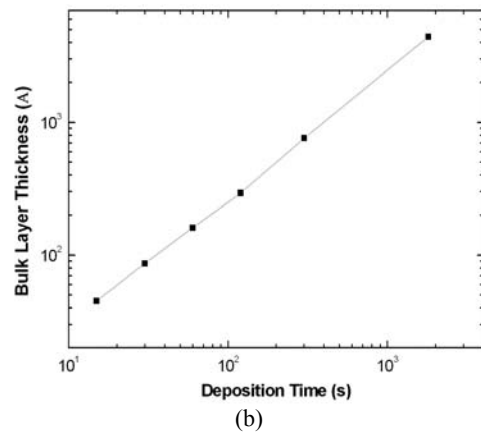
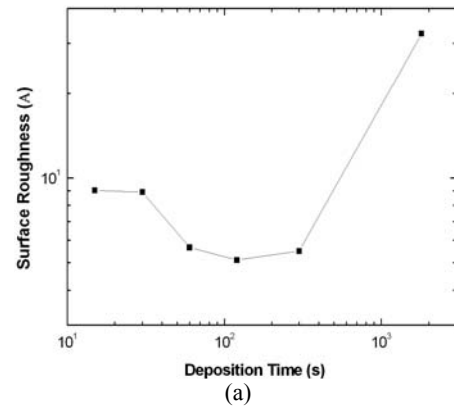


Fig. 3. (a) Variation of the surface roughness and (b) bulk layer thickness of the a-Si:H films.

Variation of the surface roughness indicates a phase transformation of the growing film. Film growth begins in an isolated nucleation sites on the substrate surface, which leads to rapid initial increase in the surface roughness. When continuous film formation starts, surface roughness rapidly decreases [9]. Fig. 3 shows variation in the surface roughness and bulk layer thickness as a function of deposition time deduced from analysis of SE measurements. Following a maximum, surface roughness decreases and starts saturating after 60s. At very long deposition times surface roughness increases again indicating there could be mixed a-Si:H and μ c-Si:H phase in the film growth. Bulk layer thickness increases linearly with deposition time.

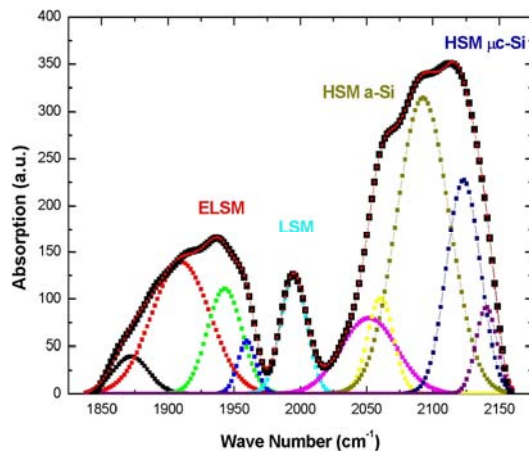


Fig. 4. Hydride stretching modes in the FTIR spectra for 15 s film.

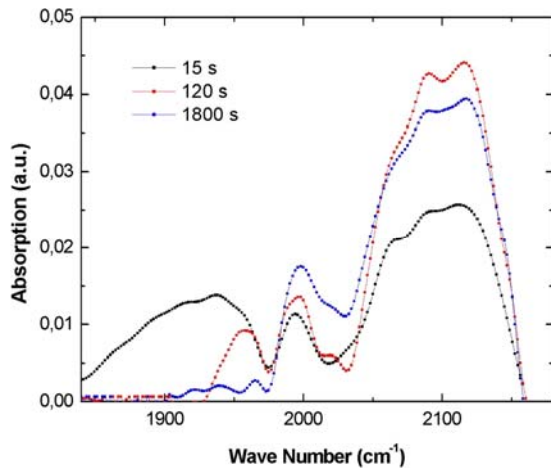


Fig. 5. Variation of FTIR spectrum of the films at different deposition times.

Hydrogen bonding configuration of the deposited films was analysed by Fourier transform infrared (FTIR) vibrational spectroscopy. During analyses we have focused on the most informative Si–H stretch region between 1900–2250 cm^{-1} . Deconvolution of IR spectrum for the 15s film is shown in Fig. 4 where observed stretching modes are indicated. These are extreme LSMs (ELSM, 1895, 1929 and 1950 cm^{-1}), the low SM (LSM,

1980–2010 cm^{-1}), the two high SM (HSM, 2070–2100 cm^{-1} , 2120 cm^{-1}) [10]. Evolution of the FTIR spectrum with deposition time is presented in Fig. 5. ESLM dominates the spectrum at early times suggesting that hydride-dense a-Si:H tissue, which either passivates the crystalline grain boundaries or fills the small pores is present in the films [10]. At 120s, where surface roughness is at a minimum value (Fig. 3) a small ELSM is observed while, HSM for both a-Si:H and μ c-Si:H remarkably increases. As deposition time further increases, HSM modes slightly decrease while LSM increases suggesting mixed growth of a-Si:H and μ c-Si:H.

4. Conclusions

Structural variation of a-Si:H on p-type, <100> c-Si wafer is investigated using SE, HRTEM and FTIR measurements. At early durations of the deposition where surface roughness is high, a mixed deposition of epitaxial, a-Si:H and μ c-Si:H growth is observed. As the deposition time is increased structure of the film becomes mostly amorphous mixed μ c-Si:H. Decrease in deposition temperature is necessary to prevent epitaxial silicon growth.

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