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Atmospheric Pressure Iodine Vapor Transport for Thin-Silicon Growth

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Atmospheric Pressure Iodine Vapor Transport for Thin-Silicon Growth

T.H. Wang, T.F. Ciszek, M.R. Page, R.E. Bauer, M.D. Landry, Q. Wang, and Y.F. Yan
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Abstract

Randomly oriented or [110]-textured polycrystalline silicon layers have been grown on foreign and silicon substrates by iodine vapor transport at atmospheric pressure with high rates (~3 µm/min) and large grain sizes (~20 µm) at a moderate temperature of ~900°C. A gravity trapping effect coupled with the cold-top vertical reactor configuration allows use of an open-tube system without much loss of the volatile gas species and offers high-speed transport of silicon in the reaction zone at the hot bottom. High quality epitaxial layers can also be grown on CZ-Si for electronic applications or on MG-Si substrates for thin-layer solar cells.

1. Introduction

The atmospheric pressure iodine vapor transport (APIVT) [1] of silicon is based on a disproportionation reaction [2] between SiI_2 and SiI_4. It is a non-vacuum, open-tube deposition system technique with potential for continuous processing, low capital cost, and no need for expensive effluent treatment. It has shown to be able to deposit polycrystalline silicon thin layers on foreign substrates at high rates (~3 µm/min) and with large grain sizes (~20 µm) at a moderate temperature of about 900°C. This is to report our recent results in advancing the technique for thin silicon solar cells.

2. Reactor

A vertical quartz tube houses the substrates, Si source, iodine, and all the resulting silicon iodides. Two heaters control the source and substrate temperatures independently. The reactor is maintained cold at the top and hot at the bottom. The deposition zone can be expanded as required to accommodate large substrates or to allow a vertical arrangement of multiple substrates. A schematic of the reactor setup is shown in Fig.1. The cloud of iodine and silicon iodides trap all the volitile gas species underneath. A continuous hydrogen purge flow keeps air from entering the system.

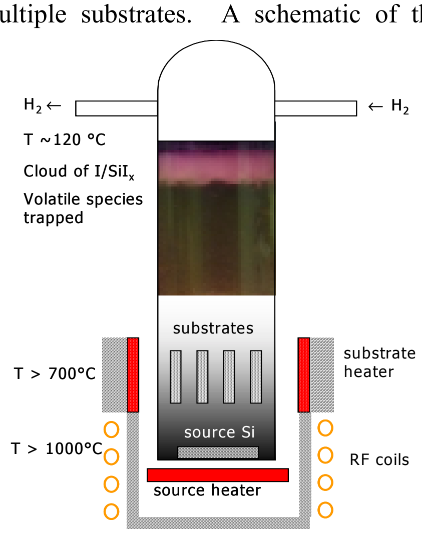

Fig 1. Schematic for a two-heater reactor

3. Large grain sizes

The average grain size strongly depends on substrate temperature. However, even at only 750°C, the obtained grain sizes are still on the order of 5 µm (Fig. 2), larger than those achieved by chlorosilane-CVD processes at 1200°C. Once the substrate temperature is increased to 950°C, the grain sizes reach over 20 µm (Fig. 3).

These large grain sizes are believed to be the result of a relatively small free-energy driving force (and thus a low density of nucleation), as evidenced by strongly faceted growth. It is also possible that the reversible nature of the disproportionation reaction between Si_2 and SiI_4 etches back small nuclei caused by any thermal fluctuation.

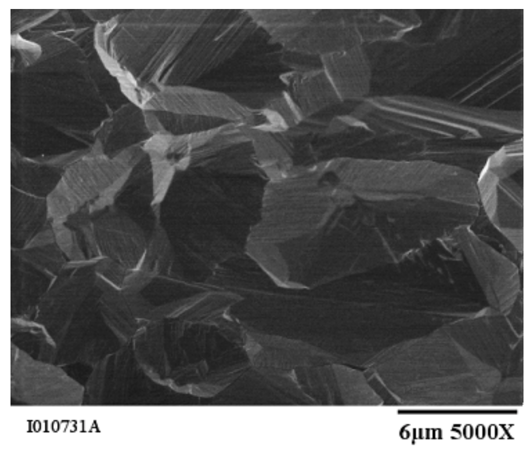

Fig 2. Poly-Si layer grown at 750°C

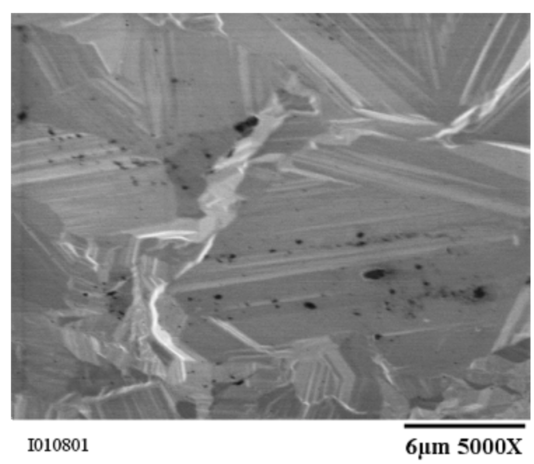

Fig 3. Poly-Si layer grown at 950°C

4. Highly [110]-textured and randomly oriented polycrystalline Si films

APIVT-grown films typically have grains with random orientations regardless of substrates used. By modifying the deposition conditions, we obtained highly [110]-oriented films. Fig. 4 shows X-ray diffraction peaks from two samples, both deposited on high-temperature glass, in comparison to standard silicon powder peaks. All the peaks were normalized to the standard [111] peak. The solid line is for a sample that was deposited under normal conditions, which showed almost random orientations, with slight [110] texturing. The dashed line, on the other hand, is a sample deposited under a different condition, but with similar grain size and thickness.

Transmission electron microscopic (TEM) observation indicates that more than 90% of the grains are within about 5° of the <110> axes. Two of the perfectly [110]-aligned grains actually allow one to see a high-resolution image of the grain boundary with dislocation cores (Fig. 5).

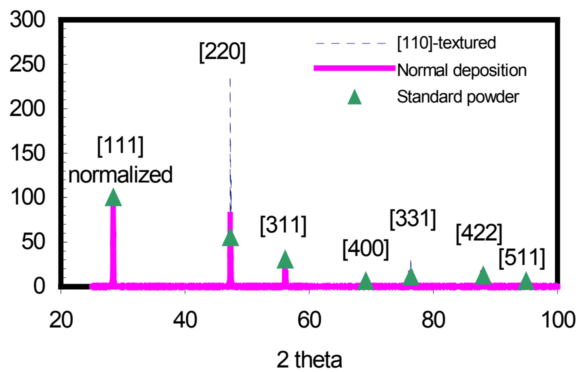

Fig 4. XRD peaks of poly-Si films

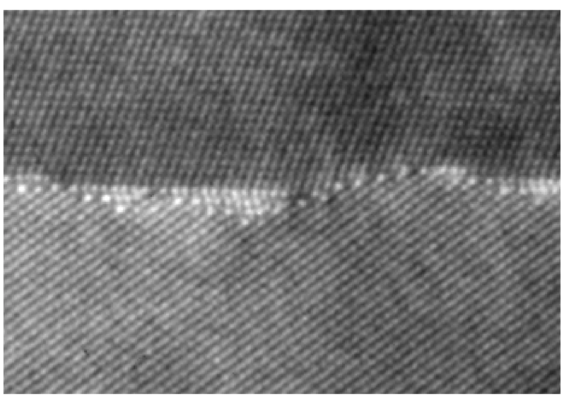

Fig 5. HRTEM image of two [110]-oriented grains

5. Epitaxial growth

We obtained high quality epitaxial growth on silicon substrates when a clean interface is maintained. This allows us to obtain high-quality active layers on low-cost metallurgical-grade silicon substrates for solar cells or different doping layers on single crystal substrates for micro-electronic applications. Epitaxial layers also give us a measure of the solar cell performance limitations of this material independent of any grain size effect. TEM studies of the layers indicate very low density of crystallographic defects (such as stacking faults and dislocations) compared to the underlying substrate.

Two hetero-junction solar cells with a-Si emitters were fabricated. One was made on a 20-µm thick epitaxial Si layer grown on a heavily doped single-crystal Si wafer (~0.0095 Ω-cm). The other was prepared on a CZ-Si control wafer. As shown in Fig. 6, the APIVT-grown epitaxial Si layer demonstrates a thickness-limited 23 mA/cm^2 and the same V_{oc} of the CZ-Si control cell.

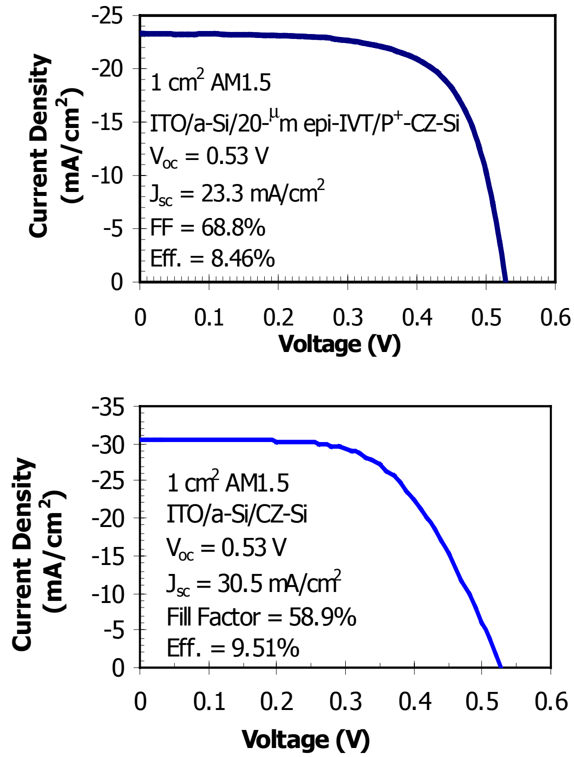

Fig 6. Diagnostic solar cell result. Top: Epitaxial-Si grown by APIVT; Bottom: CZ-Si control

6. Summary

The APIVT technique produces continuous polycrystalline silicon layers at high deposition rates (~3 µm/min) with large grain sizes (~20 µm) at a moderate temperature of 900°C on non-silicon substrates such as mullite, Corning Vycor high-temperature glass, or Corning LGA-139 glass ceramics. Randomly oriented or highly [110]-textured films can be obtained. Epitaxial growth on single-crystal Si substrates show a very low density of lattice defects and comparable device performance to CZ-Si.

Acknowledgement

We would like to thank Prof. Dieter Ast of Cornell University for providing the Corning LGA-139 glass ceramics substrates. We also thank Manuel Romero for electron microscopic characterizations of the materials.

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[1] T.H. Wang and T.F. Ciszek, “Growth of Large-Grain Silicon Layers by Atmospheric Iodine Vapor Transport,” *J. Electrochem. Society*, **147** (5) (2000) 1945-1949.

[2] R. Glang and E.S. Wajda, "Silicon" in *The Art and Science of Growing Crystals*, Ed. J.J. Gilman, John Wiley & Sons, New York, (1963) 80-92.