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Enhanced surface passivation of TiO_x with Al doping

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Titanium oxide (TiO_x) layer is currently re-emerging as a passivating material for high-efficiency crystalline silicon (c-Si) solar cells. For undoped TiO_x, it is known that the surface passivation strongly depends on the film thickness and the annealing temperature, as summarized in Table 1 [1] [2]. For example, Gad and Kasemann reported J_{0s} of 40 and 70 fA/cm^2 with 1.5 nm ALD TiO_x on p-type 1 Ω-cm and 10 Ω-cm wafers, but as the TiO_x layer increased to 5.5 nm, the passivation deteriorates significantly with J_{0s} elevated to 680 and 2000 fA/cm^2 respectively[3].The loss of surface passivation for thicker TiO_x is attributed to a phase transition inside the TiO_x during the deposition [1-5].

Table I. Summary of the thickness dependence of the surface passivation of undoped TiOx.

Doping type	Bulk Resistivity (Ω-cm)	TiO_x deposition method	TiO_x deposition Temp (℃)	TiO_x Thickness (nm)	Anneal Ambient/Temp (℃)	Passivation		Ref
						J_{0s} (fA/cm^2)	i-Voc (mV)	
p-type	5000	ALD	200	8		523		[1]
				66		5061		
p-type	10	ALD	150	1.5	FGA/350	71		[3]
				5.5		2026		
p-type	1	ALD	200	1.5	FGA/350	40		[3]
				5.5		683		
n-type	5-10	E-beam	< 100	3.5	O_2/250	100-130		[2]
				10.5		1600-2000		
n-type	3	ALD	230	5.5	FGA/250		687	[6]
				10			646	

In this abstract, to circumvent the limitation of passivation deterioration on thicker TiO_x due to in-situ crystalization of TiO_x during depostion, we investigated the impact of Al doping on the surface passivation of TiO_x. Our experiments demonstrate that the incorporation of Al ions into the TiOx films inhibits the crystallization of the as-deposited TiO_x, which in turn retains excellent passivation for thicker TiO_x. Further heat treatment significantly improves the surface passivation of Al doped TiO_x, achieving the best surface recombination at 350°C, in stark contrast to the poor passivation observed for the undoped TiO_x. We believe this study presents a promising novel strategy to improve the surface passivation quality and the thermal stability of TiO_x, providing a strong basis for further development of TiO_x to function as antireflection coating and passivation layer simultaneously.

Figure 1 (a) shows the J_{0s} of Al doped TiO_x (TiO_x:Al) as a function of doping concentration. All undoped and doped films were deposited with 500 ALD cycles (about 15 nm), and the Al doping concentration is controlled by choosing a series of cycle ratio of TTIP-H_2O and TMA-H_2O, from 1/71 1/38, 1/26 to 1/19. For as-deposited films, the undoped TiO_x shows a J_{0s} ~ 7.7 x 10^3 fA/cm^2. However, all Al doped TiO_x samples display much lower J_{0s} of ~600 fA/cm^2. Following FGA, the J_{0s} of samples passivated with TiO_x:Al decrease significantly to ~100 fA/cm^2 after FGA at 350℃, while the undoped TiO_x still exhibits a very high J_{0s} of 8.7 x 10^3 fA/cm^2. This significant difference is explained by the inhibition of TiO_x crystallization in 15 nm TiO_x films with the incorporation of Al-O cycles during the ALD deposition, as shown Figure 1 (b).

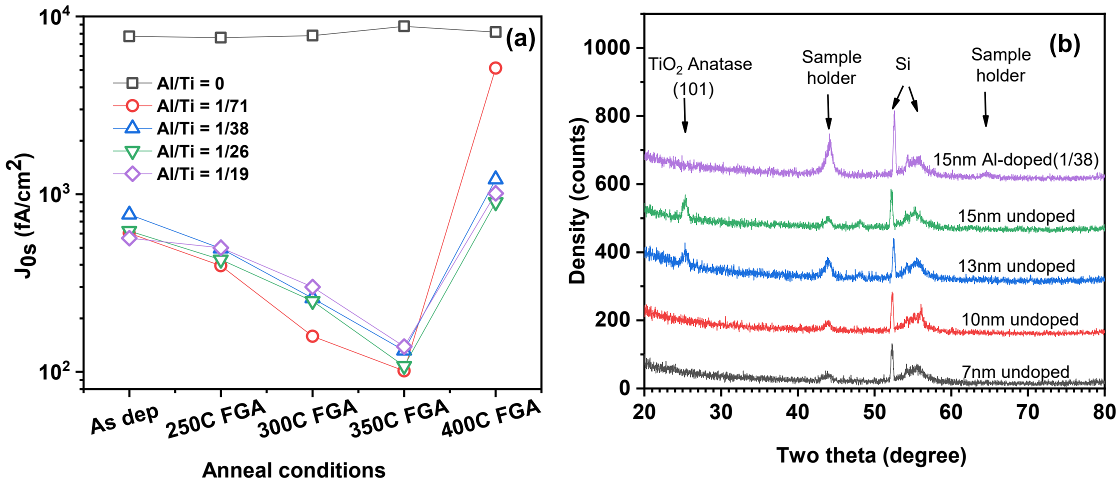

Figure 1. (a) Surface recombination factor J_{0s} of 15 nm Al doped TiOx(TiOx:Al) after successive FGA from 250 ℃ to 400 ℃ and the sample was subjected to each temperature for 5min. (b) Impact of the films thickness and Al doping on the crystalline phase of titania, where all films are as-deposited

In order to get more insight into the impact of Al doping on TiO_x passivation, GIXRD spectroscopy was carried out to disclose the crystalline nature of the as-deposited TiO_x films on c-Si (100) substrates. In Figure 1 (b), the features at 50 - 60° are found to be in good accord with the (311) plane of the c-Si (100) substrate, and peaks at 44° and 64.5° are from the sample jig that holds the sample during measurement. For the undoped TiO_x films, the anatase phase is detected from the 13 nm and 15 nm TiO_x films according to the emerging of a peak located at $2\theta = 25^{\circ}$, which is assigned to the (101) plane of the anatase TiO_x. However, we do not detect this peak for the 7 nm and 10 nm TiO_x films confirming TiO_x is amorphous. More importantly, the 15 nm Al doped TiO_x does not show any diffraction peak of anatase or rutile phase demonstrating that the crystallization of TiO_x is indeed restrained by Al doping, which is in line with the passivation results in Figure 1(a).

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