Detailed Study on the c-Si Surface Passivation Mechanism of O$_2$-Based Batch Atomic Layer Deposited AlO$_x$ for Solar Cell Applications

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AlO$_x$ films deposited by atomic layer deposition (ALD) have recently demonstrated an excellent level of surface passivation on c-Si. Such a high level of surface passivation is attributed to a strong field effect passivation induced by high negative fixed charge density (Q$_f$) at an AlO$_x$/Si interface and moderate chemical passivation resulting in the reduction of interface trap density (D$_i$) [1]. More recently, AlO$_x$ films grown by O$_2$-based batch ALD achieved an excellent level of surface passivation on low resistivity p-type c-Si wafers [2], which showed the industrial feasibility of AlO$_x$ for the surface passivation of c-Si solar cells. However, there is still lack of detailed study on the c-Si surface passivation mechanisms of AlO$_x$ grown by O$_2$-based batch ALD for solar cell applications. In this study, we found that the passivation properties are strongly dependent on the deposition temperature (T$_{dep}$) and post-deposition annealing (PDA) regardless of film thickness. For instance, the AlO$_x$ films deposited at T$_{dep}$ ≥ 200 °C contained the negative Q$_f$ in the range of (3.4–7.1)×10$^{12}$ cm$^{-2}$ and D$_i$ in the range of (4.8–10)×10$^{11}$ eV$^{-1}$cm$^{-2}$ with demonstrating some degree of surface passivation, but the AlO$_x$ films deposited at room temperature demonstrated a significantly low level of surface passivation. After PDA in N$_2$ gas, AlO$_x$ films show a high level of surface passivation regardless of film thickness and T$_{dep}$. Especially, a flat injection level dependence of the effective lifetime and a significantly high level of surface passivation (S$_{eff}$ < 7 cm/s) were achieved after annealing at 400 °C for samples passivated with 30 nm-thick AlO$_x$ films deposited at 200 °C. Such an excellent level of surface passivation is due to sufficiently low D$_i$ (= 1.1×10$^{11}$ eV$^{-1}$cm$^{-2}$) as well as high Q$_f$ (= 5.3×10$^{12}$ cm$^{-2}$). This result indicates that a field-effect passivation does not play a prominent role. Instead, the excellent surface passivation can be mainly due to low D$_i$ at a SiO$_x$/c-Si interface after PDA. In addition, we have performed atomic hydrogen treatment of 10 nm-thick samples to investigate the origin of this chemical passivation. From the result, only RT-deposited AlO$_x$ samples showed both significant increase in Q$_f$ and more reduction in D$_i$ compared to control samples annealed in N$_2$ gas. This means that the effect of hydrogen treatment is strongly dependent on the density of AlO$_x$ films and hydrogen in AlO$_x$ films should be the origin of chemical passivation. We will address these issues and the thermal stability of AlO$_x$ films in detail during a presentation. On the other hand, we found that the dramatic enhancement in the passivation performance of RT-deposited AlO$_x$ films after PDA can be attributed to the phase transformation of aluminum silicate to mullite in an AlO$_x$ interlayer and the resulting self-aligned AlO$_x$/SiO$_x$ interface [3].

