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PACS: 68.60.-p; 71.23.Cq; 72.40.+w

Manuscript

COMPLEX STUDY OF MECHANICAL PROPERTIES OF a-SI:H AND a-SIC:H BORON DOPED FILMS

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Comment [k1]:

ABSTRACT

The aim of the present work is to provide the complex study of the mechanical properties of p-doped a-Si:H and a-SiC:H thin films prepared under different plasma conditions. For the investigation of the samples we used mainly the continuous depth sensing indentation technique (DSI), pin-on-disc test and internal stress measurement. The morphology of the thin film surface and the indentation prints are studied using optical microscopy, scanning electron microscopy (SEM) and topography mode of atomic force microscopy (AFM). The dependence of the mechanical parameters upon the deposition conditions were compared with the optoelectronic properties of studied films.

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1. INTRODUCTION

The main priority when preparing the thin films for optoelectronic device application is their good optical and transport properties. However, for the final applications, the good mechanical and thermomechanical stability is not of the second order of importance. The large internal mechanical stress and/or weak adhesion can result the deterioration of the optoelectronic device (cracking, delamination). Material parameters such as microhardness, internal stress, elastic modulus, fracture toughness and adhesion have been studied more often due to their importance for the development of thermo-mechanically stable devices. In this work the above listed material parameters of doped thin a-Si:H and a-SiC:H films determined by depth sensing indentation technique were investigated as a function of boron doping.

2. EXPERIMENT

Boron doped a-Si:H and a-SiC:H, 0.54-0.68 μm thick films were deposited on Corning glass substrates at 180 ^{o}C by RF glow discharge decomposition of 10 sccm of silane mixed with either diboran or thrimethylboron diluted at 2% in hydrogen [1, 2]. The boron-doped silicon-carbon alloys (a-SiC:H) usually used as window layers in solar cells were produced by the decomposition of the mixture of 50% silane and methane. The boron containing doping gas to silane or silane + methane flow rate ratio was defined as doping level C_d.

The depth sensing indentation (DSI) method was used for determination of mechanical properties of the films. In the case of our indentation tester the applied load is registered as a function of indentation depth both during loading and unloading. From the loading/unloading curves we obtained the universal hardness HU as a measure of the resistance against elastic and plastic deformation, the total indentation work W_{tot}, the elastic deformation work W_e and the irreversible dissipated indentation work. From the load-penetration curves it was possible to determine also the material resistance against plastic deformation H_{pl} (so called plastic hardness). The DSI technique enables to calculate the effective elastic modulus Y of the tested material ($Y \approx E/(1-\nu^2)$, where E is the Young's modulus and ν is the Poisson's ratio of the measured material) from the slope to the unloading curve at maximum

depth [3]. By fitting of the load-penetration curve, we can obtain other materials parameters, for example the compressive yielding stress.

The Vickers indentation may introduce substantial cracks and adhesive failures into the thin films. Analysis of the morphology of the indentation prints enables to determine material characteristics as the fracture toughness of the films and its adhesive properties. If the interface between the film and substrate can slip or fracture the indentation method can be used to measure adhesion [4].
The fracture toughness of the film-substrate interface from the indentation could be determined according to [5].

The morphology of the film surface was studied by means of an optical microscope, an optical stereomicroscope, a scanning electron microscope (SEM) and by atomic force microscopy (AFM).

The optical properties of the films were measured by UV-visible ellipsometry. The optoelectronic properties were determined from photothermal deflection spectroscopy, constant photocurrent measurements and from conductivity measurements. From deconvolution of absorption spectra the parameters like optical gap E_g, the valence band tail slope E_{OV}, and the density of deep states (integral under gauss curve) B can be determined.

3. RESULTS

In Table 1 the basic material parameters of the studied a-Si:H and a-SiC:H are given. The films were smooth; the RMA roughness obtained from AFM was in the range from 1.8 to 2.6 nm. The indentation prints in a-Si:H and a-SiC:H imaged by AFM are presented in Figure 1.

The layers were transparent with the band gap between 1.80-1.87 eV for a-Si:H and around 1.99 eV for a-SiC:H. The a-Si:H films and a-SiC:H films differed in their static refractive index that was 3.5 and 3.2 respectively. Figure 2 shows the universal HU. The elastic modulus Y and the plastic H_{pl} microhardness dependence on the doping level are presented in Figure 3.

4. DISCUSSION

The slope of the valence band tail E_{OV} (see Table 1), which is an indicator of disorder in the material, is higher for the doped a-SiC:H films than for the doped a-Si:H. In our previous paper [1] the

poorer morphology of the a-SiC:H alloys compared to the a-Si:H and the smaller effect of the boron doping on their properties was discussed. These results are in very good agreement with the microhardness measurements. The p-doped a-Si:H films have substantially higher microhardness for low level of doping than p-doped a-SiC:H. The higher hardness of a-Si:H films compared to a-SiC:H may be explained with their higher density, deduced from the static refractive index, and with their lower disorder. The above mentioned material parameters together with the elastic modulus (Figure 3) and the elastic to total indentation work ratio (Figure 4) has decreasing tendency with the doping in the case of a-Si:H and remains almost constant (or slightly increase) for a-SiC:H. This behaviour can be explained by the effect of doping upon the hydrogen content. This is supported by the optical gap E_g that in the case of a-Si:H films shows first a slight increase and after a maximum at low doping levels decreases (Table 1). On the other hand, the band gap remained almost constant in the studied range of the doping of a-SiC:H films.

The fracture toughness of the film-substrate interface had an opposite tendency than the hardness; it was increasing with the doping. The adhesion and the fracture toughness of a-Si:H films were higher than for a-SiC:H films. The lower fracture toughness of a-SiC:H films was caused by their higher compressive stress; the low-doped films had higher compressive stress. The highest compressive stress was observed for a-SiC:H film prepared with doping level $C_d = 0.001$.

In Fig. 5 the SEM micrograph of the low-doped a-SiC:H film surface after indentation testing is shown. Because of high compressive stress typical “zig-zag” wrinkling and delamination of the film was observed around the indentation print.

At higher doping levels “pile-up’s“ were observed in AFM image (Figure 1) around the indentation prints in the case of a-SiC:H films, while the AFM micrograph for a-Si:H film with doping level 0.001 is without pile-ups, cracks and delamination.

4. CONCLUSIONS

The mechanical and optoelectronic properties of boron doped a-Si:H and a-SiC:H layers were investigated from the point of view of the mechanical stability of these films. We found a good correlation between the optoelectronic and mechanical properties of these films. The prepared a-Si:H

and a-SiC:H layers exhibited good protective properties: the high microhardness approx. 18 – 28 GPa and the high resistance against fracture and delamination. The highest hardness of a-Si:H films compared to a-SiC:H may be explained with their higher density and their lower disorder. The lower fracture toughness of a-SiC:H films was caused by their higher compressive stress. The increased doping level influenced more the mechanical properties of a-Si:H than those of a-SiC:H films; this can be related to the different degree of the disorder of the network in both cases.

Acknowledgements

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Figure 1.

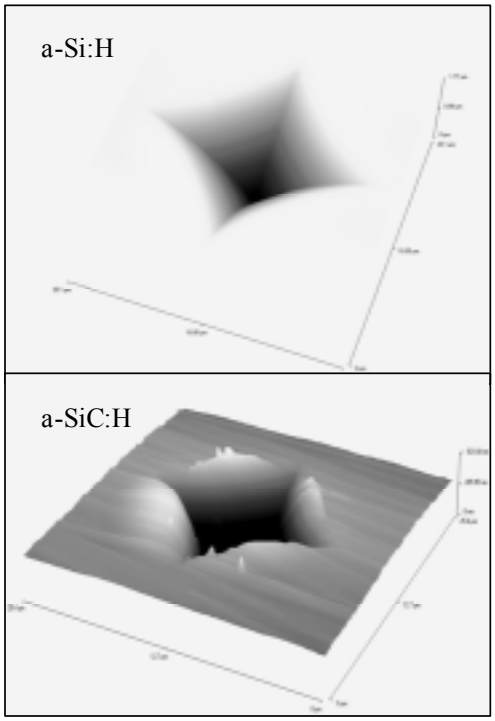

Figure 2.

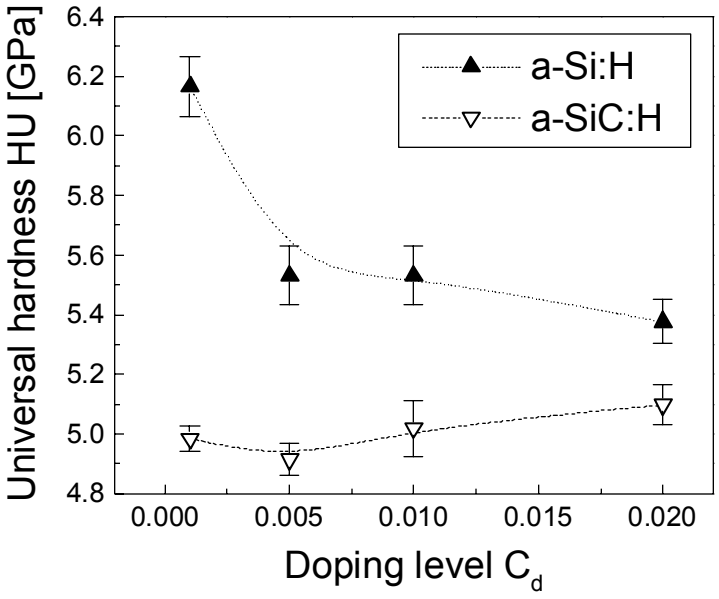
Universal hardness HU [GPa]
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
0.000
0.005
0.010
0.015
0.020
Doping level C_d
a-Si:H
a-SiC:H

Figure 3.

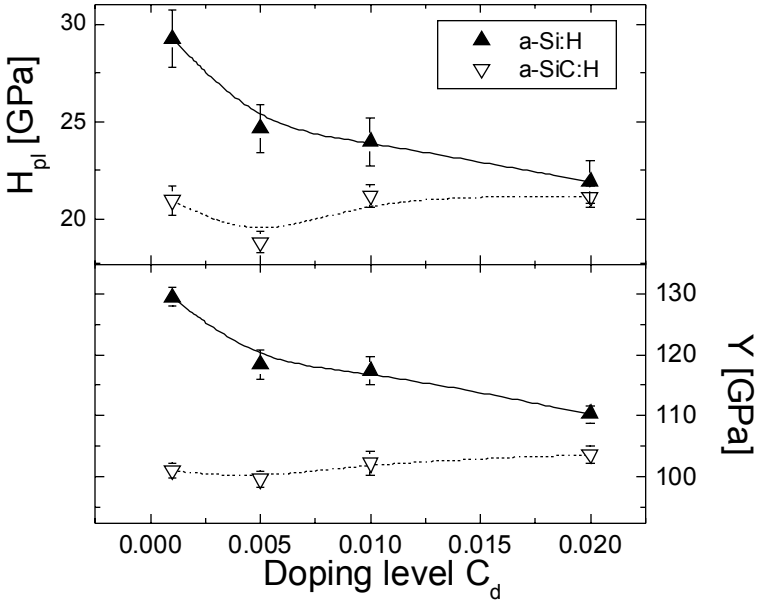
a-Si:H
a-SiC:H
H_{pl} [GPa]
Y [GPa]
Doping level C_d
30
25
20
130
120
110
100
0.000
0.005
0.010
0.015
0.020

Figure 4.

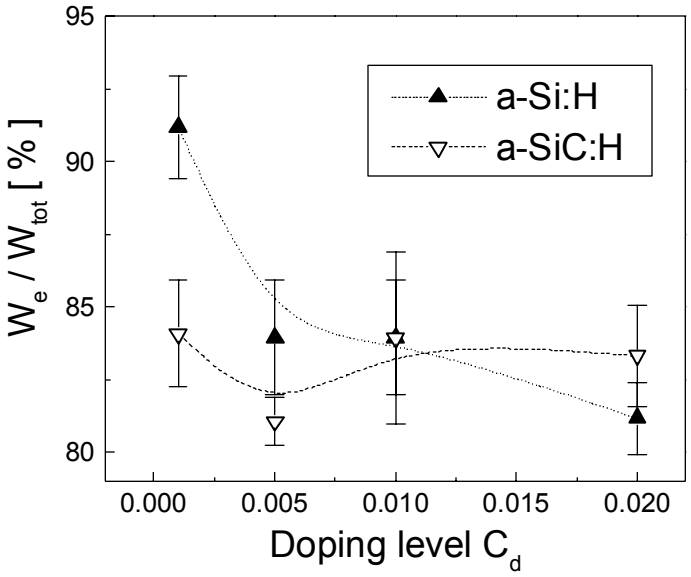
95
90
85
80
W_e / W_{tot} [%]
0.000
0.005
0.010
0.015
0.020
Doping level C_d
a-Si:H
a-SiC:H

Figure 5.

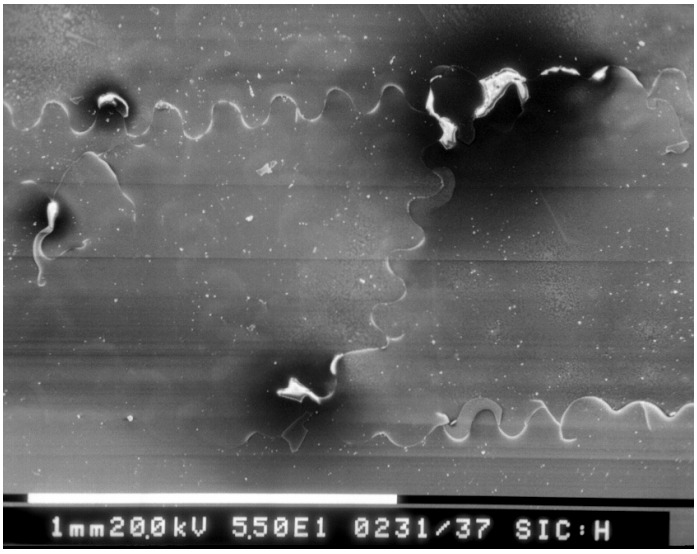

Table 1.

Type	a-Si:H	a-Si:H	a-Si:H	a-SiC:H	a-SiC:H	a-SiC:H
Doping level	$1x10^{-3}$	$5x10^{-3}$	$20x10^{-3}$	$1x10^{-3}$	$5x10^{-3}$	$20x10^{-3}$
E_G [eV]	1.84	1.87	1.80	1.98	1.98	1.99
E_{ov} [meV]	68	65	68	76	90	98
B [$cm^{-3}eV^{-1}$]	$4.5x10^{+18}$	$5.6x10^{+17}$	$2.6\ x10^{+19}$	$7.5\ x10^{+17}$	$3.0\ x10^{+18}$	$1.0\ x10^{+20}$

Captions for Figures and Table:

Figure 1.: AFM image of an indentation print in:

-up: a-Si:H film (doping level C_d = 0.01)

-down: a-SiC:H film (doping level C_d= 0.001)

Figure 2.: Universal hardness HU dependence on the doping level for a-SiC:H and a-Si:H films.

Figure 3.: Dependence of the plastic hardness H_{pl} and of the elastic modulus Y on the doping level for a-SiC:H and a-Si:H films.

Figure 4.: Dependence of the elastic to total deformation work ratio on the doping level for a-SiC:H and a-Si:H films.

Figure 5.: SEM image of the film fracture around the indentation print in a-SiC:H film (C_d = 0.001)

Table 1.: Basic material parameters – see text

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