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Highly oriented Si(111) films on lattice-mismatched single-crystalline substrates via aluminum-induced crystallization

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Abstract

In aluminum-induced crystallization, annealing of thin (t < 50nm) Al/a-Si stacks at sub-eutectic temperatures leads to the diffusion of the a-Si through the Al grains and crystallization at the substrate/Al interface. This process is typically performed on glass, or other amorphous substrates. Here, we demonstrate that the same process can be used to produce Si(111) films on lattice mismatched crystalline substrates. When the crystalline substrate has a hexagonal surface, highly aligned Si(111) films can be fabricated on the substrate surface. X-ray rocking curve full-width half-maximum values are comparable to those grown epitaxially by chemical vapor deposition.

1. Introduction

Aluminum-induced crystallization (AIC) is well-known as a method for producing polycrystalline silicon thin films on amorphous substrates. In this process, a thin (t < 50nm) aluminum film is deposited on the substrate surface, followed by a brief air exposure, and then deposition of an amorphous silicon film of similar thickness. Upon annealing at subeutectic temperatures (T < 577°) in an inert ambient, the amorphous silicon diffuses through the aluminum to the substrate interface and begins crystallizing. As more silicon crystallizes, the aluminum is displaced upwards and the layers exchange place, leaving a polycrystalline, highly (111) oriented silicon thin film on the substrate surface[1].

Well before this process was developed on amorphous substrates, a similar layer-exchange process known as solid-state epitaxy was developed for producing p+ doped silicon contacts at low temperatures. In these reports, metal-induced layer exchange on crystalline silicon substrates produced crystalline silicon thin films that matched the orientation of the underlying silicon substrate[2].

In this report, we attempt to adapt the solid-state epitaxy process to non-silicon crystalline substrates, including those lattice matched to Si(001) and Si(111). Both the substrate surface energy and the driving force for Si(111) preferential orientation are found to strongly influence the crystallization behavior of the AIC-Si film.

2. Experimental

Sample Preparation

Monocrystalline strontium titanate (STO) with a (001) surface, c-axis oriented GaN and c-axis oriented sapphire were used as substrates for this process, along with an amorphous fused quartz reference substrate. Samples were cleaned in acetone/IPA/DI water with ultrasonication, followed by piranha clean and flowing DI rinse.

For deposition, samples were loaded into and ULVAC RF sputter system that was evacuated to base pressures below 2x10-4 Pa. 30 nm aluminum and a-Si were deposited at 110 W for 300 and 500 seconds respectively, with a 3 minute air exposure between depositions.

Fabrication and Characterization

Samples were then annealed at 400-450°C in an argon atmosphere for 20-240 minutes to drive layer exchange. After annealing, X-ray diffraction characterization and electron backscatter diffraction was performed to characterize the orientation of the AIC-Si films.

3. Results

Aluminum-induced crystallization of sub-50nm Si films

As seen in Figure 1a, θ-2θ scans indicate that Si(111) is formed on all crystalline substrates, including STO(001), which has only a 3.4% lattice mismatch with Si(100). In comparison, the larger lattice mismatch between Si(111) and GaN or sapphire (18% and 27% respectively) does not hinder Si(111) formation.

Electron backscatter diffraction gives a further description of the <111> normal direction for these films, following earlier reports. As seen in figure 1b-e, films fabricated on the reference quartz sample and STO (001) substrate have uniform (111) orientation but a loose distribution around the <111> direction. In contrast the distribution is much tighter for the films grown on the GaN and sapphire films, with sharp, narrow lines indicating grain surfaces are uniformly oriented towards the <111> direction. This can be confirmed from Figure 2, which shows x-ray rocking curves of Si films on a) GaN and b) sapphire substrates with very narrow full-width half maximum values, ranging from roughly 0.3° on GaN and 0.1° on sapphire.

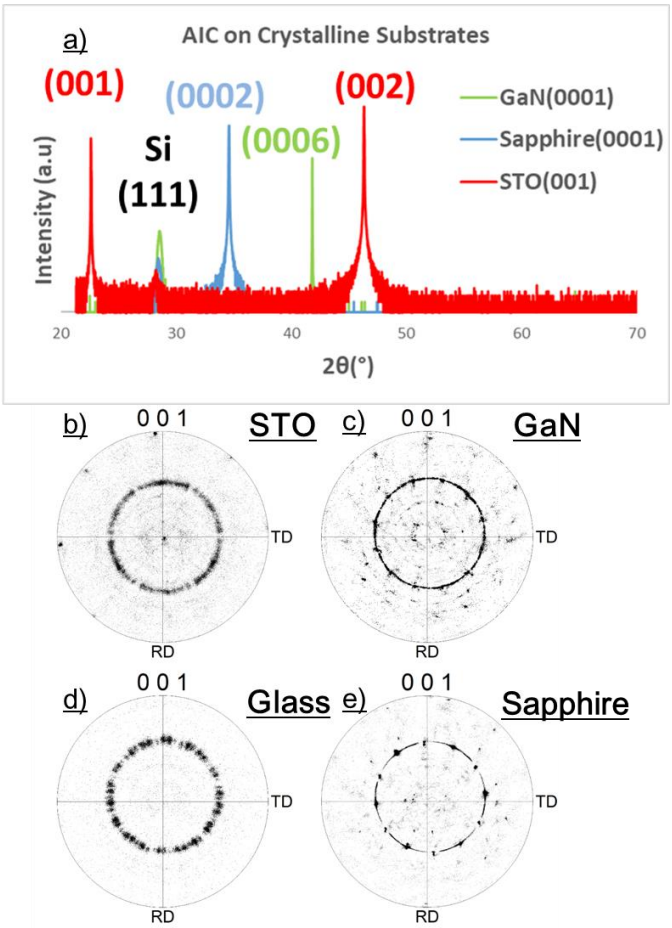

Fig. 1 - Si(111) fabricated on crystalline substrates by aluminum-induced crystallization. a) XRD showing Si(111) formed on different crystalline substrates. b-e)EBSD pole figures showing the extent of orientation or misorientation relative to the <111> for the AIC-Si films

Aluminum-induced crystallization of thicker Si films

Remarkably, these highly oriented films can still be fabricated under conditions that generally do not promote preferential Si(111) orientation during aluminum induced crystallization. Films fabricated from 90nm Al and 100nm a-Si layers in Figure 4 are shown to have a more randomly distributed orientation when formed on glass and STO, but when formed on sapphire, they maintain their selective preferential <111> orientation, suggesting that the influence of the substrate can become the dominant force driving not only misorientation, but preferential orientation in general.

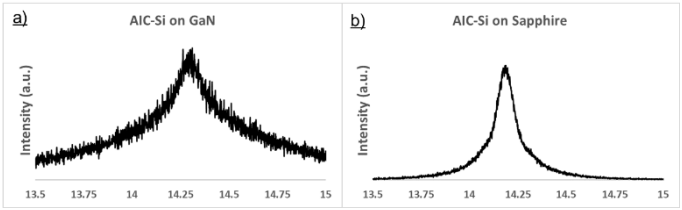

Fig. 2 - X-ray rocking curves of AIC-Si on a) GaN and b) sapphire showing narrow full-width half-maximums.

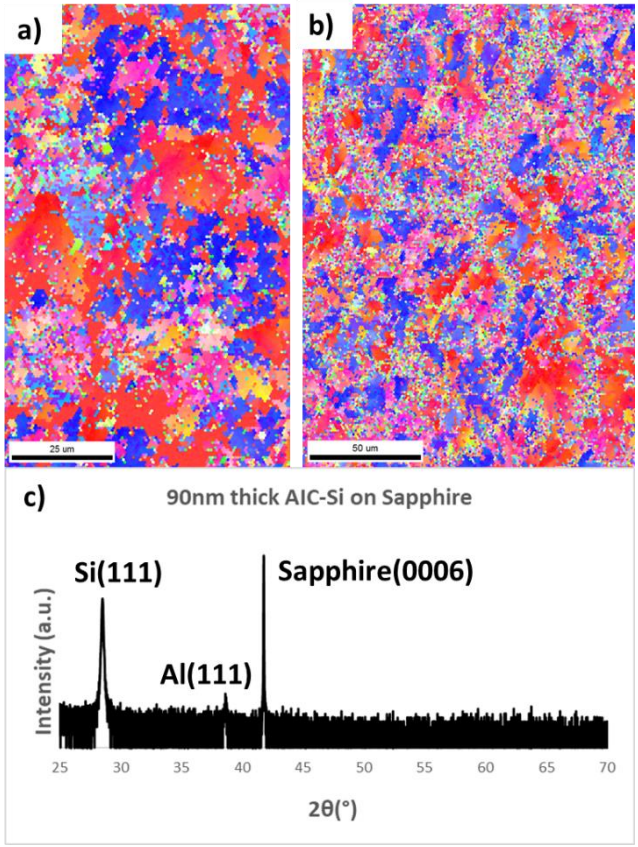

Fig. 3 - Substrate effects on thicker Si films. EBSD of ~100nm AIC-Si on a) STO(001) b) glass showing a loss of preferential orientaiton with increasing thickness. c) XRD of thicker AIC-Si on sapphire showing that preferential Si(111) orientation is preserved. Note the Al peak is present because Al was not etched from the film surface.

3. Conclusions

In summary, aluminum induced crystallization on monocrystalline substrates lattice matched to both Si(100) and Si(111) produces Si(111) films for film thicknesses below 50nm. On hexagonal GaN and sapphire substrates, these films become highly oriented, with very narrow full-width half-maximum peaks. The orientation-promoting effects of these substrates is strong enough to promote Si(111) orientation even in thicker films that typically do not form with a preferential Si(111) orientation.

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