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Optical modeling of microcrystalline silicon deposited by plasma-enhanced chemical vapor deposition on low-cost iron-nickel substrates for photovoltaic applications

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Abstract

This paper deals with the optical modeling of thin hydrogenated microcrystalline silicon films grown on flexible low-cost iron-nickel alloy substrates by low-temperature (175 °C) plasma-enhanced chemical vapor deposition. This material serves as the absorber in solar cells and hence it has direct impact on the resulting solar cell performance. Since the crystallinity and the material quality of hydrogenated microcrystalline silicon films evolve during the growth, the deposited film is inhomogeneous, with a rather complex structure. Real-time spectroscopic ellipsometry has been used to trace the changing composition of the films. In-situ ellipsometric data taken for photon energies from 2.8 to 4.5 eV every 50 seconds enabled us to study the evolution of the monocrystalline silicon fraction of the hydrogenated microcrystalline silicon films.

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Keywords: In-situ ellipsometry; optical modeling; thin films; plasma-enhanced chemical vapor deposition; microcrystalline silicon; solar cells.

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1. Introduction

Photovoltaic industry is today driven by a constant pressure on the decrease of price per watt to less expensive and more efficient solar cells (Branker et al., 2011). Since the photovoltaic module cost depends on the total manufacturing cost of the module (Razykov et al., 2011), innovations leading to the reduction of the solar panel cost and the increase of the energy conversion efficiency are needed. This requires substantial effort towards searching for new materials and designs which can push limits of existing solar cells.

The most recent development of complex materials and nanostructures for solar cells requires more effort to be put into their characterization and modeling. The quality of deposited materials can be monitored by characterization of materials and nanostructures during the growth process using e.g. in-situ ellipsometry [(Kumar et al., 1986), (Jellison Jr. et al., 1993), (Layadi et al., 1995), (Collins et al., 2003)]. However, the model for the in-situ characterization is not always straightforward, because dielectric function as well as the surface of the deposited microcrystalline silicon thin film change during the growth [(Matsuda, 2004), (Fujiwara et al., 2002)].

In this work we deal with the optical modeling of a thin hydrogenated microcrystalline silicon (μc-Si:H) film deposited on a flexible low-cost iron-nickel (Fe-Ni) alloy substrate by low-temperature (175 °C) plasma-enhanced chemical vapor deposition (PECVD), which is promising for a low-cost high-efficiency solar cells production [(Torres-Rios et al., 2011), (Djeridane et al., 2007)]. We focused particularly on a closer analysis of the optical model with a special attention dedicated to the study of the impact of the surface roughness layer composition on the quality of the fit.

2. Experiments

2.1. Deposition of microcrystalline silicon thin film

The studied sample of thin μc-Si:H film on a Fe-Ni alloy substrate was deposited in a PECVD rf power system working at 13.56 MHz. The temperature, the rf power, and the pressure were kept during the deposition at 175 °C, 25 W and 4 Torr, respectively. The deposition was realized using a mixture of silicon tetrafluoride (SiF_4) diluted in hydrogen and argon with an H_2/SiF_4 ratio equal to one.

The iron-nickel alloy (called N42) suitable for a PECVD deposition of μc-Si:H is a low-cost flexible industrial steel with 41 at.% of nickel (Torres-Rios et al., 2011). It has a cubic structure with more than 95 % of the surface oriented in the <100> crystallographic direction (Torres-Rios et al., 2011). Although the lattice constants of N42 substrate and silicon are $a_{N42} = 3.59$ Å and $a_{Si} = 5.43$ Å, respectively, the misfit of only 6.4 % can be achieved by rotation of one of the lattices by 45° with respect to the other. Moreover, both these materials have very similar coefficients of thermal expansion in a wide range of temperatures [(ARCELLORMITTAL, 2007), (Mazur and Gasik, 2009)].

2.2. Real-time spectroscopic ellipsometry

A set of 160 ellipsometric spectra (see Fig. 1) measured by the in-situ spectroscopic phase modulated ellipsometer UVISEL (Jobin-Yvon Horiba) during the material deposition was studied. Each spectrum contains 16 points from the range of photon energies between 3 eV and 4.5 eV with the step of 0.1 eV. The integration time was 300 ms and every spectral measurement took about 48 s. The angle of incidence was 71.20° and the standard ellipsometric configuration with angle of 0° for modulator and +45° for analyzer was used.

3. Results and discussion

Each spectrum was modeled using a separate model with free parameters as in Fig. 2. We have started the fitting from the last measured spectrum and proceeded towards the first measured one. The fitted values of parameters from the previous spectrum were used as the initial parameter values for the subsequent one. Figure 2 shows the schematic drawing of the used optical model. Deposited layer consists of a mixture of monocrystalline silicon (c-Si), the reference highly crystallized hydrogenated microcrystalline silicon prepared by PECVD at hydrogen dilution