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## Preprint

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# APIVT Epitaxial Growth on Zone-Melt Recrystallized Silicon

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## Introduction

Single-junction thin-film silicon solar cells require large grain sizes to ensure adequate photovoltaic performance. Using 2D silicon solar cell simulations on the quantitative effects of grain-boundary recombination on device performance [1], we have found that the acceptable value of effective grain boundary recombination velocity is almost inversely proportional to grain size. For example, in a polycrystalline silicon thin film with an intragrain bulk minority-carrier lifetime of 1 μs, a recombination velocity of $10^4$ cm/s is adequate if the grain is 20 μm across, whereas a very low recombination velocity of $10^3$ cm/s must be accomplished to achieve reasonable performance for a 2-μm grain. For this reason, large grain size on the order of hundreds of μm is currently a prerequisite for efficient solar cells, although a more effective grain-boundary passivation technique may be developed in the future.

One way to achieve such large-grained silicon layers is by zone-melt recrystallization (ZMR) to make a seed layer on an inexpensive high-temperature substrate, followed by device-quality epitaxial layer growth. The ZMR silicon seed layer is heavily contaminated due to the high-temperature melt process, even though its crystallinity may be excellent. Epitaxy preserves the crystallinity and maintains low impurity levels in the active absorber layer by a lower-temperature process. Even with the relatively high-temperature (1150°C) trichlorosilane atmospheric pressure chemical-vapor deposition (APCVD) technique, Sims et al. [2] demonstrated over 9%-efficient solar cells in an epitaxial layer on a ZMR seed layer using an AstroPower-developed ceramics substrate. An inexpensive and fast epitaxy process at a lower temperature (~900°C) may be able to further improve the material quality by reducing impurity contaminations. We report here on epitaxial silicon film growth on ZMR silicon seed layers by the atmospheric-pressure iodine vapor transport (APIVT) [3] with such desired characteristics.

## Experimental

*AstroPower, Inc*. - A silicon layer was deposited onto a proprietary ceramics substrate by CVD. This special ceramics is high-temperature compatible, chemically stable, and closely matched to silicon in thermal-expansion coefficient. It is fabricated by a low-cost tape cast process with an estimated material cost of ~$10/m$^2$. This silicon layer is then zone-melt recrystallized to make a large-grained 40-μm-thick seed layer with the grains elongated along the scanning direction of the line heater/substrate transport. Typical grain width is about a few tenths of a mm. APCVD with trichlorosilane was used to grow 26-μm-thick epitaxy films for comparison to APIVT growth.

*NREL* - The ceramics substrates with ZMR silicon seed layers were cut into 2.5-cm x 2.5-cm squares to fit our experimental APIVT reactor. The general APIVT deposition process has been described elsewhere [3]. However, maintaining a clean interface is critical to obtain epitaxial growth. In the current experimental system, this clean condition is accomplished by heating the substrate to the source temperature before actual growth starts, which avoids the build-up of silicon iodides at the film/substrate interface. An oxygen-free ambient in the reactor is also critical. Combining cycle-purging and continuous-purging is effective in removing oxygen from the reactor. We also used a resin-based gas purifier for the argon and hydrogen purge gases. During growth, the substrate temperature was lowered to 900°C to minimize impurity contamination and to still be able to maintain low defect density. Dopant boron is incorporated into the films from the pre-doped source silicon at a 1-to-1 ratio. Epitaxial film thickness ranges from 25 μm to 50 μm. Grown films are characterized by secondary-ion mass spectrometry (SIMS), transmission electron microscopy (TEM), scanning electron microscopy (SEM), and optical microscopy.

**Surface morphology**

Figures 1a, 1b, and 1c show different appearances of the epitaxial silicon film sur-

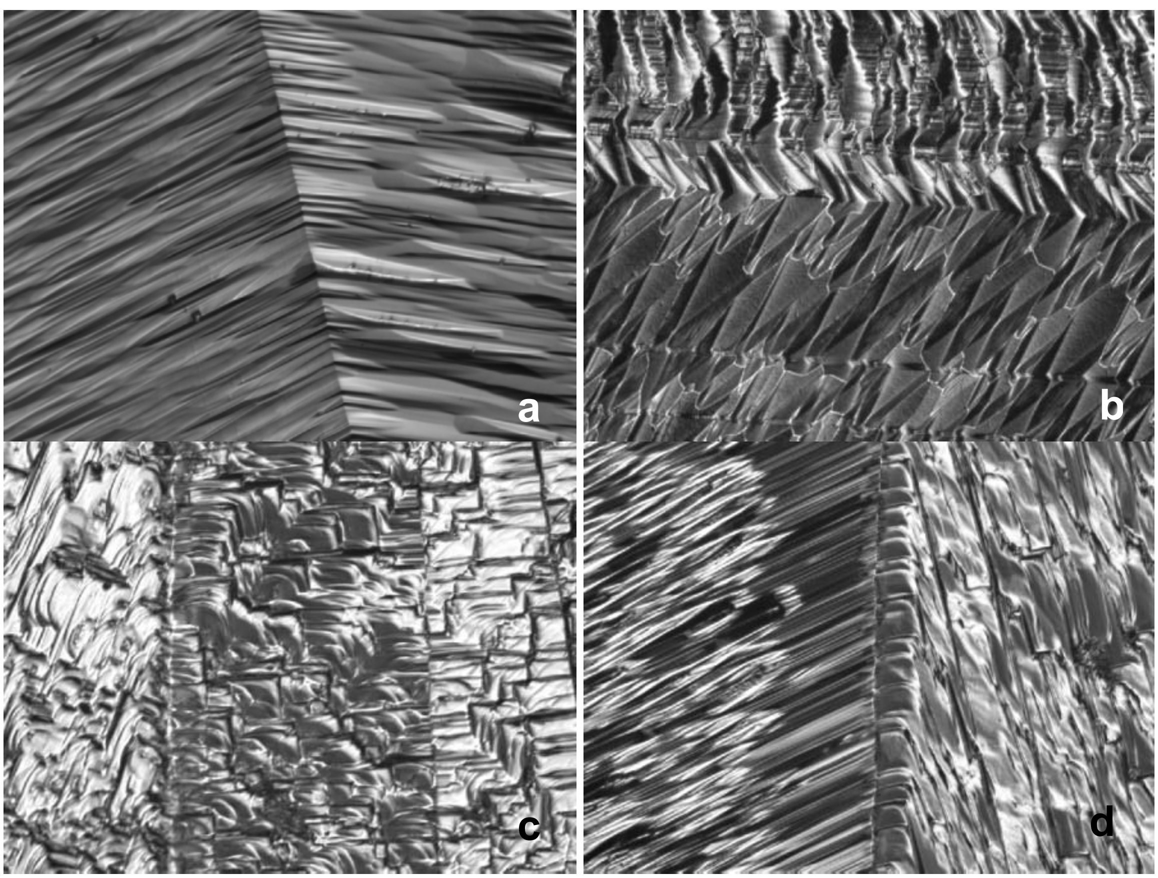


Fig. 1. Nomarski photomicrograph showing surface morphology of APIVT epitaxial silicon films grown at 900°C on a ZMR seed layer. Picture width = 350 μm.

faces. Depending on their orientations, some grains have smooth surfaces (only 1-2-μm variations); others have rough ripples or ridges as high as 10 μm in a 45-μm-thick film. Growth at grain boundaries appears to be very conformal; there are no apparent voids or holes at grain boundaries. At some large-angle grain boundaries (Fig. 1d), thicker growth was seen, probably due to locally higher free energy that leads to faster growth. These films were grown at 900°C with an average rate of 1 μm/min.

### Comparison with high-temperature APCVD

Films grown by trichlorosilane APCVD at 1150°C at 4.3 μm/min generally show macroscopically smoother surfaces (Figs. 2a and 2b). This is to be expected, as higher temperature tends to increase microscopic roughness and reduce macroscopic roughness. A thermal CVD process in principle also has a higher free-energy driving force than the near-equilibrium APIVT process.

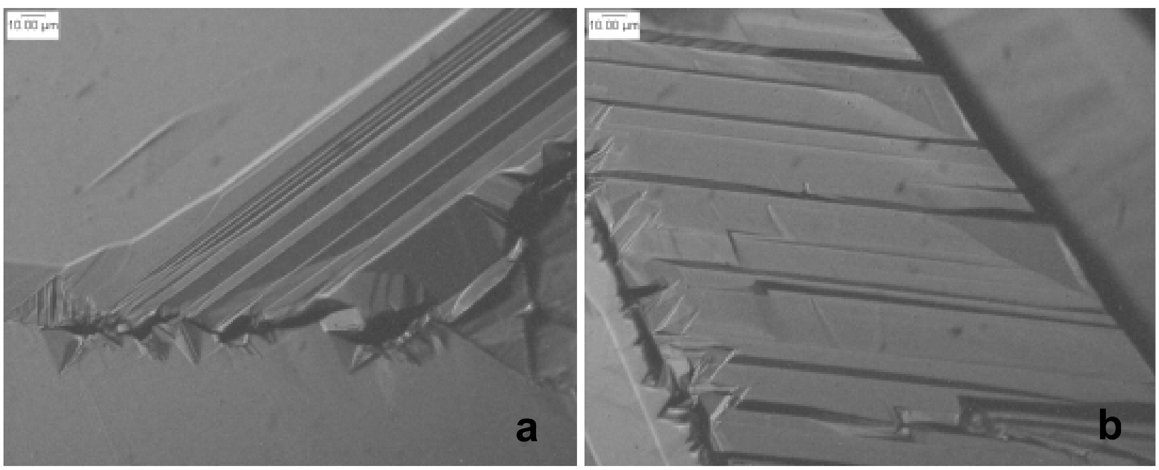


Fig. 2. Nomarski photomicrograpgh showing surface morphology of trichlorosilane APCVD epitaxial silicon films grown at 1150°C on a ZMR seed layer.

### Orientation-dependent growth rate

Examining an entire surface after APIVT epitaxy on a 2.5-cm x 2.5-cm substrate, we observed that some grains grew at nearly twice the rate as some neighboring grains. This was also evident in a trichlorosilane APCVD film in Fig. 2b. In some APIVT films grown at faster than 1 μm/min, polycrystalline deposition occurred on one single grain, while the next grain showed epitaxy at a faster rate, as shown in Fig. 3. The photomicrograph to the left in Fig. 3 is focused on the epitaxially grown grain, whereas the one to the right is focused to the polycrystalline growth on the neighboring substrate grain. The epitaxy grain is 45 μm thick, as compared to a 30-μm average thickness for the polycrystalline part, after 25-min growth. This implies that because of the lower temperature of 900°C that we used, some grains of special orientations cannot grow at a fast enough rate to keep up with the incoming silicon atoms. Reducing the overall growth rate to ~1 μm/min eliminated any polycrystalline deposition. Therefore, we may define 1 μm/min as approximately the maximum epitaxial growth rate for all grains at 900°C. This maximum rate is obviously higher with a higher growth temperature.

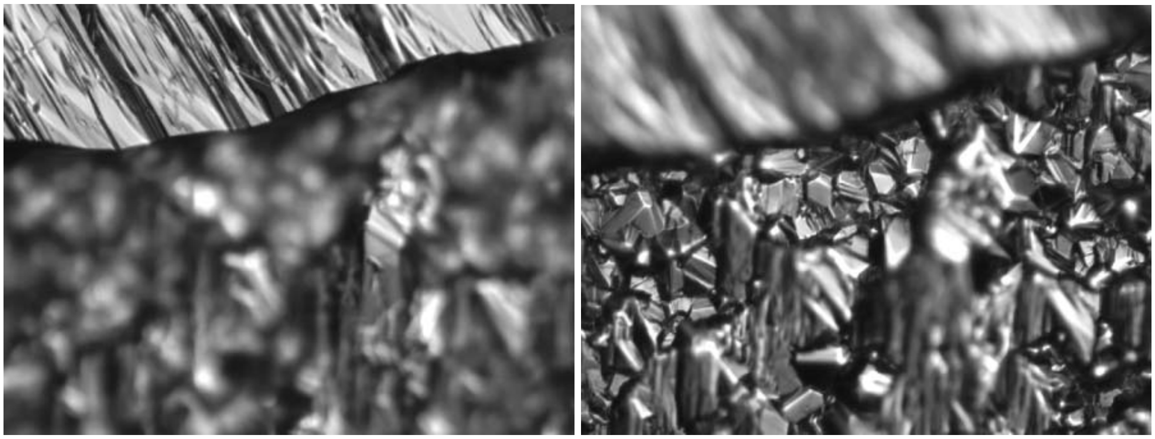

Fig.3. Photomicrograph of aerial view in the same area, showing two adjacent substrate grains that resulted in epitaxy and polycrystalline growth with focal points at the respective surfaces. Picture width = 350 μm.

**Summary**

We report successful epitaxial silicon film growth on ZMR silicon seed layers by the inexpensive and fast epitaxy process of atmospheric-pressure iodine vapor transport at a lower temperature of ~900°C than the previous growth at 1150°C by trichlorosilane APCVD. Maintaining a clean interface is critical to obtaining epitaxial growth by any method, and it is particularly important for the APIVT technique because there are no in-situ cleaning gas agents available. In the current experimental system, this clean condition is accomplished by heating the substrate to the source temperature before actual growth starts.

Surface morphology depends strongly on the orientations of individual grains and the growth temperature. The APIVT films generally have rougher surfaces than the trichlorosilane APCVD films due to the lower temperature used and the near-equilibrium growth nature of APIVT. A maximum deposition rate to ensure epitaxial growth on all grains is determined to be about 1 μm/min for a growth temperature of 900°C.

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