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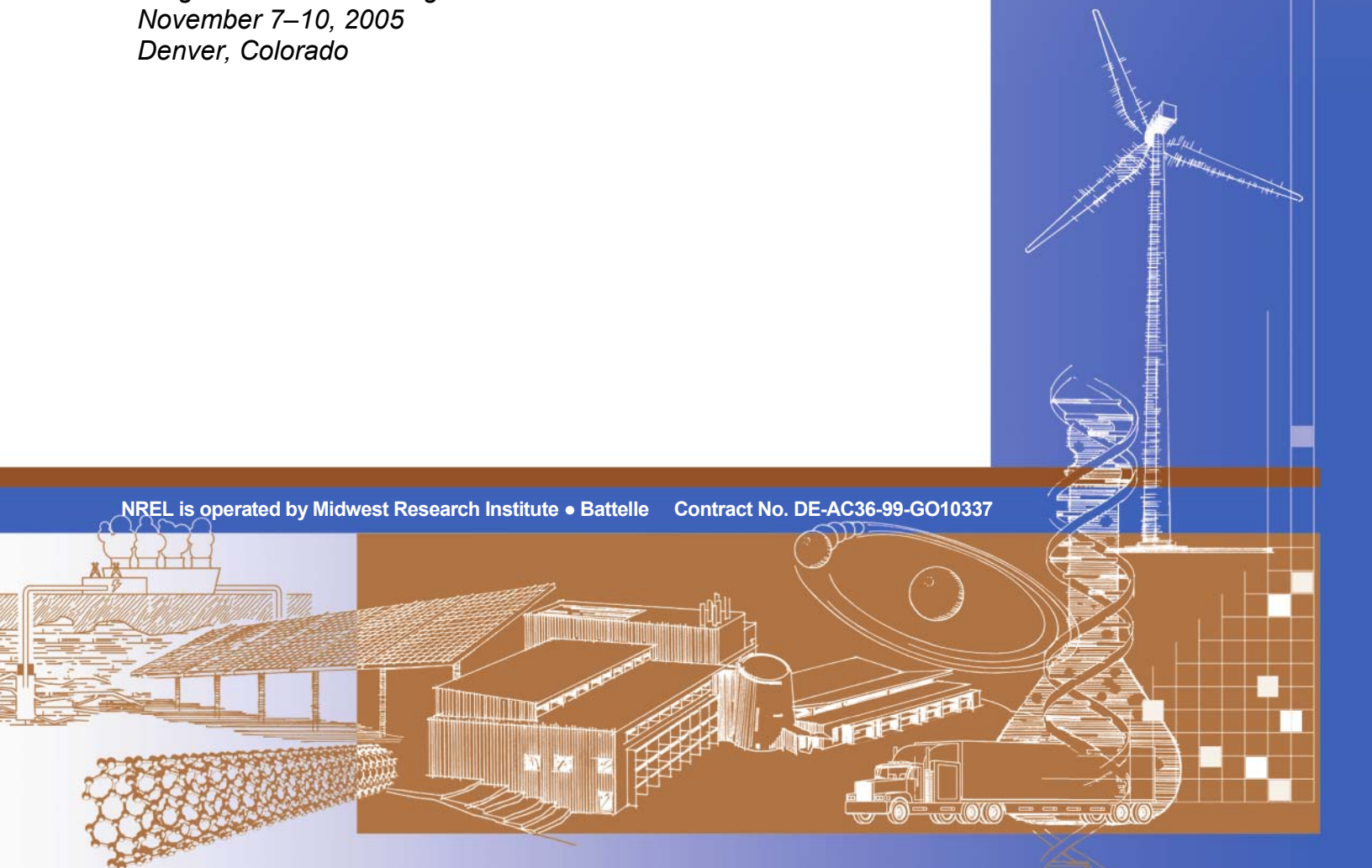

Rapid Thermal Annealing of HWCVD a-Si:H Films: The Effect of the Film Hydrogen Content on the Crystallization Kinetics, Surface Morphology, and Grain Growth

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ABSTRACT

We report the effect of the hydrogen (H) content (C_H) on the crystallization kinetics, surface morphology and grain growth for Hot Wire CVD a-Si:H films containing 12.5 and 2.7 at.% H which are crystallized by rapid thermal anneal (RTA). For the high C_H film we observe explosive H evolution, with a resultant destruction of the film for RTA temperatures >750C. At RTA temperatures ~600C, both films remain intact with similar morphologies. At this same lower RTA, the incubation and crystallization times decrease, and the grain size as measured by X-Ray Diffraction increases with decreasing film C_H. SIMS measurements indicate that a similar film C_H (<0.5 at.%) exists in both films when crystallization commences. The benefits of a two-step annealing process for the high C_H film are documented.

1. Objectives

The ability to crystallize thin a-Si:H into large grain Si can lead to significant improvements in Si solar cells. We are examining what factors play a role in determining crystallite grain size and/or defect density when a-Si:H films undergo RTA to induce crystallization. Such factors include film H content, crystallization anneal temperature, higher temperature post anneals to possibly reduce the film defect density, and how to rehydrogenate the grain boundaries. This work addresses these first two factors.

2. Technical Approach

0.8-1.0μm thick a-Si:H films with different initial hydrogen content (C_H) were deposited on 1737 corning glass by the HWCVD method.[1] Films were annealed at temperatures (T_A's) between 600°C to 800°C in a custom built RTA system for times ranging from 6 sec to 400 min.[2] The shift of the reflection fringes in the visible region and the saturation of the c-Si reflectance UV peak intensities were used as indictors of the completeness of crystallization.[3] XRD spectra of all films were measured for 2θ between 20-60° to define the amorphous incubation time, confirm completeness of crystallization and determine the grain size from the (111) diffraction peak FWHM using Sherrer's formula. The experimental procedure was to anneal the same piece of each film consecutively at each T_A, and measure the reflectance and XRD after every step. SIMS was also employed to measure the hydrogen profiles. Finally, optical micrographs of the Films were taken to examine changes in the surface morphology of the films due to different T_A's.

3. Results and Accomplishments

While the incubation (T_I) and crystallization (T_C) times are similar for films of different C_H for a T_A >750C, the significant H evolution has a dramatic effect on the surface morphology for the high C_H film at this T_A. In particular, for the high C_H film we observe explosive H evolution, with a resultant destruction of the film. This does not occur for the low C_H film, as the surface morphology remains unaffected by the much smaller amount of H evolved. Optical photographs of these films are seen in Figure 1. On the other hand, the T_I and T_c

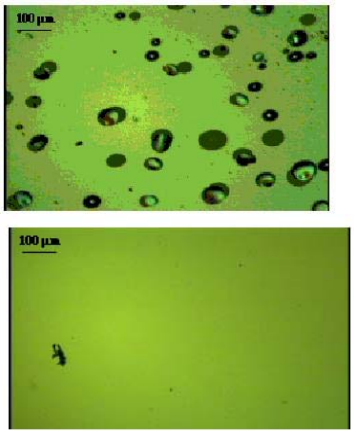

Fig. 1. Surface morphology of the high C_H (top) and low C_H (bottom) films annealed at 800C for 6 s.

times are markedly affected by the C_H at a lower T_A of 600C.[2] In particular, T_I and T_C decrease from 11,400s and 24,000s to 6,000s and 13,500s respectively as the film C_H is lowered from 12.5 to 2.7 at. %. At the same time, the XRD grain size is also quite different at low T_A. As seen in Figure 2, the maximum grain size for the 12.5 at.% C_H film is ~500Å, while that for the 2.7 at.% C_H film is ~800Å. We note that XRD linewidth broadening relates to the development of structural order on a scale longer than that existing in amorphous films. We are currently examining identically deposited and RTA annealed films by TEM to determine whether this measure of long-range order extends entirely across a 'grain', as defined in the

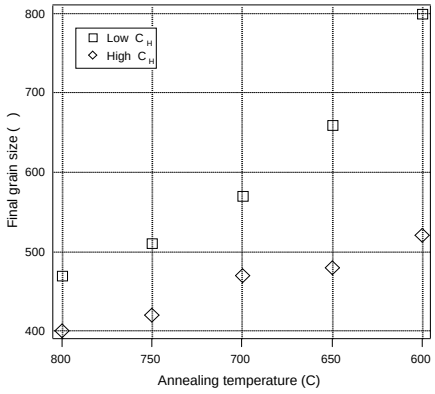

Fig. 2 . XRD grain size versus film C_H for different T_A.

usual sense of a 'crystallo graphic region separated by high angle grain boundaries'. However, in the present work we use the term 'grain size' to indicate the spatial context of the long range order as measured by XRD line broadening.

Figure 3 shows SIMS H profiles for the two films annealed at 600C. Shown are the as grown C_H, the film C_H when nucleation is first observed by XRD, and also the film C_H at complete crystallization. Two points of interest can be noted. First, irrespective of the initial film C_H, both films exhibit a similar C_H (~0.1-0.2 at.%)

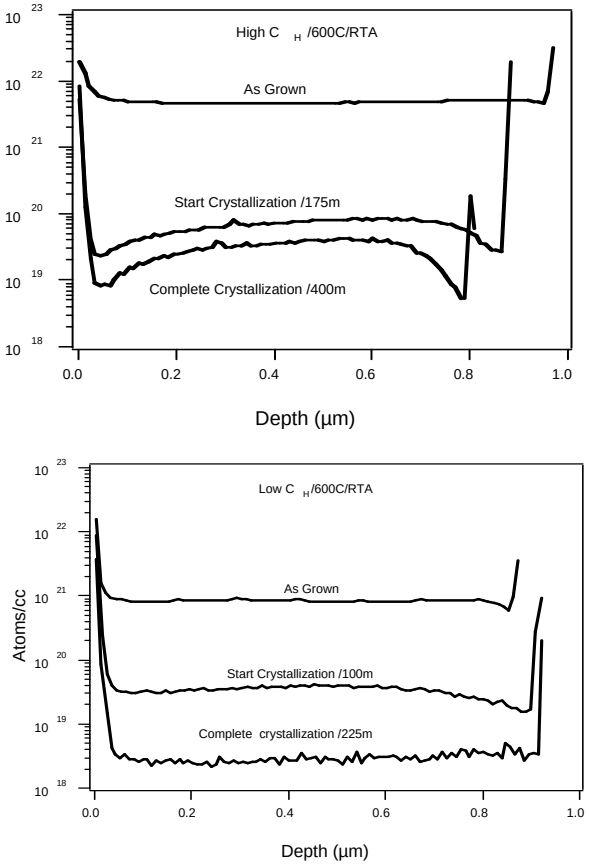

Fig. 3. SIMS H depth profiles for the 12.5 (top) and 2.7 (bottom) at.% C_H films.

when nucleation first occurs. Further, since most of the initial C_H is lost very early in the incubation period,[2] we suggest that nucleation may be initiated not be evolution of the more loosely bound, or 'mobile' H, proposed to assist in a-Si:H crystallization,[4] but by evolution of the more tightly bonded H which generates a larger number of dangling bonds upon evolution.[5] Second, the high C_H film retains most of this ~0.1 at.% C_H as it is annealed to complete crystallization, while the low C_H film looses all its remaining C_H following a similar 600C anneal. Since the XRD grain sizes are roughly similar when nucleation commences,[2] the data of Fig. 1 suggest that the C_H retained by the high C_H film may act to retard grain growth and/or grain coalescence as the film is annealed to complete crystallization.

Finally, we investigate whether a two–step anneal of the high C_H film might result in a final grain size similar to that of the low C_H film. Accordingly, we pre-annealed our high C_H film for 50 hours in a conventional furnace at 400C to evolve a significant fraction of the 12.5 at.% H. This film was then RTA annealed at 650C in a fashion identical to the previous experiment, and the grain size was examined. We observed that the grain size increased using this two-step procedure (from ~475Å to ~625Å), to a value more comparable to the results for the low C_H film. This promising preliminary result suggests an avenue to further improve the crystallization of our high C_H HWCVD films.

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