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Replacing NRA by fast GD-OES measurements as input to a model based prediction of hydrogen diffusion in a-Si

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Abstract

In order to predict hydrogen diffusion in hydrogenated amorphous silicon (a-Si:H) layers, Gerke *et al.*[1] proposed a model which requires just one nuclear resonant reaction analysis (NRA) and one Fourier transform infrared spectroscopy (FT-IR) as input. This contribution presents the possibility to substitute this single NRA measurement by a calibrated glow discharge optical emission spectroscopy (GD-OES) measurement. In the hydrogen concentration range of 2-30 at% relevant for a-Si:H layers there are currently no commercial calibration standards available, leading to the necessity of laboratory standards. Hydrogen depth profiles of a-Si:H layers exhibit plateaus of constant hydrogen concentration in a range large enough to qualify them as calibration standards. Therefore, six plasma enhanced physical vapor deposited (PECVD) a-Si:H layers with different hydrogen concentrations were prepared as laboratory standards. The absolute hydrogen concentration was determined using the NRA technique and the layer thickness was determined with a focused ion beam (FIB) in a scanning electron microscope (SEM). These results enabled a calibration of the GD-OES setup for a-Si:H, which successfully reproduced the NRA measurements of Gerke *et al.* [1].

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Keywords: GD-OES; a-Si:H; hydrogen diffusion; NRA

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1. Introduction

Hydrogenated amorphous silicon (a-Si:H) is frequently used in photovoltaics, especially as thin layer. Since hydrogen has a significant impact on the electronic and optical properties of such layers, a fundamental understanding of the hydrogen diffusion processes is required, including the measurement of hydrogen depth profiles. A widely used method to determine precise depth profiles is the nuclear reaction analysis (NRA) [2]. Since it is hardly accessible and costly, huge efforts are necessary to measure hydrogen depth profiles of a series of samples. To reduce these efforts Gerke *et al.* proposed a model based prediction of the diffusion of hydrogen in post-hydrogenated a-Si:H [1]. With this model it is possible to predict the hydrogen depth profiles of layers exposed to post-hydrogenation processes of different durations with just one single NRA measurement and one Fourier transform infrared spectroscopy (FT-IR) measurement. In this contribution the glow discharge optical emission spectroscopy (GD-OES) [3] is introduced to replace even this single NRA measurement in the sense of further minimizing the efforts. GD-OES is a fast and cost effective technique for obtaining depth profiles of hydrogen in a-Si.

The basis of the model proposed by Gerke *et al.* [1] is the assumption, that the hydrogen diffusion in a-Si can be described according to Fick's law by a complementary error function [4]:

$$H_x(x_l) = H_i + (H_s - H_i) \cdot erfc\left(\frac{x_l}{2\cdot\sqrt{D_H \cdot t_t}}\right) \tag{1}$$

Except for the depth of the calculated hydrogen concentration x_l and the treatment duration t_t, the other parameters are determined using the results of the NRA and FT-IR measurements. The parameters are namely H_i the hydrogen concentration at the interface of a-Si and the bulk material, H_s the hydrogen concentration at the surface and D_H the diffusion coefficient. A consideration of a possibly initial hydrogen concentration H_0 prior to the post-hydrogenation treatment leads to a more accurate prediction of the hydrogen depth profiles. Fig. 1 presents several NRA measured hydrogen depth profiles and the corresponding calculated depth profiles using the model prediction (for experimental details see [1]).

2. GD-OES

2.1. Measurement principle

The GD-OES technique determines depth profiles of the elemental composition by applying a glow discharge argon plasma to the sample surface. The argon ions sputter the atoms of the surface which are then excited in the plasma and emit a characteristic spectrum. The intensities of this characteristic light carry information about the initial elemental composition which is determined by a comparison with the light intensities of certified calibration standards. The resulting composition and the corresponding densities of the pure elemental solids are then used to transform the sputter process duration into depth information [3]. For the atmospheric elements, *i.e.* hydrogen, nitrogen and oxygen, this procedure is not possible, because they are gaseous at room temperature and so no density of the elemental solid is available. The depth information has to be determined individually for each sample type containing these elements.

In fact, once the GD-OES device is calibrated, it has powerful advantages. The most important advantage is the very short measurement duration, typically in the range of 10-100 s for layers up to several µm thickness, depending on the chosen plasma conditions. Also these plasma conditions are highly reproducible and hence a reliable comparison with the intensities of the calibration samples is possible. A resolution down to 100 ppm is achievable, depending on the chosen emission line and specific detector setup. In principle it is possible to achieve depth resolution in the order of 1 nm. But this depth resolution is limited by the specific detector setup and the shape of the crater sputtered into the sample, which in turn is defined by the plasma conditions. The shape of the crater as well as the crater bottom roughness may reduce depth resolution with increasing measurement duration or at interfaces of two materials with different sputter rates.