Excellent Surface Passivation of Crystalline Silicon by Atomic Layer Deposition

Al_xMg_{1-x}O_y Thin Films

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[Introduction]

In the field of crystalline silicon (c-Si) photovoltaics, trends toward lighter dopant diffusions, thinner substrates, and higher lifetime substrates have placed an increased importance on surface passivation. Recently, AlO_x has been intensively studied and enhanced solar cell efficiencies largely by providing excellent surface passivation on highly and lowly doped p-type silicon surfaces.¹ Meanwhile, to achieve high conversion efficiencies, advanced silicon solar cell architectures such as interdigitated back contact (IBC) solar cells demand that both the n^+ and p^+ doped Si surfaces are passivated simultaneously by a single passivation scheme. However, on heavily doped n⁺ Si surfaces, the AlO_x passivation is compromised because the minority carrier (i.e., hole) concentration at the surface is increased by the significant negative fixed charges of the AlO_x passivation. Therefore, the absence of significant negative fixed charges and high chemical passivation are expected to be beneficial for the passivation of n⁺ surfaces. In this study, we focused on a ternary oxide, $Al_xMg_{l-x}O_y$ (AMO) to make a solution for the passivation of both the n^+ and p^+ doped Si surfaces because MgOx has not only excellent properties such as high permittivity (κ ~9.8), large band gap (7.3 ~7.9 eV), and higher breakdown field (12 MV/cm) but also positive fixed charges on Si surfaces.²⁻⁵ In addition, magnesium aluminate fabricated by atomic layer deposition is hydrogen-rich and amorphous below 800 °C.6 Hence, based on these facts, we have developed ternary Al_xMg_{1-x} O_y as a new class of passivation materials through the use of plasma-enhanced atomic layer deposition (PE-ALD).

[Experimental]

 $Al_xMg_{1-x}O_y$ thin films were fabricated on p-type (100) Si substrates by PE-ALD at 200 °C. Bis(ethylcyclopentadienyl) magnesium [Mg(CpEt)2], trimethyl aluminum [Al(CH₃)₃], and O₂ plasma were used as the Mg, Al, and O sources, respectively. Fig. 1 shows the pulse sequence used to deposit the $Al_{y}Mg_{l-y}O_{y}$ thin films. A super-cycle consisted of a number of sub-cycles of AlO_x (n_{Al}) and a cycle of MgOx. The Mg concentration in the films was controlled by the Mg and Al precursor cycle ratio, R_{pc} (= $[n_{Mg}']/[n_{Mg}'+n_{Al}']$, where n_{Mg}' and n_{Al}' are the numbers of total sub-cycles of Mg and Al precursors, respectively). Rpc was varied from 1/10 to 1/80. Annealing was performed in a tube furnace under N2 ambient at temperatures ranging from 450 $^\circ C$ to 800 $^\circ C$ to activate the surface passivation after depositing AlOx and AlxMg1-xOy. A level of surface passivation and optical and interface properties of the samples were investigated by a lifetime tester, spectroscopic ellipsometer, capacitance-voltage (C-V) measurements and so on.

[Discussion]

From the experiment above, we found that a level of surface passivation and interface properties of $Al_xMg_{I-x}O_y$ thin films can be controlled by varying the Al and Mg

precursor cycle ratio, R_{pc} . In addition, we also found that $Al_xMg_{I-x}O_y$ thin films are superior to pure AlO_x thin films for the passivation of c-Si under a given experimental condition. In particular, we can obtain very low S_{max} of ~5.5 cm/s using $Al_xMg_{J-x}O_y$ thin films on a p-type Czochralski (Cz) (100) Si wafer after post deposition annealing at 500 °C in N₂. Therefore, we can conclude that ALD with a super-cycle consisted of a number of sub-cycles of AlO_x (n_{Al}) and a cycle of MgO_x can be applied for effective engineering of physical properties of the ternary $Al_xMg_{J-x}O_y$ thin films and provide excellent surface passivation on p-type c-Si. During our presentation, we will demonstrate detailed study on the ternary $Al_xMg_{J-x}O_y$ passivation on c-Si and discuss its passivation mechanism for c-Si.

[References]

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Figure 1. Schematic diagram of ALD process of $Al_xMg_{I-x}O_y$ thin films (upper) and measured effective minority carrier lifetime, τ_{eff} of $Al_xMg_{I-x}O_y$ passivated samples fabricated with different R_{pc} at different post deposition annealing time at 500 °C in N_2 (lower).