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Small-Angle Neutron Scattering Studies of a-Si:H and a-Si:D

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ABSTRACT

The heterogeneity of hydrogen and deuterium on the nanometer scale has been probed by small-angle neutron scattering (SANS) from a-Si:H and a-Si:D films. Films were deposited by two techniques, plasma-enhanced chemical vapor deposition (PECVD) and hot-wire chemical vapor deposition (HWCVD) using conditions that yield high quality films and devices. Two important results are that no detectable light-induced changes were observed, in contrast with an earlier result, and that significant differences in SANS were observed between the samples made with various deposition conditions.

1. Introduction

Extensive small-angle x-ray scattering (SAXS) studies of a-Si-based materials have provided new information on the structure of these materials on the nanometer scale [1]. The purpose of this research is to complement the SAXS-based information with small-angle neutron scattering (SANS) measurements which are, in principle, much more sensitive to the hydrogen distributions [2]. Also, the possibility of substituting D for H allows additional information due to the large differences in scattering of neutrons by these two isotopes [2]. Although there has been previous SANS research with a-Si-based materials [3-5], there has been little documentation of the device quality of the material used in these investigations. Typically, good SANS signals were obtained with the poorer quality material. One intriguing result obtained in the mid-1980's was the observation of a light-induced change in the SANS [6], which could be explained only by a rather large-scale change in the H distribution [7]. We wanted to try to reproduce this result due to the implication for models of the Staebler-Wronski effect. We also wanted to test whether useful SANS data can be obtained from device-quality material using the high-flux SANS facility at the NIST Center for Neutron Research (NCNR) [8].

2. Experimental

The SANS measurements were done at the NCNR on beamline NG-3. Data were collected over a momentum transfer range from q = 0.05 nm^{-1} to 3 nm^{-1}, using neutrons with wavelength 0.6 nm and two detector positions (2 m and 13 m from the sample). Several special samples were prepared, some with deuterated gases (SiD_4, D_2) used in place of SiH_4 and H_2. Special, high purity FZ c-Si substrates were used with surface roughness below 0.5 nm (checked via AFM measurements) in order to prevent extra background scattering. Multiple films of 1 to 2 μm thickness were prepared to allow stacking of up to 20 layers. Four samples made under conditions that yield high quality material (high hydrogen or deuterium dilution in PECVD, and high substrate temperature in HWCVD) were examined in both a light-soaked state (300 h, AM1) and an annealed state (190°C, 1 h). The latter was done *in-situ* with a special annealing chamber and insured that no changes in measurement geometry occurred between the two states.

3. Results and Discussion

Example SANS data from two samples are shown in Fig. 1. Note the range of intensities over several orders of magnitude and the significant differences in the SANS intensities versus q for the PECVD and the HWCVD samples. Also note the good statistical quality of the data. The lower intensity at high q for the HWCVD sample is due to a much lower H content. We found significant differences in the SANS from the deuterated samples, partly due to the formation of microcrystalline material via the PECVD technique when using the high D_2 dilution condition. Fitting of the data with various models is underway to extract details of the H(D) nanostructure such as sizes of the scattering features and the variation in H(D) concentrations needed to explain the intensities observed. The latter is made possible by the use of absolute cross-section intensity units ($cm^{-1}ster^{-1}$) in processing the data.

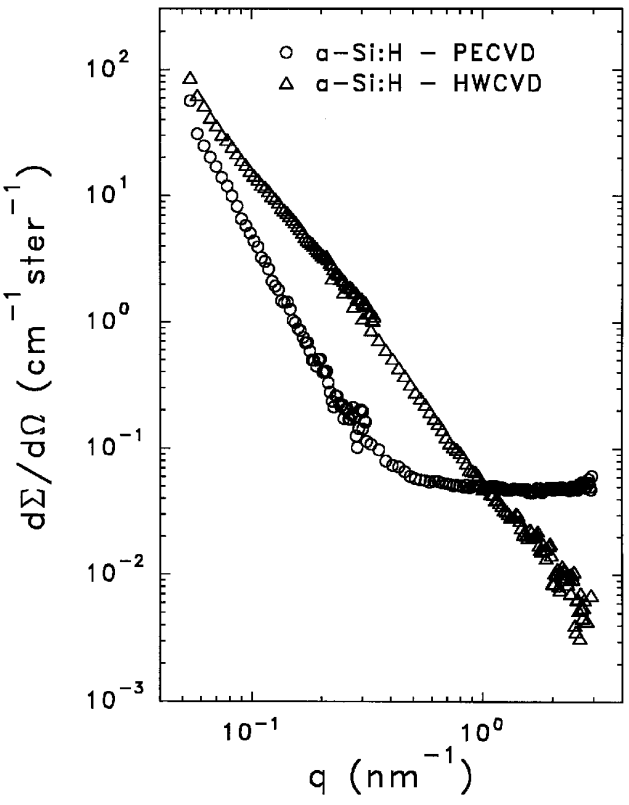

Fig. 1. Example SANS data from films of a-Si:H.

There was no obvious change in the SANS intensities caused by annealing the four light-soaked films. The previous result indicated an increase of 25% in the intensity at all q upon light soaking [6]. In order to examine our data more carefully, the ratio of light-soaked/annealed intensities was computed for each sample over all experimental q's. The ratios are unity within an experimental scatter range of about ± 2%.

4. Conclusions

The previous Staebler-Wronski-effect-induced change in nanostructure reported several years ago [6] could not be reproduced in the present study. No detectable changes were found. We also established that statistically-significant SANS data can be obtained from device-quality films. Analysis of such data should lead to improved understanding of the non-uniform H distributions and their ultimate connection with the opto-electronic properties.

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