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Title:	Combining Periodic Nanoimprint Lithography and Disorder for Light Trapping in Polycrystalline Silicon Solar Cells on Foreign Substrates	Abstract/Summary:
Author(s):	I. Abdo, C. Trompoukis, A. Abass, B. Maes, R. Guindi, V. Depauw, D. Van Gestel, I. Gordon, O. El Daif	Experimental and theoretical investigations of two dimensional (2D) periodic photonic nanostructures fabricated by nanoimprint lithography (NIL) and dry etching on polycrystalline silicon (PolySi) layers are presented. PolySi layers are fabricated using the Aluminium induced crystallisation (AIC) layer exchange process and epitaxy. The optical properties of the nanopatterning and in particular its impact on absorption are studied. Nanoimprint lithography is performed on ultra-thin PolySi films grown on rough alumina substrates. The 2D periodic photonic nanostructures combined with the disordered substrate result in an enhanced light absorption in the photoactive material. The results are modelled thanks to an original model based on the finite element method combining coherent and incoherent simulations. The developed model shows that significant absorption enhancement can be achieved by combining front gratings and a back diffuser in a solar cell structure.
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COMBINING PERIODIC NANOIMPRINT LITHOGRAPHY AND DISORDER FOR LIGHT TRAPPING IN POLYCRYSTALLINE SILICON SOLAR CELLS ON FOREIGN SUBSTRATES

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ABSTRACT: Experimental and theoretical investigations of two dimensional (2D) periodic photonic nanostructures fabricated by nanoimprint lithography (NIL) and dry etching on polycrystalline silicon (PolySi) layers are presented. PolySi layers are fabricated using the Aluminium induced crystallisation (AIC) layer exchange process and epitaxy. The optical properties of the nanopatterning and in particular its impact on absorption are studied. Nanoimprint lithography is performed on ultra-thin PolySi films grown on rough alumina substrates. The 2D periodic photonic nanostructures combined with the disordered substrate result in an enhanced light absorption in the photoactive material. The results are modelled thanks to an original model based on the finite element method combining coherent and incoherent simulations. The developed model shows that significant absorption enhancement can be achieved by combining front gratings and a back diffuser in a solar cell structure.

Keywords: Polycrystalline Silicon, nanoimprint, Aluminum induced crystallization, light trapping.

1 INTRODUCTION

In the route towards reducing the cost of crystalline silicon photovoltaic cells, Polycrystalline Silicon (PolySi) based on Aluminum induced crystallisation (AIC) [1,2] is an interesting material that can be grown on inexpensive non silicon substrates thanks to its possible deposition on a cheap foreign substrate. In this work, thin layers of PolySi of 3 microns are fabricated on an alumina substrate thanks to the AIC layer exchange process.

Given the absorption properties of crystalline silicon (cSi), a slab of thickness in the order of a few microns loses most of the incident light leading due to poor light absorption of the cSi. Light trapping is therefore inevitable for such thin film structure. One of the most extensively used light trapping techniques is random pyramid texturing, used in most commercial solar cells nowadays. It enhances light absorption but, as it is based on the fabrication of pyramids of several micron height, it is only usable for thick active layers. As for ultra-thin technologies of few microns, such conventional light trapping techniques cannot be used because they consume a lot of material which is not affordable. One other technique used for texturing is the random plasma texturing that yields randomly rough surfaces on a nanoscale. Application of plasma texturing on AIC-based polySi layers resulted in cells with a current density of 20mAcm^{-2} and efficiency of 8% [1,3]. However, this technique still consumes ~1micron of silicon, and it yields a very rough surface that is difficult to passivate. Finally, from the pure optical point of view, a random surface yields a Lambertian profile of light scattering that could be in principle surpassed by diffractive optics [4].

Light manipulation using periodic photonic nanostructures with dimensions within the range of solar wavelengths that silicon absorbs (0.3 to 1.17 μm) is now possible thanks to the progress in nanophotonics [5,6].

Experimental and simulation results have been shown, demonstrating the effect of nanopatterning on the optical properties of various materials [8-14]. Fabrication of surface nanopatterning requires a nanopatterning technique of high resolution, high throughput, large patterning area and at the same time of low cost. All these characteristics could be found in the nanoimprint lithography (NIL) technique [15,16] which now has started to be used for Si PV applications [6,7].

In this work, we propose the use of NIL to fabricate the two dimensional (2D) surface periodic nanopatterning, in order to enhance the light absorption properties of polySi active layers of a thickness of 3 microns based on the AIC process. And at the same time, get a light absorption higher than that resulting from the use of random plasma texturing technique. A full wave simulation technique that evades the traditional large-scale computational domain typical in simulations of disordered systems is also developed. The benefit of the use of surface nanopatterning is confirmed using these simulations. In section 2, the nano-imprint lithography (NIL) process used for nano-patterning will be discussed. In section 3, optical and topographical results will be shown. In section 4, the simulation results and theoretical discussion is then presented.

2 EXPERIMENTAL DETAILS

Thin-film PolySi solar cell technology tries to combine the cost benefit of thin film technology and the quality potential of crystalline Si technology. For this type of solar cells the challenge is to fabricate crystalline Silicon layers on non-silicon substrates. We propose to use AIC in order to increase the grain size of the

crystalline material as described in previous publications [1,3].

In order to fabricate the 2D periodic photonic nanostructures, nanoimprint lithography (NIL) was used as shown in Fig. 1. It's based on the deformation of a thermal resist by compression using a hydraulic press and a soft Polydimethylsioxane (PDMS) stamp. The soft stamp is first fabricated in a mold using a Silicon master stamp (previously patterned by deep UV lithography) and PDMS at a temperature of 80°C. The PolySi layer to be nanoimprinted is then spin coated with the thermal resist which is then deformed at 130°C by the hydraulic press using the PDMS soft stamp. Reactive ion etching (RIE) is then used to etch the PolySi layer through the nanopatterned thermal resist. The resist is then removed by Acetone and isopropanol to finally have the nanopatterned PolySi layer [6].

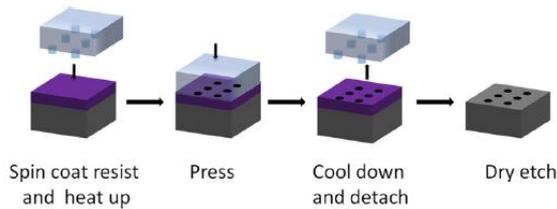


Fig. 1. Schematic representation of the soft thermal-nanoimprint lithography process flow [6]

3 EXPERIMENTAL RESULTS

The result of the periodic nanopatterning process is shown in Fig. 2. For comparison, a picture of a surface patterned by random plasma etching is shown. The periodic nanopatterning has a period of 900 nm, the diameter of the nanopatterning is 800 nm with a depth of 550 nm. The period is predefined from the used master stamp. The depth and the diameter-to-period ratio depend on the etching conditions. The plasma texturing shown in Fig. 3 was done in a prototype reactor from Secon using micro-wave antennas positioned above the substrates, with SF6 and N2O as precursor gases [3].

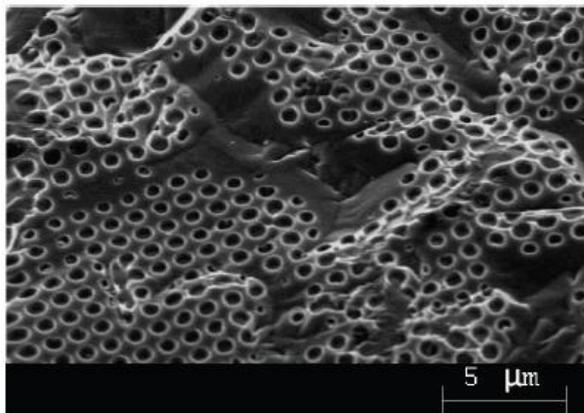


Fig. 2. SEM picture of a nanopatterned PolySi layer

As can be seen from Fig. 2 the nanopatterning is covering most (>70%) of the surface despite the latter's roughness. This is possible thanks to the fact that the stamp is soft. The remaining 30% mainly consists of steep sidewalls of hillocks at the grain boundaries.

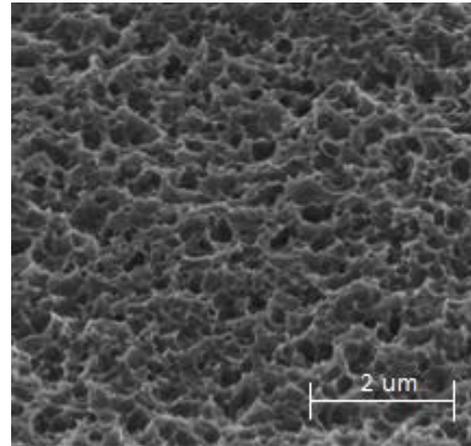


Fig. 3. SEM picture of a plasma textured PolySi layer [3]

Optically, reflectance reduction is achieved thanks to nanopatterning compared to random plasma texturing. The reflectance curves as well as the integrated reflection values are shown in Fig. 4a. We are able to bring the integrated reflectance down to 17% for the nanoimprinted samples compared to 19% for the reference samples which had a random plasma texturing. This decrease in reflectance is expected to be translated at the cell level by an increase of 15% in short-circuit current compared to non-patterned cells.

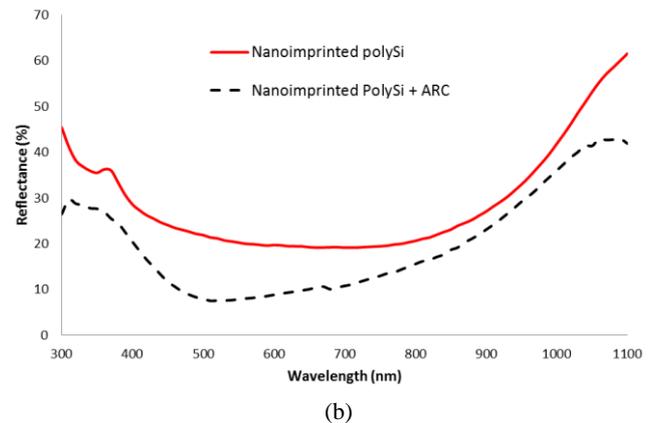
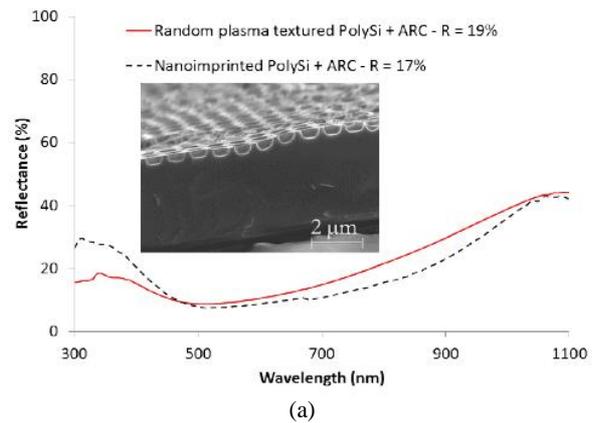


Fig. 4. Optical characterization: (a) Reflectance comparison between nanopatterned and plasma textured PolySi (b) Effect of adding ARC on reflectance of nanopatterned PolySi

Fig. 4b shows that adding an anti-reflection coating (ARC) to nanopatterning actually decreases the reflection

in a complementary way; both effects of ARC and nanopatterning are superimposing in a way that they are not acting in different directions.

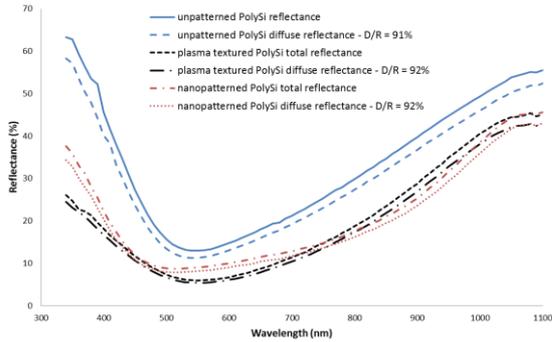


Fig. 5. Total and diffuse reflectance of an unpatterned, plasma textured and nanopatterned PolySi layer

Optical measurements further show that surface roughness has a big influence on the reflectance's angular distribution. Fig. 5 compares the diffuse components of the reflectance for unpatterned, plasma textured and nanopatterned PolySi. The diffuse-over-total reflectance ratio (D/R) is relatively high for all studied samples, it is however the lowest for the unpatterned layer reaching 91% as the flatter surface enhance the specular component of the reflectance. The D/R has an integrated value of 92% for *both* plasma textured and nanopatterned layers. Going to a finer study, one can see that the plasma texturing shows a lower reflectance at intermediate wavelengths, which may show a better ARC behaviour. On the other hand, the periodic nanopatterning surpasses at long wavelengths, that can be interpreted as a consequence of the diffraction allowed by the periodicity of the nanopatterning, which should act at longer wavelengths given the period of ~ 900 nm.

4 SIMULATION RESULTS AND THEORETICAL DISCUSSION

To study and understand further the light trapping effect of a combined top grating and bottom diffuser structure, numerical simulations were done utilizing the one pass coherent (OPC) method which takes advantage of the incoming light's limited coherence [17]. The OPC method takes into account coherent scattering effects of the top grating while avoiding a large computational domain in simulating the bottom diffuser by working directly with the Fourier components of diffuse wave fronts. In the PolySi thin film system investigated here, coherence of incoming light is broken due to the random nature of the bottom diffuser and additionally due to the optical path length is larger than the natural light coherence length. This is well approximated in the OPC calculations as light coming back from the bottom reflector is considered to have lost its phase relation with light from the top.

2D reflectance plots of combined grating-diffuser structures are shown in Fig. 6. We compare the light trapping effect of top grating only structures with that of combined structures assuming a lossless bottom reflector and a reference unpatterned flat structure. The results in Fig. 6 show that significant reflectance reduction is already obtained by patterning the top surface as can be

seen in Fig. 6 when one compares the black square plots with the circle plots. Additionally, having a lambertian diffuser at the bottom can significantly further reduce the reflectance of a top patterned solar cell structure. A notable reduction of the integrated reflectance of the AM 1.5G spectrum throughout the wavelength range of 300-1200nm can be achieved with the combined structure. For example, for the period of 400nm, a top grating only structure can have an integrated reflectance of 28% whereas the combined structure has an integrated reflectance of 22%.

The further reduction of reflectance in the combined structure comes from the additional increase of optical path length by diffuse scattering of light to larger angles. Though the grating structure gives diffraction scattering effects aside from anti reflection graded index effects, the resulting angular spread of light is limited due to the high refractive index of silicon. Furthermore, conventional grating structures tend to not diffract light efficiently to high diffraction orders. For the wavelength of 900nm, the first order diffraction of normal incidence light by gratings with a periodicity of 400nm leads to an angle of 38.5° inside the silicon. Thus, even with a grating that can impart high in-plane momentum, the angular spread of light is still limited and leaves a lot of room for a bottom diffuser to contribute.

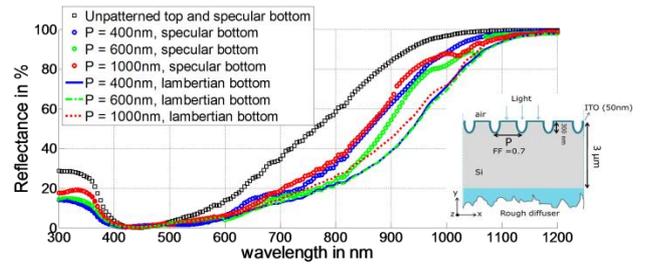


Fig. 6. Reflectance of PolySi solar cell structures calculated with the OPC method. Structures with patterned top surface only are compared to structures with combined top grating and bottom diffuser for different periodicity. The inset shows the simulated structure. Periods are varied without changing the fill factor and grating depth.

5 CONCLUSION AND OUTLOOK

The results of integrating nanopatterning using NIL into AIC-based PolySi layers was shown experimentally and theoretically. We were able to nanopattern 70% of the whole surface. The patterning was shown to decrease the reflectance from 19% for plasma texturing down to 17% and the effect of both ARC and patterning are superimposing. A 15% increase in short circuit current is expected as a result of this decrease in reflectance. The diffuse reflectance was found as the dominating part of the total reflectance as a result of the surface roughness. Simulations demonstrate that combining top grating pattern with a bottom diffuser can lead to significant absorption enhancement. The top grating pattern mainly gives better antireflection properties while the bottom diffuser increases optical path length of light by increasing the angular spread inside the material.

To make cells of nanopatterned PolySi active layers, good surface passivation is inevitable due to the probable increase of dangling bonds after etching. Increasing the nanopatterning area and optimizing the patterning

dimensions, in particular in order to improve the optical effect at shorter wavelengths, are also challenges for better absorption enhancement and light coupling into the active layer for more current gain.

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