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Double layers of ultrathin a-Si:H and SiN_x for surface passivation of n-type crystalline Si wafers

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Abstract

Surface passivation by double layers made of hydrogenated amorphous silicon (a-Si:H) and hydrogenated silicon nitride (SiN_x) on float zone n-type Si substrates was investigated. The thickness of the a-Si:H layers was varied from 0 to 4 nm and they were deposited at low temperature by plasma-enhanced chemical vapour deposition. The structure and composition of the double layers was determined by a combination of spectroscopic ellipsometry and glow discharge optical emission spectroscopy. The minority carrier effective lifetime and the uniformity of the surface passivation of the wafers were measured by calibrated photoluminescence imaging. The lifetime was observed to increase with increasing a-Si:H thickness. An excellent lifetime value of 7.3 ms was measured on the double layers with an a-Si:H layer thickness of 3.4 nm, corresponding to surface recombination velocity below 2 cm/s. Capacitance-voltage and conductance-voltage measurements were used to determine the densities of fixed charge and interface states at the interface between the Si substrate and the a-Si:H/SiN_x stacks. The fixed charge density of the initial SiN_x was positive, as expected. However, the overall fixed charge density of the double layers was observed to decrease when a layer of a-Si:H was inserted beneath the SiN_x, and eventually reaches negative values when the a-Si:H thickness exceeds 2 nm. The conductance-voltage measurements revealed that the interface state density (D_{it}) is significantly lowered when adding the ultrathin a-Si:H film between the substrate and the SiN_x layer, providing a significant improvement of the chemical passivation, thus reducing the overall surface recombination velocity.

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1. Introduction

Recently, several solar cells with efficiencies approaching or above 25% have been demonstrated. These, include the HIT solar cell from Panasonic with a conversion efficiency of 25.6%, and the TOPCon silicon solar cell from Fraunhofer ISE with an efficiency of 25.1%, both of which have been realized using stacks as surface or contact passivation material [1, 2]. It is well known that a-Si:H yields good surface passivation because of its low density of interface states resulting in good chemical passivation on silicon surfaces. However, a-Si:H shows poor thermal and UV stability and exhibits some parasitic optical absorption. [3] To overcome these limitations, stacks like SiO_x/SiN_x [4], a-Si:H/SiN_x [5,6] and a-Si:H/Al₂O₃ [7] have been developed for high efficiency solar cells. For the capping layer, low absorption, high stability, as well as high fixed charge are desirable properties. SiN_x is a prominent candidate because of its good thermal and temporal stability, tunable refractive index and a fairly high density of fixed, positive charge. Koyama et al. reported that a surface recombination velocity (SRV) of 1.5 cm/s and 9.0 cm/s could be obtained for n-type and p-type wafers, respectively, with a-Si:H/SiN_x stacks deposited by catalytic chemical vapor deposition (Cat-CVD). [8] A similar SRV value of 3.5 cm/s for plasma-enhanced chemical vapour deposition (PECVD) deposited a-Si:H/SiN_x stacks passivated n-type silicon has been obtained by Stepanov et al [9]. The passivation yielded by an a-Si:H/SiN_x stack is very sensitive to the a-Si:H layer thickness. [10] In this report, we focus on ultrathin a-Si:H films with a thickness between 0 and 4 nm capped by a SiN_x film with a thickness of 100 nm, which is good for avoiding parasitic absorption of a-Si:H.

2. Experiments details

In this work, double layers of a-Si:H/SiN_x, where the a-Si:H layer thickness was below 4 nm, were made. The thickness variation was controlled by adjusting the deposition time during the PECVD process and estimated based on predetermined deposition rates. The SiN_x layer thickness was kept constant at 100 nm while the a-Si:H thickness was varied from 0 to 4 nm. One 40 nm a-Si:H and one 100 nm SiN_x single layer were deposited for reference separately. The thicknesses were measured by variable angle spectroscopic ellipsometry (VASE). For the experiments, six halves of 4 inch float zone (FZ) n-type silicon wafers with a resistivity of approximately 2.8 Ω cm were used. The wafers were double-side polished with a thickness of 290 µm and a crystal orientation of (100). The double layers of a-Si:H/SiN_x were deposited on both sides of the wafers in a PlasmaLab 133 system from Oxford Instruments including a direct parallel plate reactor and an automatic wafer loading system. Before deposition, all wafers were cleaned in HF (5%) for 1 min, whereafter the a-Si:H films were deposited using a power density 9 mW/cm² and a temperature of 230 °C. In order to obtain a clean surface before deposition of the rear side, the wafers were subjected to a 5 s HF-dip before the second deposition of a-Si:H. In order to avoid cross contamination between a-Si:H and SiN_x, the PECVD was conditioned by performing a long (20 min) deposition of SiN_x on a dummy sample before the outermost 100 nm thick SiN_x layers were deposited on both sides with a power of 46.5 mW/cm² at 230 °C, the same deposition temperature as for the a-Si:H. After deposition, all wafers were cut into two pieces. One quarter was kept for lifetime measurements to determine temporal stability. Another quarter was used to deposit metal to form metal-insulator-semiconductor (MIS) structures for capacitance-voltage (C-V) and conductance-voltage (G-V) measurements.

The effective carrier lifetime was measured by photoluminescence imaging (PL-imaging) calibrated using the quasi steady-state photoconductance (QSSPC) method at an injection level of $10^{15} \mathrm{cm}^3$. VASE was used to characterize the film thickness and glow discharge optical emission spectroscopy (GDOES) was performed to investigate the composition of the samples as a function of thickness. The ellipsometry was performed using a variable angle spectroscopic ellipsometer from J. A. Woollam Co., Inc. A GDOES setup from Horiba Jobin Yvon was used to characterize the hydrogen depth profile of the samples. The C-V and G-V measurements were carried out at room temperature at a frequency of 100 kHz using a Keithley 4200-SCS semiconductor characterization system.

GDOES is a well-established spectrochemical approach for detecting trace elements. GDOES has many benefits including a high depth resolution, fast sputtering rate, low limits of detection and no need for high vacuum. [15] Here we applied GDOES to determine the H distribution in the c-Si/a-Si:H/SiN_x system for the first time.

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