Analysis of amorphous-nanocrystalline silicon thin films by High Resolution Transmission Electron Microscopy and Time-of-Flight Elastic Recoil Detection Analysis

K. Juraić[1], D. Gracin[1], Z. Siketić[1] and M. Čeh[2]

1. Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia
2. Jozef Stefan Institute, Jamova 11, Ljubljana, Slovenia

Presenting author: kjuraic@irb.hr
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Amorphous-nanocrystalline silicon (a-nc-Si:H) is mixed-phase material consisting of silicon nanocrystals embedded in amorphous silicon (a-Si:H) matrix. It has promising technological applications in photovoltaic devices and thin film transistor. Electrical and optical properties of a-nc-Si:H can be controlled by silicon nanocrystals size distribution and ratio of amorphous/nanocrystalline volume contribution. Because of better resistivity to Staebler-Wronski degradation, sufficient electrical conductivity, variable energy bandgap and absorption coefficient of the same order, compared to amorphous silicon, a-nc-Si:H are promising candidate for application in "third generation" thin film solar cells.

100 nm thick a-nc-Si:H/a-Si:H bilayer structure (Figure 1) are prepared by Plasma Enhanced Chemical Vapour Deposition (PECVD) using radio frequency discharge in gas mixture of silane (90%) and hydrogen (10%) for amorphous layer while dilution was enhanced up to 94% hydrogen in gas mixture for formation a-nc-Si:H [1]. The substrate was glass and glass covered with SnO_x thin film. The power density during the formation of a-nc-Si:H layer was 20 mW/cm^2 resulting in film growth rate of 2 nm/min.

As seen by high resolution transmission electron microscopy (HRTEM), the films contained nanocrystals of silicon (2-10 nm in size) embedded in a-Si:H matrix. The size of nanocrystals and crystal to amorphous fraction are increased starting from substrate towards surface of the film. Amorphous matrix looked uniform except in the area close to a-Si:H/a-nc-Si:H interface where spots brighter than average appeared (Figure 1). These areas can be attributed to less density material, presumably voids. It is assumed that the surface of voids is "decorated" with hydrogen that saturates silicon "dangling bonds" [2]. That is why distribution of hydrogen should indicate density fluctuation in material.

The in-depth distribution of hydrogen atoms in 100 nm thick a-nc-Si:H/a-Si:H with 10 nm resolution was estimated by Time-of-Flight Elastic Recoil Detection Analysis (TOF ERDA) using previously described setup [3]. TOF-ERDA (Figure 2) showed non uniform distribution of hydrogen across the depth with maximum close to a-Si:H/a-nc-Si:H interface that coincidence with less density material seen by HRTEM. This supports the idea about important influence of voids in crystal formation, in particularly in nucleation phase.

References:

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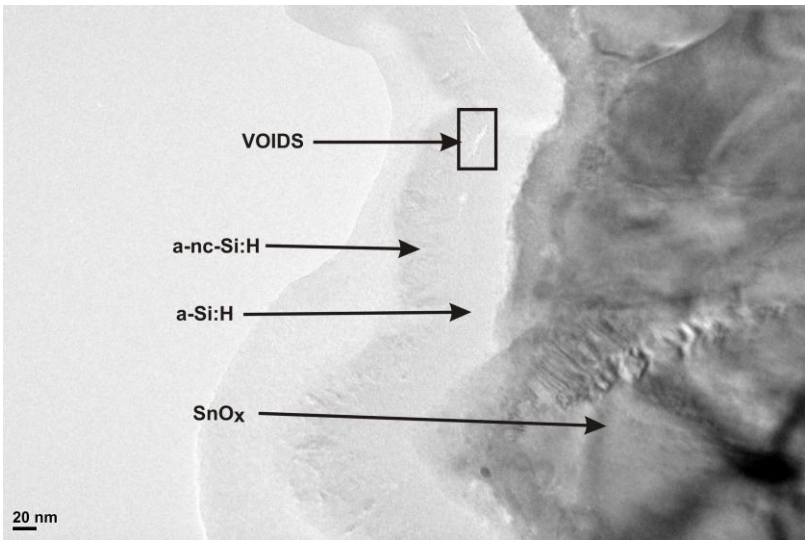

Figure 1. TEM micrograph of a-nc-Si:H sample deposited on SnO + glass substrate.

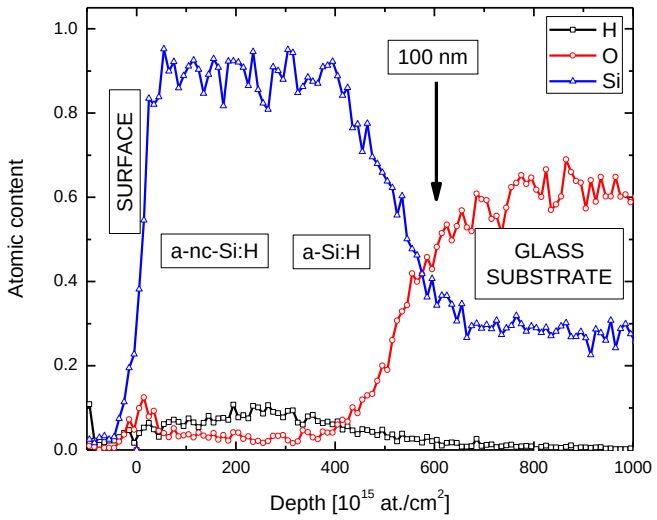

Figure 2. Results of TOF-ERDA elemental analysis of a-nc-Si:H/a-Si:H as function of depth