Finite element method modeling applied to laser crystallization of amorphous silicon

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ABSTRACT:

The crystallization by laser of amorphous or microcrystalline silicon films allows to obtain thin, high-quality, polycrystalline Si films, being a very promising method for diminishing costs in the microelectronic and solar cells sectors. During a laser crystallization process, light is partially absorbed in the amorphous silicon film, heating the sample and, if the temperature rises high enough, causing the reorganization of the film structure into a crystalline one.

In this work we show both experimental results on the crystallization of non-hydrogenated silicon thin-films performed by a continuous wave infrared laser are included, as well as a study of the process with a simple finite elements (FEM) numerical model based in the dimensional non-linear heat transfer equation with a steady heat source.

Key words: Laser crystallization, polycrystalline silicon, FEM modelling.

1.- Introduction

Laser crystallization and annealing of amorphous silicon (a-Si) to produce high quality crystalline-silicon thin films has been a subject of great interest for applications as thin-film transistors, sensors, or solar cells. Especially in the latter field, as thin-film polycrystalline silicon solar cells have long been considered a potential competitor to wafer-based silicon devices. Electron-beam and laser crystallization of a-Si are regarded as the most promising methods for fabricating thin-film polycrystalline silicon solar cells from crystallization of amorphous material. With the aim of improving the efficiency and lowering the cost of these solar cells, intensive research has been done to enhance the quality of laser crystallized silicon films deposited on low-cost substrates such as glass.

A major advantage of laser crystallization and annealing over conventional heating methods is its ability to induce rapid heating and cooling of thin surface layers. During laser crystallization, laser energy is used to heat the amorphous or microcrystalline silicon thin film, melting it and changing the microstructure to crystalline silicon (poly-Si) as it cools. Phase change from a-Si to c-Si thus depends on the absorbed energy from the incident laser-pulse.

Different laser sources has previously been used in laser crystallization experiments of a-Si, as pulsed excimer lasers emitting in the UV range or pulsed Nd:YAG lasers (532 nm, 355nm and 1064 nm) [1-4], although the best results have been obtained with continuous wave (CW) lasers emitting in the IR range [5-7]. Also, as a way to understand the physics underlying the process, it usual to found works about crystallization modelling [8, 9].

In this work we show the results of experiments with a CW infrared laser source, as well as a thermal study by FEM modelling of the laser crystallization.

2.- Crystallization experiments

The samples used consisted of Borofloat 33 glass substrates with a buffer layer of about

200 nm and 10 microns of hydrogenated amorphous silicon (a-Si:H) deposited by PECVD. The samples are thermally annealed previous to the laser treatment to effuse the hydrogen from the a-Si:H. During the laser crystallization process the samples are heated up to 700ºC with a heater plate to prevent cracks due to thermal stress in the substrate. A continuous wave (CW) laser emitting at 980 nm has been used in the experiments. The laser have a cylindrical lens, leading to a line spot of 2,16 cm (Gaussian) × 19,6 cm (Top hat), allowing the crystallization of large areas. Laser beam is scanned along the sample at a constant speed. The samples were morphologically characterized by optical and electronic microscopies, and its internal structure was studied by Raman and XRD spectroscopy.

2.1.- Crystallization results

A parametrization of the silicon laser crystallization was performed for process velocities ranging from 0 to 25 mm/s. Fig 1 show the parameter window obtained for different velocities and laser light intensities.

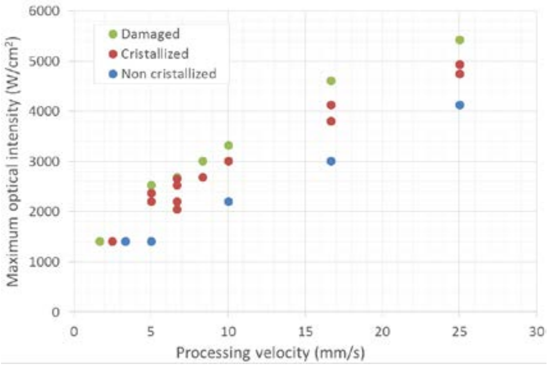

Fig 1: Parameter window for the silicon laser crystallization process.

For too low intensities (show as blue dots in the figure) the film surface do not show any change. As the laser intensity increases, small areas appear in the sample surface, corresponding to a partial melting and a subsequent solidification of the silicon. That is the beginning of the liquid phase crystallization process (see Fig 2). For slightly higher intensities the sample crystallizes completely in crystal grains of great area (up to mm^2). Finally, too high intensities (green dots in Fig 1) led to the dewetting of the silicon film (i.e. the separation of the Si film from the glass substrate).

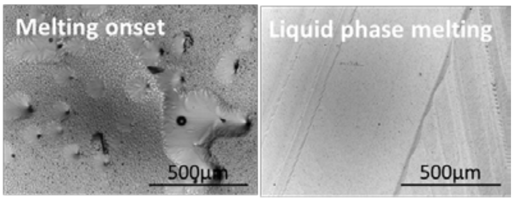

Fig 2: Onset of the silicon melting (left) and crystallized samples (right) obtained for different process parameters.

3.- Finite elements method (FEM) modelling

To have a better understanding of the crystallization process we used a finite elements method (FEM) model. Using COMSOL Multiphysics Software we developed a 2D stationary model based in the non-linear heat transfer equation, taking the laser as a Gaussian heat source, and including the phase change for silicon at 1687 K (show as a red line in Fig 3).

We selected some of the parameters used in the experiments and calculate the temperature distribution for a stationary process in the whole system (silicon film + glass substrate). Fig 3 show the model results using a maximum optical intensity of 2700 W/cm^2 and a process velocity of 8.3 mm/s. As can be seen in the temperature profile, as the laser reaches a sample point the temperature of that point rise quickly, being slightly over the melting temperature for about half a second, and cooling afterwards.

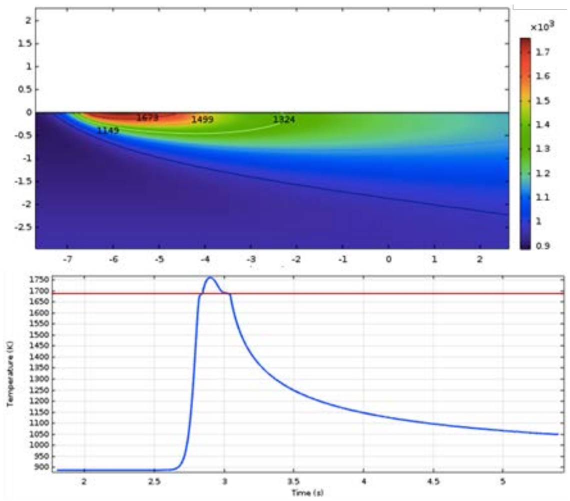

Fig 3: Temperature in the sample (top) and at a point versus time (bottom) obtained from the FEM model for a maximum optical intensity of 2700 W/cm^2 and a process velocity of 8.3 mm/s

The obtained temperatures are consistent with the experimental results. From the calculations we concluded that the irradiation time (i.e. the process speed) is identified as a key variable in the crystallization process. In addition, the model can predict the start of the liquid phase crystallization process with diode laser, and can be used to study the thermal conditions for the onset of the dewetting of the silicon.

4.- Conclusions

In this work we present a study of the influence of irradiating time and laser power in laser crystallization of amorphous silicon thin films, using continuous wave IR laser source emitting at 980 nm. Different results are show for different process parameters, but laser-annealed films with high crystalline quality (grains of several mm wide) have been obtained.

A simple thermal finite element model (FEM) has been developed in COMSOL Multiphysics to simulate the process by solving numerically the two dimensional non-linear heat transfer equation with a steady heat source. The local temperature evolution in the irradiated area given by the FEM model show good agreement with the experiment results. The numerical model developed helps to understand the physics underlying and determine the process parameters in which crystalline silicon is obtained without damage or ablation of the silicon surface.

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