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Performance of microcrystalline silicon single and double junction solar cells of different degrees of crystallinity

M. Nath [a,*], S. Chakraborty [a], E.V. Johnson [b], A. Abramov [b], P. Roca i Cabarrocas [b], P. Chatterjee [a]

[a] Energy Research Unit, Indian Association for the Cultivation of Science, Kolkata 700 032, India
[b] Laboratoire de Physique des Interfaces et des Couches Minces, CNRS, Ecole Polytechnique, 91128 Palaiseau, France

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ABSTRACT

Hydrogenated microcrystalline silicon (μc-Si:H) solar cells show decreasing open-circuit voltage with increasing crystalline volume fraction (F_c). Therefore, most research groups focus on μc-Si:H films produced close to the transition with amorphous silicon. Three cells with varying F_c and large-grain fraction, F_{lg} have been studied experimentally and by modeling. The large grained fluorinated μc-Si:H cell appears to be an exception to the above rule, and modeling is used to understand why low and high F_c μc-Si:H and μc-Si:F:H are used as the second intrinsic-layer in hypothetical double junction cells. Modeling suggests possible efficiencies of 11.3%, 8.4% and 13%, respectively. Three methods of double junction cell thickness optimization are discussed.

1. Introduction

Hydrogenated microcrystalline silicon (μc-Si:H) solar cells generally show decreasing open-circuit voltage (V_{oc}) with increasing crystalline volume fraction, F_c (Fig. 1). In a previous article [1] we had identified three contributing factors to the decrease of V_{oc} with increasing F_c, namely, an increase in both mid-gap and tail defects as well as a decrease in the mobility gap. We also explained that in the limiting case of crystalline silicon cells, with an even lower band gap, a higher V_{oc} is possible due to a sharply reduced gap defect density and a lower effective density of states (N_c, N_v) at the band edges. In this work, we model fluorinated μc-Si:H solar cells [2], with very high F_c as well as a significant fraction of large grains (F_{lg}), which appears to violate the general rule (Fig. 1). A material containing large grains is a dense material with low oxygen content, which can be obtained when using SiF_4 based plasma processes [2]. μc-Si:H with (i) F_c=79%, F_{lg}=0%, (ii) F_c=93%, F_{lg}=27% and (iii) μc-Si:F:H (F_c=100%, F_{lg}=50%) are used as the second I-layer in hypothetical double junctions and the optimized efficiencies are calculated. Three methods of thickness optimization are discussed.

2. Experiments and modeling

Microcrystalline PIN solar cells having the structure: textured ZnO/P-μc-Si:H/I-μc-Si:H/N-a-Si:H/Aluminum have been deposited in a multiplasma monochamber RF-PECVD reactor, employing different ratios of silane to hydrogen flow rates during the intrinsic (I) layer deposition – SiH_4:H_2=4:200, and SiH_4:H_2=6:200 [1]. This results in different F_c and F_{lg} (sa and sb in Table 1). The P-μc-Si:H and N-a-Si:H layers were deposited under the same conditions for the two cases. A third set (sc) has a fluorinated μc-Si:H I-layer, where hydrogen plasma treatment has been done both before and after deposition of the I-layer, since the latter procedure is shown to improve cell performance [2]. The composition of the films was obtained from the Bruggeman effective medium approximation modeling [3] of the pseudo-dielectric function of the films, deduced from spectroscopic ellipsometry measurements. This approach has been shown to be well adapted to the modeling of μc-Si films [4]. In this approach we used as components for the model the dielectric functions of (i) amorphous silicon; (ii) voids to take into account the porosity of the films; (iii) small grain μc-Si; and (iv) large grain μc-Si material produced by chemical vapor deposition (CVD) at high temperature. (The dielectric function of large grain μc-Si taken corresponds to that of a material produced by CVD at high temperature (~650 °C) – Ref [5].) The presence of significant fraction of large grains in a material produced by plasma enhanced CVD (PECVD) at 175 °C has been shown to correlate with improved transport properties of the films [6]. In Table 1 we report the values of the total crystalline fraction F_c (which is the sum of the small grain and large grain fractions) and F_{lg}, which is the parameter of interest in this study. Indeed, achieving a high value of F_{lg} indicates that the films obtained by PECVD at 175 °C have a grain size similar to that of polycrystalline layers produced by CVD at ~650 °C [5].

The one-dimensional electrical–optical model Amorphous Semiconductor Device Modeling Program (ASDMP) [7] used in

* Corresponding author. Tel.: +91 33 2473 4971x612; fax: +91 33 2473 2805.
E-mail address: madhumitanath_21@yahoo.co.in (M. Nath).

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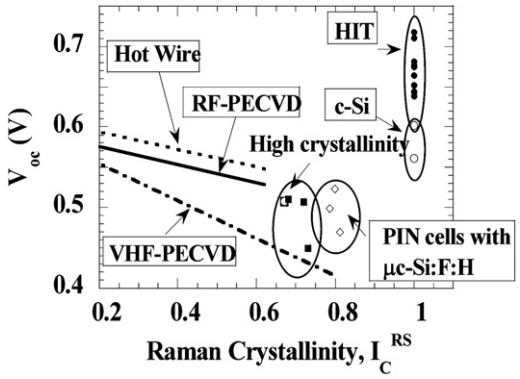

Fig. 1. The V_{oc} of silicon solar cells with varying Raman crystallinity.

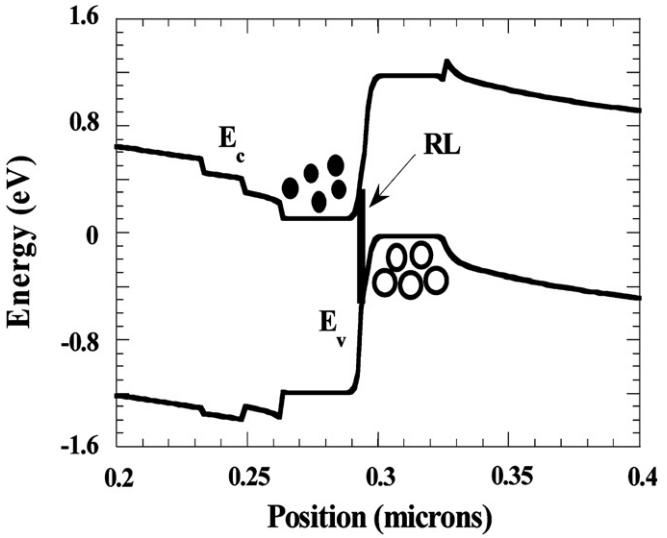

Fig. 2. Energy band diagram under short-circuit conditions and AM1.5 bias light around the inter-cell recombination layer (RL – shaded black in the figure), indicating our approach for simulating this contact region. The conduction band edge (E_c) and the valence band edge (E_v) are indicated.

Table 1
Comparison between the measured (Expt) and modeled (Model) solar cell output in PIN devices (sa, sb, sc), having different F_c and F_{lg}. da, db and dc are hypothetical double junctions with an a-Si:H top-cell and different μc-Si:H materials in the bottom-cell. The optimized thickness (in μm) of the top and bottom sub-cell I-layers in double junctions are d_1/d_2=0.23/1.71 in da, d_1/d_2=0.147/1.01 in db and 0.7/1.2 in dc, showing the importance of an intermediate reflector when using this high F_{lg} material.

Case	F_c (%)	F_{lg} (%)		J_{SC} (mA/cm^2)	V_{OC} (V)	*FF*	η (%)
sa	79	0	**Expt**	16.76	0.54	0.687	6.22
			Model	16.76	0.54	0.685	6.20
sb	93	27	**Expt**	19.94	0.46	0.631	5.79
			Model	19.85	0.45	0.640	5.72
sc	100	50	**Expt**	23.2	0.523	0.680	8.30
			Model	22.9	0.526	0.704	8.50
da				10.86	1.45	0.72	11.34
db				9.47	1.27	0.70	8.42
dc				13.92	1.37	0.69	13.16

this study solves Poisson's equation and the two carrier continuity equations under steady state conditions for the given device structure and yields the resulting *J–V* characteristics and the quantum efficiency. The electrical part of the modeling program is described in Ref. [8]. The gap state model used in our calculations consists of the tail states and Gaussian distribution functions to simulate the deep dangling bond states. The junction between the P–I–N cells of the stacked structure is modeled by Palit and Chatterjee [9], and Hou et al. [10] a heavily defective "recombination" layer (RL) with a reduced mobility band gap. The potential barriers for carriers moving towards this junction are reduced by band gap grading. Fig. 2 represents the blow-up of the area surrounding this inter-cell contact region and our approach to simulating the junction region.

The generation term in the continuity equations has been calculated using a semi-empirical model, that has been integrated into the modeling program [7]. Both specular interference effects and diffused reflectances and transmittances due to interface roughness are taken into account. The complex refractive indices for each layer of the structure are required as input and have been measured in-house by SE.

3. Results and discussion

The experimental solar cell output parameters for "low F_c", "high F_c" μc-Si:H and fluorinated μc-Si:H are compared to the modeling results in Table 1. From these simulations, typical parameters that characterize the intrinsic μc-Si:H layers of these cells have been extracted and are given in Table 2. Modeling indicates that high F_c μc-Si:H cell (sb) has a lower band gap, higher carrier mobilities, and both higher mid-gap defect density and broader band tails as compared to the cell having low F_c μc-Si:H (sa) [1]. In order to simulate the improved cell performance (Table 1) of the μc-Si:F:H cell, we had to take higher carrier mobilities, lower mid-gap defects and lower effective DOS at the band edges (similar to crystalline silicon). Indeed, the use of SiF_4 as a gas precursor allows to reduce the concentration of oxygen in the films and leads to a material with a higher fraction of large grains. This in turn results in better transport properties. In particular we have shown that the electron mobility, as measured by time resolved microwave conductivity, increases with the fraction of large grains [6]. The lower defect density in μc-Si:F:H is confirmed by Fourier transform photocurrent spectroscopy (FTPS) measurements (not yet published); and a decrease of the band gap of μc-Si:H with increasing F_c (Table 2) has been observed by Hamma and Roca i Cabarrocas [11]. The vastly improved spectral response at long wavelengths confirms the very high crystalline volume fraction of μc-Si:F:H [2]. Since the highly crystallized μc-Si:F:H cell violates the general trend of lower V_{oc} with increasing F_c, we checked the experimental results on various sets of solar cells all having very high F_c and F_{lg} and found the results reproducible. These cell results have been confirmed independently by measuring at the Jülich research center.

The parameters of μc-Si:H (low and high F_c) and of μc-Si:F:H are then used as input to calculate the efficiency of hypothetical double junctions (da, db, and dc, respectively), with a standard a-Si:H top-cell. After suitable thickness optimization, the cell outputs are given in Table 1. The results indicate that the double junction cell dc, with fluorinated μc-Si:H as bottom sub-cell has the potential to give a higher efficiency ($\eta \sim 13\%$), compared to the low F_c cell da ($\eta \sim 11.3\%$) and the high F_c cell db($\eta \sim 8.4\%$), but requires an exceptionally thick top-cell. This is due to the fact that current capacity of the bottom cell with μc-Si:F:H is very high (22.9 mA/cm^2 in the single junction, sc); so to match the current between the two sub-cells, the first cell has to be very thick. This suggests that we need an intermediate reflector to selectively reflect the short wavelength light into the top cell, so that higher current can be achieved with a thinner top sub-cell.