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A study of crystallinity in amorphous Si thin films for silicon heterojunction solar cells

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ABSTRACT

In this work we analyzed the crystallinity of hydrogenated amorphous Si thin films deposited on n-type Si substrates using the effective medium approximation (EMA) method of a spectroscopic ellipsometer (SE) and evaluated their passivation quality by measuring effective carrier lifetime (τ_{eff}) and implied V_{oc} using quasi-steady-state photo conductance decay (QSSPC) simultaneously. The crystalline volume fraction of doped a-Si:H layers using RF-PECVD was controlled from ~0% (nearly full amorphous phase) to above 90% (nearly polycrystalline phase) through varying deposition conditions. The passivation property depended on the crystallinity more strongly for p-a-Si:H than n-a-Si:H of which crystallinity was more sensitive to deposition rate relatively. The implied V_{oc} above 650 mV was achieved with crystallinity less than about 5% for p-a-Si:H and 20% for n-a-Si:H. The HRTEM images confirmed the reliability of SE analysis with EMA modeling and showed the maximum part of crystalline phase exists at the interface of a-Si:H and c-Si in the form of epitaxial growth configuration. By the optimization of each a-Si:H deposition conditions 17.17% the cell efficiency was accomplished on non-textured substrate.

1. Introduction

An amorphous Si/crystalline Si heterojunction solar cell has a simple layer structure and can be processed at a relatively low temperature compared to a conventional crystalline Si solar cell generally; moreover, the heterojunction solar cell has low temperature coefficient of efficiency and high open circuit voltage at the same time. Therefore, the silicon heterojunction technology is expected to be one of the most advanced solar cell technology for high efficiency and low cost production recently. The heterojunction with intrinsic thin layer (HIT) [1] of Sanyo Electric. Co. Ltd in Japan has already achieved efficiency exceeding 22% [2]and high open circuit voltage over 0.7 V that adopted hydrogenated intrinsic amorphous thin layer, which yields outstanding performance for passivating crystalline Si substrate surface.

Recent works reported that it is very important to maintain the abruptness in a-Si:H/c-Si interface (so called hetero-interface) for high open circuit voltage(V_{oc}) and fill factor [3,4]. Various methods were developed to achieve high quality hetero-interface passivation, which could be attained by hydrogen termination. These are hydrogen contained chemical solution or plasma treatment and thin film deposition [5] containing hydrogen atoms such as a-SiO_x:H [6], SiN_x:H [7] and a-Si:H.

On a single crystalline silicon substrate, epitaxial growth or micro-crystalline phase growth is more likely to happen than amorphous phase [8,9] because an amorphous Si/crystalline Si heterojunction is making amorphous phase on single crystal silicon substrate. The crystallinity in a hetero-interface creates many states and defect sites that trap the generated carriers. Therefore, this leads to the decrease in effective carrier lifetime and concentration of mobile carriers and induces band structure deformation through Fermi energy level pinning at hetero-interface [10].

In this study, we focused on evaluating the crystallinity of amorphous Si thin films, which deposited on c-Si substrates. We verified the accuracy of spectroscopic ellipsometric (SE) measurement as a non-destructive method clearly and established relationships between the crystallinity of a-Si:H films and its passivation properties.

2. Experiment procedure

For the experiments, 300 μm thick phosphor-doped floating zone (FZ, (1 0 0)) n-type 4" Si wafers with relatively low resistivity (3.0 cm) were used. Both surfaces of the substrates were mirror polished to eliminate the influence of substrate surface roughness

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on the passivation properties and for the convenience of SE measurements. The cells (1 cm^2) were fabricated on polished (non-textured) Si wafers also. Surface cleaning was conducted by RCA cleaning process basically, before the deposition of a-Si:H thin films. The substrates were immersed in a $HCl:H_2O_2$ and $H_2SO_4:H_2O_2$ solution to eliminate contaminants and to grow a chemical oxide, which were followed by a rinse in de-ionized water each and then dipped for removing oxide in buffered oxide etchant. After drying, the substrates were immediately transferred to the load lock of the deposition system.

For amorphous Si thin film deposition, a parallel plate direct PECVD reactor operating at radio frequency (RF13.56 MHz) power was used. The 10–20 nm thick doped amorphous Si thin film was deposited on both sides of the Si wafer identically to evaluate the passivation property. Hydrogen diluted PH_3 and B_2H_6 gases were used for doping the a-Si:H films and then the deposition parameters including power density, working pressure, dilution ratio (H_2/SiH_4) [11] and so on were modified to control the crystallinity of a-Si:H thin films. The $ZnO:Al_2O_3$ 0.5wt% was deposited to make a front transparent electrode by RF sputtering method and Ag/Al was evaporated as front finger and backside electrode in the cell structure.

The spectroscopic ellipsometer (SE, J.A.Woollam, M-2000U) was used to measure the thickness and optical property of the amorphous Si thin film and the quasi-steady-state photo conductance decay (QSSPC), Sinton consulting Co. Ltd, WCT-120) [12] method was used to evaluate the passivation property. The effective carrier lifetime (τ_{eff}) and implied open circuit voltage(V_{imp}) were obtained by the QSSPC method operated in the generalized mode [13].

In SE measurement, we made good use of effective medium approximation (EMA) modeling for estimating the crystalline volume fraction of a-Si:H thin films especially. High resolution transmission electron microscope (HRTEM) analysis was performed to visualize the hetero-interface and to verify the exactitude of ellipsometric analysis. The cell performance was evaluated under the AM1.5G (100 mW/cm^2) standard irradiation condition.

3. Result and discussion

The SE measurement result is presented in Fig. 1 where the EMA modeling is based on the polarization dispersion as for the Clausius–Mosotti relationships and assumes that the crystalline Si phase is dispersed in an amorphous silicon matrix uniformly with sphere shape as the Bruggeman theory [14–16]. The thickness measuring results of a-Si:H thin films by SE were well matched with TEM results.

In this work, we analyzed the passivation quality with the variation of crystallinity in a-Si:H thin films. The passivation quality can be represented by the implied open circuit voltage deduced from photo generated current and we can estimate the open circuit voltage of the real device from the implied open circuit voltage.

The lower the crystallinity was, the higher the implied open circuit voltage irrespective of doping types, but the range of the crystallinity where the implied V_{oc} is over 650 mV was significantly different (Fig. 2(a)). In the case of p-a-Si:H, we should maintain very low crystallinity less than 5% (volume fraction) for over 650 mV of implied *Voc*, in contrast to the case of n-a-Si:H that showed an equal passivation capability up to near 20% (volume fraction) of crystallinity. This means that the process window can be wider when the passivating layer and the substrate have the same semiconductor type on account of field passivation effect. If n-a-Si:H thin film has higher doping concentration than Si substrate (10^{15-16} $/cm^3$), n-a-Si:H layer

a

4	srough	0.458 nm
3	EMA(p)/4.98% polysi_a	23.437 nm
2	p	0.000 nm
1	intr_jaw	0.207 nm
0	si_jaw	0.23 mm

b

4	srough	0.705 nm
3	EMA(n)/8.07% polysi_a	10.605 nm
2	n	0.196 nm
1	intr_jaw	0.331 nm
0	si_jaw	0.5 mm

Fig. 1. EMA model for ellipsometric analysis, which is composed in 4 layer constitution in which surface roughness/amorphous and crystalline Si mixed phase/amorphous Si/interface/c-Si substrate. (a) p-a-Si:H has about 4.98 crystalline volume fraction (%) in 23.4 nm thickness, (b) n-a-Si:H has about 8.07 crystalline volume fraction (%) in 10.6 nm thickness.

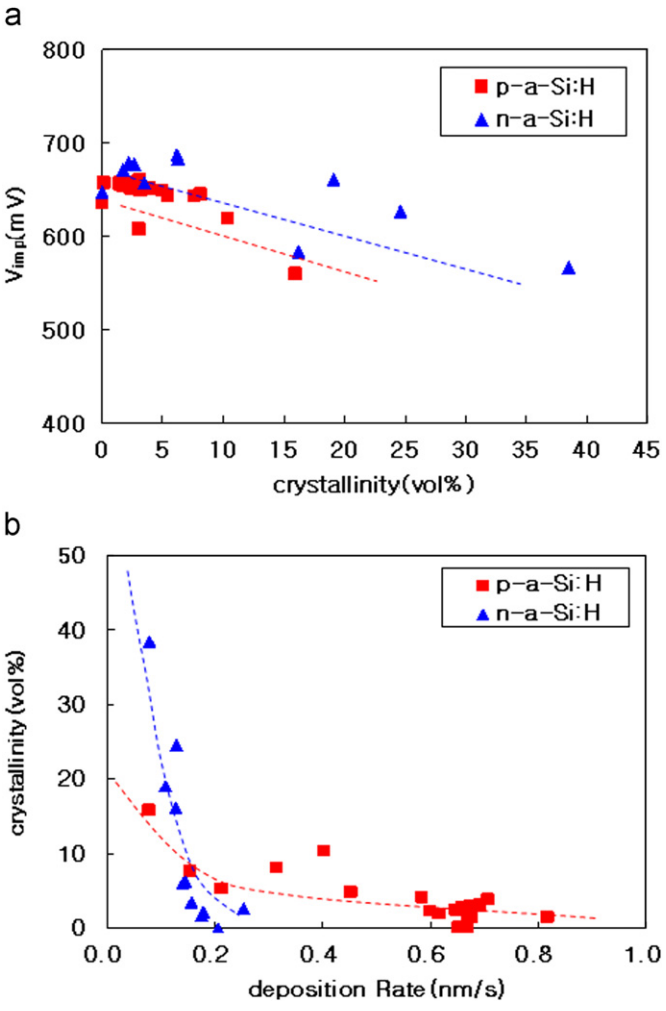

Fig. 2. (a) The relationship between the implied open circuit voltage and crystalline volume fraction in each a-Si:H thin film. (b) The relationship between the deposition rate and crystalline volume fraction in each a-Si:H thin film.