

Restricted epitaxial growth during thermal crystallization of nanocrystalline silicon: experiments and modeling

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Hydrogenated nanocrystalline silicon (nc-Si:H) has attracted greater attention because of its improved transport properties with respect to hydrogenated amorphous silicon (a-Si:H) [1]. In addition, its deposition conditions are compatible with amorphous silicon technology which makes it possible to use both materials in the same device. In this sense, it has been proposed as a candidate for the circuits connecting amorphous thin film transistors (TFTs) in active matrix liquid crystal displays [2] and has been used as a part of a-Si:H photovoltaic solar cells and other devices [3]. Essentially, the high crystalline fraction (up to 90%) of nc-Si:H results in high carrier mobility and electrical conductivity. However, in contrast with polycrystalline silicon obtained by crystallization of a-Si:H [4], the conductivity of nc-Si:H cannot be described by a simple law of mixtures between the values for its amorphous and crystalline phases [5]. Deviations from this simple behaviour are explained by the important role of grain boundaries between crystallites and the amorphous phase [6]. They act as potential barriers to charge transport. Important changes in conductivity are observed when the grain boundaries are modified by thermal annealing [7, 8].

In the present work, we study the thermal crystallization of nc-Si:H by means of differential scanning calorimetry (DSC). Experiments reveal that the amorphous phase crystallizes by solid phase epitaxy around the pre-existing crystallites. However, and in contrast with the usual crystallization of wafers partially amorphized by ion implantation, only a small fraction of the interface contributes to the epitaxial growth. This conclusion relies on two main results: a) the crystallization temperature is much higher and b) the crystallization peak is sharper than expected. Both features result in the characteristic dependence of the interface area active for epitaxy versus the epitaxial distance plotted in Fig.1.

To test the correctness of our conclusion, we have modelled the restricted epitaxial growth of nc-Si [9]. The model assumes that all pre-existing crystallites are identical squares randomly distributed inside the amorphous phase (Fig. 2). This 2D model successfully describes the dependence of the active interface area on the epitaxial distance and delivers a fraction of the interface area coherent with the experimental results. Furthermore, the numerical simulation provides information about the spatial distribution of the active a-c interface sites and about the grain morphology development during crystallization. A calculated microstructure cross section corresponding to a transformed fraction of 84% relative to the initial amorphous volume fraction is given in Fig 2.

The restricted epitaxial growth revealed by our study can be useful for understanding the microscopic mechanisms of carrier transport in nc-Si:H.

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Figures:

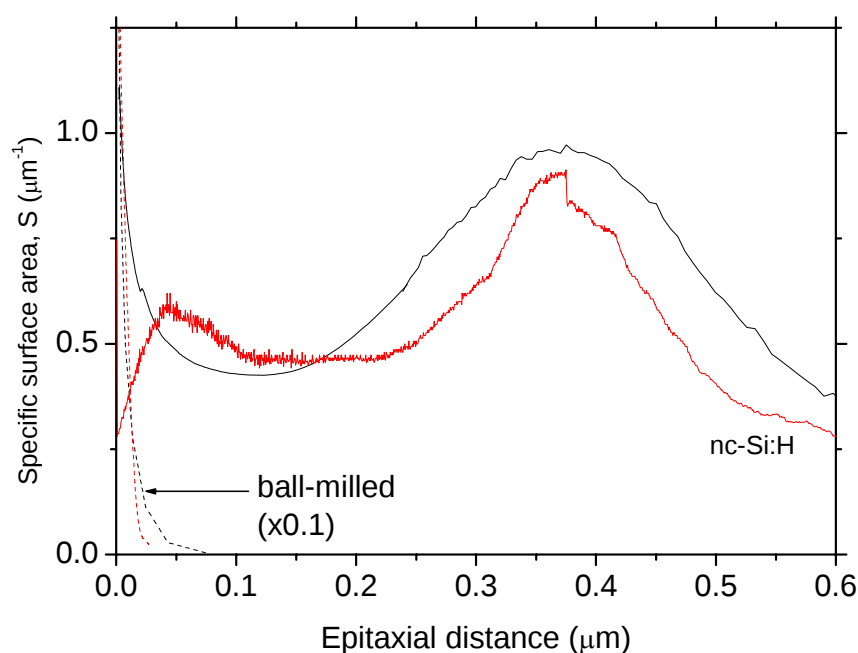


Fig 1. Specific surface area of the crystallization front vs epitaxial distance for the nc-Si:H (solid line) and ball-milled Si (dashed line). Black lines correspond to experimental data while red lines are numerical results.

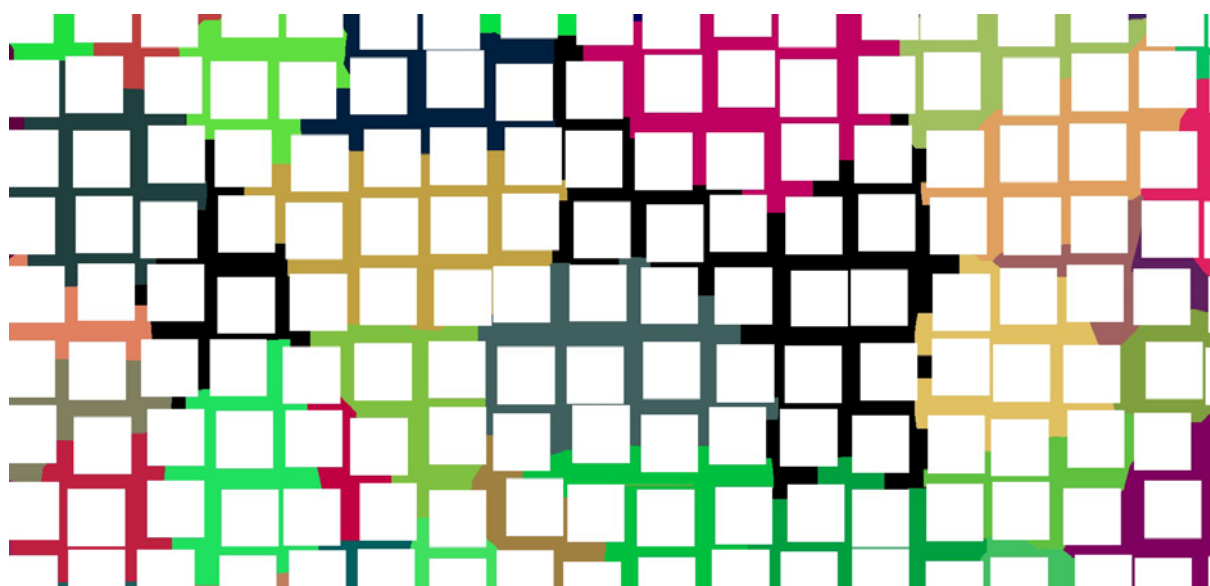


Fig 2. Calculated microstructure cross section; transformed fraction of 84%. White squares are pre-existing crystallites, black regions are untransformed amorphous phase and colored regions correspond to thermally crystallized regions.