PROPERTIES OF THIN-FILM SILICON IN THE TRANSITION REGION FROM THE AMORPHOUS TO NANOCRYSTALLINE PHASE

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Amorphous hydrogenated silicon (a-Si:H) solar cells represent a promising solar cell technology of the second generation. Advantages of this technology are its low cost and the possibility to manufacture the cells on flexible substrates. By combining the a-Si:H cell with a microcrystalline bottom cell, in the so-called micromorph configuration, efficiencies of up to 14% can be achieved [1].

A drawback of a-Si:H solar cells is the light-induced degradation that is a manifestation of the Staebler-Wronski effect in a-Si:H. There is a strong research effort to prepare a-Si:H material with improved stability. So far it has been demonstrated that a-Si:H deposited from silane diluted with hydrogen shows an improved stability against light soaking. Increasing the dilution ratio R, defined as $R=[H_2]/[SiH_4]$, results in films with increased stability, which is attributed to the increase of the medium range order in the material.

However, under these deposition conditions the growth of a silicon film is inhomogeneous and the film evolves from the amorphous (a-Si:H) to the microcrystalline (μc-Si:H) phase [2,3]. The properties of the films in the transition phase strongly depend on the deposition parameters, especially the dilution ratio R. A phase-diagram of silicon films deposited at different R, which was obtained by monitoring the surface roughness using spectroscopic ellipsometry measurements, is shown in Figure 1 [2].

We present results of a structural characterization of a series of hydrogen diluted silicon films deposited with rf-PECVD. Figure 2 shows Transmission Electron Microscopy (TEM) images of 1μm thick Si:H films deposited with a hydrogen to silane dilution ratio from R=0 to R=40. It can be seen from these images that the layers are completely amorphous up to a hydrogen dilution of R=20. For higher dilution ratios a phase transition occurs in the films, which is more abrupt when the dilution is increased.

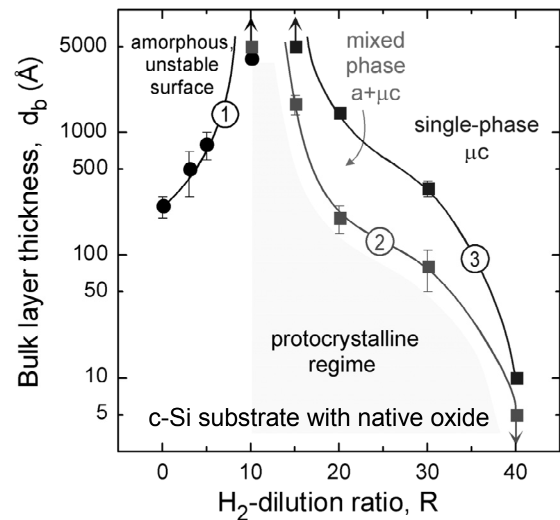

Figure 1. Phase transitions in Si:H as a function of the hydrogen dilution [2]

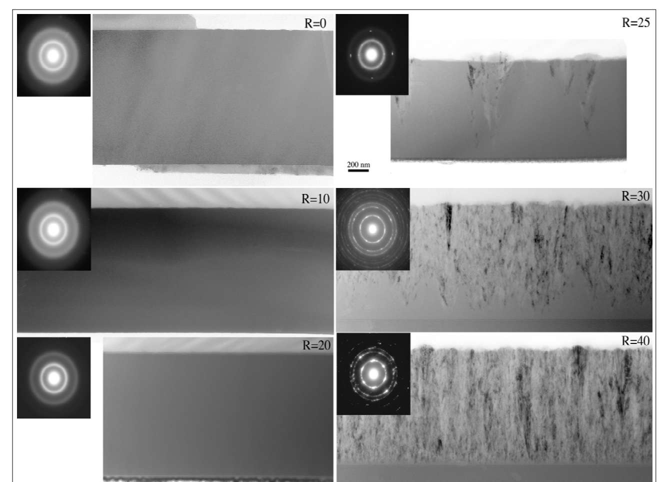

Figure 2. TEM images of 1μm thick Si:H layers with dilution ratio R as indicated

In addition to the TEM technique, Raman spectroscopy was used to evaluate the phase transition in the films. From the Raman spectra of the films the crystalline fraction in the material can be estimated. Figure 3 shows the crystalline fraction determined from thickness series of Si:H layers. The results correspond well with the TEM images.

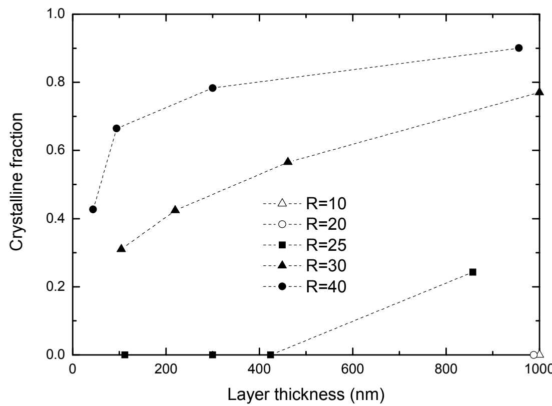

Figure 3. Surface crystalline fraction determined with Raman spectroscopy as a function of layer thickness

Since the electronic quality of the Si:H is strongly related to the amount of dangling-bond defects in the material, the defect density was estimated from the absorption spectra. These spectra are obtained using Dual Beam Photoconductivity measurements combined with Reflection and Transmission measurements. Figure 4 shows the absorption coefficients as function of photon energy for 400 nm thick layers with a dilution of R=0, 10, 20, 25, 30 and 40. The layers deposited with R=30 and R=40 show a typical microcrystalline curve, whereas the other layers display a typical amorphous absorption profile.

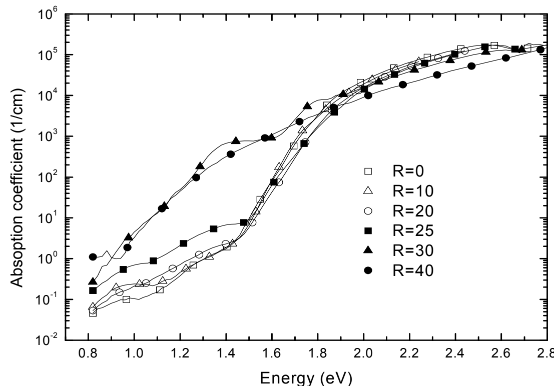

Figure 4. Absporption coefficient spectra for 400 nm Si:H layers deposited with different R

Table 1. Properties of 400 nm Si:H layers

R		E_{04} [eV]	E_u [eV]	α(1.2eV) [cm^{-1}]	α(0.8eV) [cm^{-1}]	Nd [cm^{-3}]
0	a-Si	1.88	0.048	0.38		9×10^{15}
10	a-Si	1.92	0.045	0.46		1×10^{16}
20	a-Si	1.94	0.051	0.71		2×10^{16}
25	mixed	1.96		2.12		5×10^{16}
30	μc-Si	1.88			0.26	4.4×10^{16}
40	μc-Si	2.02			1.0	1.7×10^{17}

Table 1 presents the calculated defect densities in amorphous and microcrystalline material from the absorption spectra, according to the methods described in [4, 5]. It can be seen from Table 1 that higher diluted films have an increased defect density, which can be attributed to the inhomogeneous growth.

Circumvention of the phase transition is a key issue for Si:H materials, both for μc-Si:H and a-Si:H. Several methods have been used to approach homogenous Si:H layers with high hydrogen dilution. One of them is hydrogen dilution profiling, in which the dilution is adjusted during deposition. For this method the use of in-situ characterization by spectroscopic ellipsometry is almost indispensable to prevent the phase transition by monitoring the surface roughness. The best μc-Si:H and a-Si:H materials grown with this method are reportedly deposited close to either side of the transition.

We focus on a layer-by-layer approach, in which thin undiluted interlayers are used to interrupt the microcrystalline growth and achieve amorphous Si:H layers with sufficient thickness for application in solar cells. Raman spectroscopy measurements have shown that application of 10 nm undiluted amorphous interlayers can effectively reduce the crystal growth in films deposited with a dilution ratio of R=30.

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