

Detailed Study on the c-Si Surface Passivation Mechanism of O₃-Based Batch Atomic Layer Deposited AlO_x for Solar Cell Applications

Meiji Univ.¹, Univ. of Hyogo², National Institute for Materials Science (NIMS)³, JST-CREST⁴,
 °Hyunju Lee^{1,4}, Tomihisa Tachibana^{1,4}, Norihiro Ikeno^{1,4}, Hiroki Hashiguchi^{1,4}, Yuki Tsuchiya^{1,4},
 Koji Arafune^{2,4}, Haruhiko Yoshida^{2,4}, Shin-ichi Satoh^{2,4}, Toyohiro Chikyow³, Atsushi Ogura^{1,4},
 E-mail: tz10021@meiji.ac.jp

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_{it}) [1]. More recently, AlO_x films grown by O₃-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 O₃-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 $T_{dep} \geq 200$ °C contained the negative Q_f in the range of $(3.4\text{--}7.1) \times 10^{12} \text{ cm}^{-2}$ and D_{it} in the range of $(4.8\text{--}10) \times 10^{12} \text{ eV}^{-1} \text{ cm}^{-2}$ 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 N₂ 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 ($S_{eff} < 7 \text{ cm/s}$) 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_{it} ($= 1.1 \times 10^{11} \text{ eV}^{-1} \text{ cm}^{-2}$) as well as high Q_f ($= 5.3 \times 10^{12} \text{ cm}^{-2}$). 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_{it} 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_{it} compared to control samples annealed in N₂ 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].

[1] B. Hoex et al., Appl. Phys. Lett. **89**, 042112, 2006.

[2] G. Dingemans et al., Electrochem. Solid-State Lett. **14**, H1, 2011.

[3] H. Lee et al., Appl. Phys. Lett. **100**, 143901, 2012.