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Multifractal analysis of textured silicon surfaces

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ABSTRACT

Pyramidal textures with random distribution of texture shapes on crystalline Si wafers substantially reduce reflection losses of substrates for high-efficiency solar cells, detectors and similar applications. In this work random pyramids on n-type Si wafers were prepared by anisotropic surface etching in potassium hydroxide (KOH) solution. The morphology of pyramidal shapes was examined by the AFM method and reveals high complexity of the surface structure. Properties of AFM observed pyramidal textures were characterized by the statistical and multifractal methods. This approach provides good platform for the distinguishing between fine details in the pyramidal distributions. Significant correlation between the fractal properties of surface texture and its optical properties characterized by the spectral reflectance function is observed.

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1. Introduction

The worldwide solar cell production is based mainly on crystalline silicon. In the development of economically attractive silicon solar cells the light trapping in the solar cell structure plays important role. One of possibilities for decreasing of reflection losses and increasing the absorption probability by light trapping is the solar cell surface texturization [1-6]. Random pyramidal textures are usually prepared by wet chemical etching of the silicon wafers in alkaline solution. Produced pyramidal texture contains large variety of surface shapes depending on the technological treatment operations. Such a complex morphology is difficult to describe by the Euclidean geometry methods. Different approach used in this work is based on fractal geometry, providing valuable results in the description of irregular surface shape distributions when the self-similarity of structural shapes is observed. Statistical and fractal properties of prepared pyramidal textures are formed by applied steps of etching procedure and directly influence the optical properties of textured surface. In this work several textures with different distributions of pyramidal shapes were prepared. Properties of these distributions are investigated with a goal to optimize

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2. Multifractal analysis

Based on experimental observation of semiconductor surfaces at various scales there is increasing evidence that for the description of the surface structure the Euclidean geometry is not appropriate enough. The reason is that processes of forming the semiconductor surface generate complex structures whose topological dimension is different from the Euclidean one. One of the definitions of fractal dimension is Hausdorff–Besicovitch dimension *D*. It is based on Hausdorff measure consisting in defining measure as covers of sets [7–9]. The Hausdorff measure provides formal extension to measure irregular sets that cannot be "fitted" in a collection of some Euclidean covering sets. The *s*-dimensional Hausdorff measure diverges for *s* smaller than certain threshold *D* and equals zero for *s* greater than *D*. The critical value *D* is used as the fractal dimension. *D* is the only real value that may provide a finite Hausdorff measure for studied set.

Zooming in on a fractal surface reveals roughness details that cannot be constrained by a collection of Euclidean surfaces. Fractal dimension is directly related to surface roughness and for extremely rough surfaces it has significantly higher values.

Multifractal analysis of the AFM images was performed by using a box-counting method. The AFM image was divided into boxes



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Fig. 1. 3D AFM image of pyramidally textured Si surface: (a) distribution A and (b) distribution B.

with the size of the square box side ε . The height distribution function μ_{ij} in box(ij) is computed by

$$\mu_{ij} = \frac{h_{ij}}{\sum h_{ij}} \tag{1}$$

where h_{ij} is the average value of the AFM height function in box(ij) measured with respect to the reference plane. The partition function $\chi_q(\varepsilon)$ is expressed as a power law of ε with an exponent $\tau(q)$ by equation

$$\chi_q(\varepsilon) = \sum P_{ij}(\varepsilon)^q = \varepsilon^{\tau(q)}$$
⁽²⁾

where exponent q is a real valued moment. The $\chi_q(\varepsilon)$ function can be used for description of the surface texture properties. By equation

$$D_q = \frac{\tau(q)}{q-1} \tag{3}$$

the spectrum of generalized fractal dimensions D_q is defined. There is no direct information provided by D_q on the surface texture. We can obtain this information indirectly. For homogeneous, not rugged surface topography the D_q values are high. On the other hand for rugged textures the D_q values are low. If D_q values change with q, the structure is multifractal characterized by some nonlinear dependency $\tau(q)$ in the partition function χ_q . The multifractal singularity spectrum $f(\alpha)$ is computed by equation

$$f(\alpha) = \alpha q - \tau(q) \tag{4}$$

where $\alpha = d\tau(q)/dq$ is a singularity. For the multifractal structure the $f(\alpha)$ function has concave shape with single maximum point [10]. The box-counting method is used also for determination of the fractal dimension D_f [11] and determination of the probability distribution $P(D_f)$.

3. Experimental

Monocrystalline p-type Si(100) wafers (1.0–1.5 Ω cm) were cleaned by RCA [12] and treated in KOH solution at 80 °C to obtain a texture consisting of randomly distributed Si(111) pyramids. Formed textures were measured by the NT-MDT SPM system Solver Pro in semicontact mode at relatively large surface areas 100 × 100 μ m² and some specific details were examined at smaller areas. Spectral reflectance of textured surfaces was measured by fibre optics spectrophotometer Avantes 2048 at various incidence

angles measured from the surface normal in step 5°. The distance between sample and spectrophotometer was identical for all measurements. Data were taken in ambient air. The conventional quantitative analyses and multifractal spectra were used to characterize the AFM images. The NT-MDT software solution Nova was used for instrument control, Fourier analysis (FFT) and statistical analysis of height function from the AFM images.

4. Results and discussion

In this work we present results from analysis of two different distributions of pyramidal shapes at observed Si surfaces. The textures are identified as A and B type. For the texture of A type quasi uniform distribution of pyramidal shapes at the surface is essential (Fig. 1a). In the texture of B type the fraction of small pyramids is dominant but very high pyramidal shapes occur randomly at various surface positions too (Fig. 1b). Fig. 1b shows the distribution B surface in smaller detail in order to illustrate the shape and seldom occurrence of the bigger texture shapes.

The shape of pyramidal objects generated by anisotropic etching of silicon are regular in distribution A as well as in distribution B as can be seen in Fig. 2 in a cross section plots at the AFM images.

The 2D FFT maps of the surface height function obtained by the AFM are shown in Fig. 3. Each point of the FFT spectra corresponds to the spatial frequency (represented by colour) contained in the measured structure. The spectral pattern is symmetrical in relation to the centre of the image with the zero frequency in the central point. Spectral points near the centre correspond to low frequencies (large "wavelengths" of the surface periodicities) and points in a far zone correspond to higher spatial frequencies [13]. With increasing of the heights of pyramids in distribution A samples the FFT map shows enhanced structure in the high spatial frequency area (see Fig. 3a and b). Resulting pyramidal texture is more complicated and higher fractal dimension can be anticipated. Fourier domain image of distribution B pyramidal texture is simpler, seldom occurrence of high pyramids do not enhance the FFT space significantly.

Fractal dimension will be lower in comparison to distribution A with larger amount of high pyramids in correspondence to the Hausdorff–Besicovitch concept of fractal dimension.

The results of the multifractal analysis are shown in Fig. 4. The shape of the general fractal dimension D(q) curves is decreasing and therefore all pyramidal textures are multifractal. Different position of D(q) curve for distribution B in Fig. 4a enables exact distinguishing between the two pyramidal textures. Moreover

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