INTERRELATION OF BOND CONFIGURATION AND OPTICAL PROPERTIES OF μc-SiC THIN FILMS BY SPECTROSCOPIC ELLIPSOMETRY

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Amorphous (a-SiC:H) and microcrystalline μc-SiC:H hydrogenated silicon carbon alloys are of great importance in photovoltaics and electronics because of their optical gap tunability depending on the carbon content. From a fundamental point of view, silicon carbon alloys represent an intriguing system because, even for a given stoichiometry, the optical and transport properties of films could be strongly dependent on the microstructure and carbon configuration.

The general approach to analyze a-SiC:H alloys optically consists in parameterization of the dielectric function $\varepsilon(E) = \varepsilon_1(E)+i\varepsilon_2(E)$ as a function of the photon energy, E, using the Tauc-Lorentz equation (1). However, this approach only results in the dependence of optical functions on the total carbon content in the alloy. Indeed, not only the overall C-content in the alloy, but also the C-carbon configuration is important. Therefore, we have performed an analysis of the $\varepsilon(E)$ spectra in terms of dielectric functions of various Si- and C-centered tetrahedron (2) that are combined in optical model based on the Bruggeman effective medium approximation (BEMA) to determine the optical response of films and correlate it to microstructure (i.e. amorphous and microcrystalline phases volume fraction) and C-bond configurations.

μc-SiC:H were deposited by r.f. (13.56 MHz) PECVD using gas mixtures of SiF_4 and CH_4 diluted in H_2 and He. Spectroscopic ellipsometry data were measured with a phase-modulated ellipsometer in the energy range 1.5 – 5.5 eV. The effect of H_2 dilution on the alloy composition and microstructure was investigated.

Figure 1 contrasts the SE spectra of the imaginary part, $\langle\varepsilon_2\rangle$, of the pseudodielectric function of films with the same total carbon content of 14% (as estimated by XPS chemical analysis). The different SE spectra are indicative of different optical properties and microstructure, as shown by the corresponding best-fit BEMA models reported in the same figure for an amorphous a-$Si_{0.86}C_{0.14}$:H and microcrystalline μc-$Si_{0.86}C_{0.14}$:H film. The C-bond configurations are also shown. In the microcrystalline film, it is found that Si-microcrystallites are embedded in a Si-Si2C2 tetrahedrom matrix with larger bandgap.

In the SiF_4-CH_4-H_2 plasma system, the amorphous-to-microcrystalline transition in SiC:H alloys has been found to depend on H_2 flow rate. Figure 2 shows spectroscopic ellipsometric spectra and the corresponding microstructural analysis of SiC alloys deposited at different H_2 flow rates. It is found that H_2 promote the formation of μc-Si embedded in a-SiC matrix, but reduce the overall alloy C-content. This is explained in the frame of an etching/growth competition chemical model where fluorine atoms are etchant of the silicon amorphous phase better than hydrogen atoms, promoting the amorphous-to-microcrystalline phase transition, while hydrogen atoms are effective in the etching of the carbon phase (especially C-sp2). Details of the mechanism responsible for growth of μc-SiC:H will be discussed.

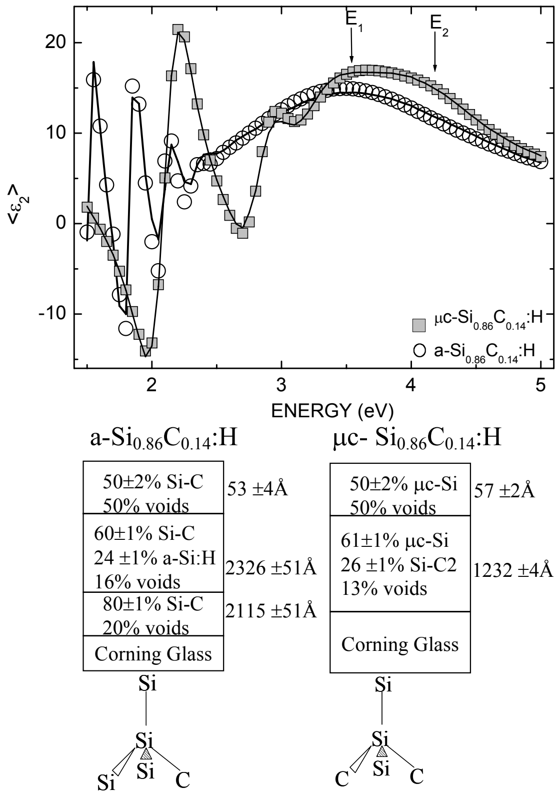

Figure 1. Experimental and calculated ellipsometric spectra of the imaginary, $\langle\varepsilon_2\rangle$, part of the pseudodielectric function of an a-$Si_{0.86}C_{0.14}$:H and a μc-$Si_{0.86}C_{0.14}$:H samples; the corresponding best-fit BEMA models evidencing the different microstructure of the two films with the same overall carbon content are also shown.

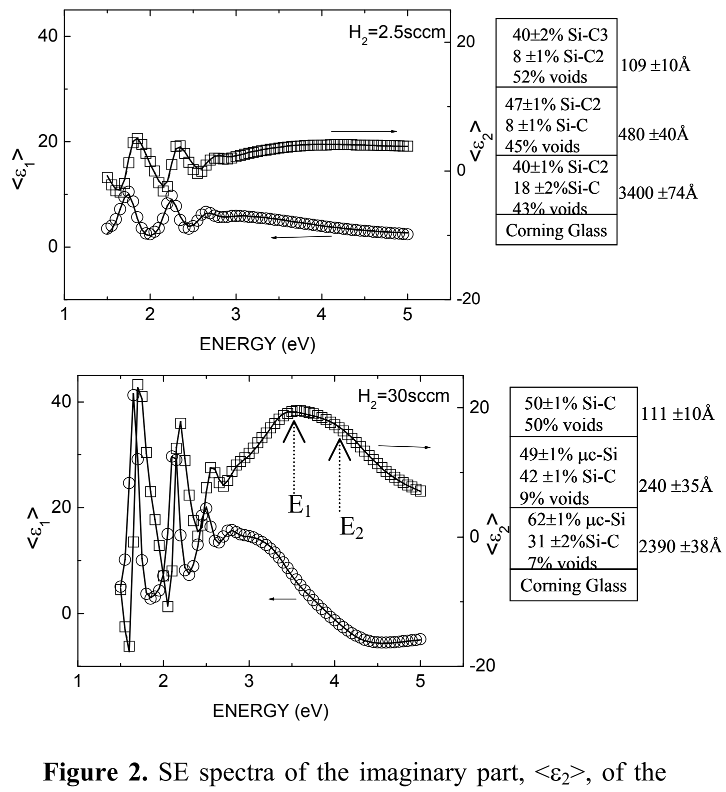

Figure 2. SE spectra of the imaginary part, $\langle\varepsilon_2\rangle$, of the pseudodielectric function of films deposited at (a) SiF_4:CH_4:H_2=20:0.2:2.5 and (b) SiF_4:CH_4:H_2=20:0.2:30 sccm gas flow ratios.

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