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Characterization and modeling of electrical transport in undoped hydrogenated microcrystalline silicon

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ABSTRACT

In this paper, we present the characterization and modeling of the electrical transport of hydrogenated microcrystalline silicon (μc-Si:H). Electrical conductivity measurements for several crystalline fractions have been carried out. The latter have been combined with surface potential measurements from atomic force microscopy in order to investigate the electrical transport in the heterogeneous structure. We propose a new numerical model based on a three-dimensional electrical circuit to extract the parameters involved in the transport. A physical based model of tunneling at large grain boundary is implemented. Combining the latter with other conductivities in the large electrical circuit, the percolation behavior in respect to crystalline fraction is fully simulated. A benefit of such a model is that it captures the fundamental physics phenomena with only a few comprehensible parameters.

1. Introduction

Hydrogenated microcrystalline silicon (μc-Si:H) is a promising material to improve the performance of transistors [1] and photovoltaic devices [2] based on hydrogenated amorphous silicon (a-Si:H). Since μc-Si:H can be prepared at low temperatures using equipment similar to that used for a-Si:H, this material is positioned as a potential candidate for low cost applications. Many publications have reported improvement in conductivity with the increase in the crystalline volume fraction [3,4]. This behavior is related to the creation of percolation conduction paths through the silicon crystallites embedded in the a-Si:H.

Temperature dependence of the dark conductivity has been investigated mainly for high crystallinity samples. For such a crystalline fraction, Konezny has considered the film to be homogeneous and the transport is modeled by an array of tunnel junctions at the region of closest approach between the crystallites [5]. The percolation behavior of this mixed-phase compound cannot be taken into account and renders questionable the physical meaning of the extracted parameters.

Many authors have reported the percolation behavior of the μc-Si:H and the effective medium approximation (EMA) has been used to investigate the electrical properties of the film [3,4,6,7]. The main objective is to predict the global conductivity of a random mixture of particles of two different conductivities. The EMA can randomly describe an inhomogeneous medium with various sizes of spherical or ellipsoidal inclusions. The EMA correctly predicts the percolation phenomena for high crystalline volume fractions. However, the prediction of the percolation threshold strongly depends on the choice of EMA theory e. g. Bruggeman theory, Maxwell Garnett or Wood-Ashcroft mixing rule. All these models predict a percolation threshold from 30% to 70% [4]. Due to the wide range of predicted thresholds, the EMA appears to be inaccurate when investigating the complex structure of the μc-Si:H, especially for crystalline volume fractions around the percolation threshold.

A three-dimensional (3D) model has been proposed by Overhof [8]. Based on a conductance network calculation, the authors simulate the percolation behavior for the conductivity and Hall mobility with a percolation threshold around 30%. However, the material, modeled as a homogenous random mixture of two phases, is far from the actual microstructure of the μc-Si:H and the microscopic behavior of the transport (especially tunneling at grain boundary) is not included in this model.

In this paper, we present a study of the electrical properties of μc-Si:H films. Atomic force microscopy (AFM) measurements and electrical characterizations have been carried out for several crystalline volume fractions. Based on this experimental data, we are able to present a numerical 3D model of the electrical transport. The main feature of this model is to unify the different approaches and provide a comprehensive tool capable of investigating the microscopic and macroscopic behavior

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of μc-Si:H.

In order to obtain realistic simulations and to eliminate the limitations of the Overhof's model, we have implemented the 3D discrete dynamical growth model of the μc-Si:H originally proposed by Bailat [9]. This model provides a 3D description of the film, including transition from the amorphous to the crystalline phase, conical shape of the crystalline domains, crystalline fraction and roughness evolution with respect to the layer thickness.

The numerical model of transport deals with a very large conductance network, taking into account the transport in amorphous and crystalline phases and also transitions at grain boundary so that we are able to obtain both microscopic understanding of the transport phenomenon as well as macroscopic percolation behavior of the film.

2. Experimental details

Argon diluted a-Si:H and μc-Si:H thin films were deposited in a conventional RF (13.56 MHz) PECVD chamber at a substrate temperature of 200 °C. Various crystalline volume fractions were achieved by modifying the gas pressure and RF power [10,11]. The crystallinity was characterized by Raman scattering measurements with an argon laser at a wavelength of 473 nm. Surface native oxide was removed by HF etching followed by evaporation through a photolithographic mask with a 300 nm thickness of aluminum contacts having a width of 200 μm and a length of 2500 μm. The conductivity measurements were carried out in dark and vacuum in a coplanar configuration. Before the measurements, all samples were heated at 425 K for 30 min to remove the impurities present on the surface. The conductivity has been measured using an Agilent 4156C semiconductor parameter analyzer.

Experimental data on Figs. 2, 4 and 9 are presented with bidirectional error bars. We have grouped similar crystalline fraction samples, leading to horizontal error bars. The vertical error bars provide the average value and upper/lower limits of the experimental data.

3. Electrical conductivity measurements

Fig. 1 shows typical examples of the variation of conductivity versus temperature for the samples of crystalline fractions 0%, 21%, 54%, 61% and 70%. The sensitivity of the experimental set-up reduces the temperature range studied according to the conductivity of each sample. It goes down to 285 K for the more amorphous and to 175 K for the more crystalline samples. Over the range studied, a thermally activated conductivity is observed, from which we can extract the activation energy (E_a) and conductivity prefactor (σ_0) according to the Arrhenius equation:

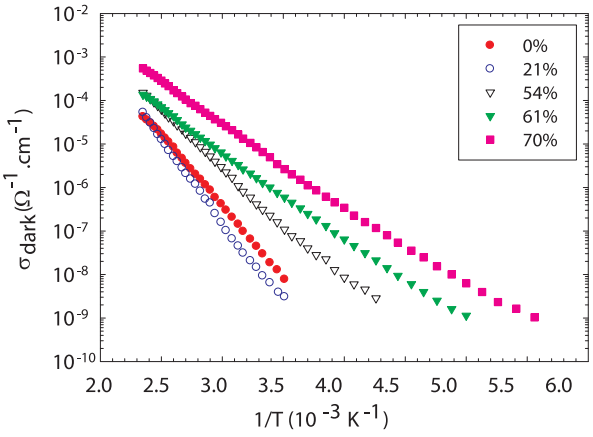

Fig. 1. Examples of Arrhenius plot of the dark conductivity for different crystalline fractions.

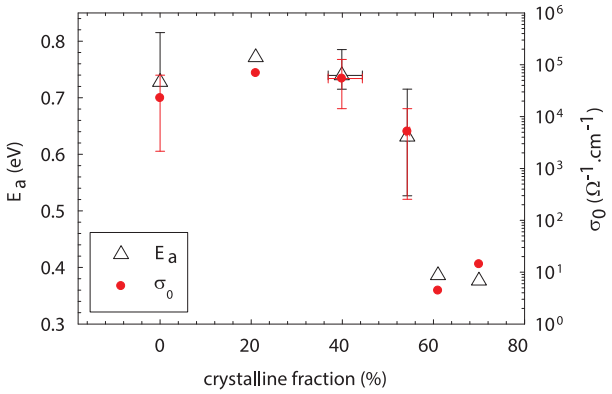

Fig. 2. Variation of the activation energy (triangle) and the conductivity prefactor (closed circle) as a function of the crystallinity.

$$\sigma = \sigma_0 \exp\left(-\frac{E_a}{K_B T}\right) \quad (1)$$

We present in Fig. 2 the dependence of E_a and σ_0 on the crystalline fraction. The variations of E_a are correlated to the structure of the material. Below the percolation threshold, E_a has an average value of 0.75 eV, above the percolation threshold this value is 0.37 eV.

This sharp drop in E_a and σ_0 is related to the change of the microstructure and the formation of percolation paths through a network of crystalline grains.

These experimental results are in agreement with most published data relative to undoped μc-Si:H [12–15].

4. AFM characterizations

In order to investigate the microscopic properties of the samples, characterizations of the morphology and the surface potential of the samples have been carried out with an atomic force microscope Nanoscope Multimode from VEECO Instruments. The scans were carried out using a platinum coated silicon tip in 2 × 2 μm^2 area.

Fig. 3 shows the surface morphology in tapping mode for the sample of crystalline fraction 60%. The scan reveals crystalline conglomerates (large grains) and encapsulated crystallites within them. The root mean square (RMS) surface roughness and average large grain diameter were determined using image analysis software "Guiddyon". Results are shown in Fig. 4.

Surface potential measurements were carried out on two samples of crystalline fractions of 21% and 54%. A constant voltage is applied between two aluminum coplanar contacts spaced 50 μm apart. The AFM tip measures the surface potential of an area of 2 μm^2 located between the contacts. Figs. 5 and 6 show the morphology and the corresponding surface potential of these two samples.

The potential in the sample of crystallinity 21% is almost linear (Fig. 5(b)) without any correlation to the surface topography. This result suggests that the transport takes place mainly in the homogeneous amorphous phase of this sample.

The potential in the sample of crystallinity 54% (Fig. 6(b)) shows a correlation with the topography: potential drops are located at the large grain boundaries.

The surface potential measurements provide a fundamental result to identify current routes in this material. This experimental data suggests that the transport mainly takes place through the large grain boundaries where a potential drop is measured. The quasi constant potential inside the grains suggests that the conductivity inside the grains is high compared to that of the boundary, so that the conductivity inside the large grain has a minor influence and represents no barrier for transport inside a large grain, as reported in [16,17].

Moreover, these observations are consistent with many published