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Research on mechanism for high light absorption of micro-structured silicon

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ABSTRACT

The mechanism of the high light absorption of surface-microstructure silicon is discussed using optical simulation based on Monte Carlo method in this article. Calculation results indicate that the micro-structured surface and high refractive index of material are the two key factors that effectively reduce the reflection, especially transmittance, of the material instead of surface wave and sulfur. In addition, this shows clearly a development in direction for manufacturing new type detectors and increasing the efficiency of traditional detector effectively in the future.

1. Introduction

Surface-microstructure silicon which is also called “black silicon”, which has been paid to much more attention for its excellent performance, absorbs incident light more than 90% in the 0.25–10 μm light band [1,2]. Such a wide spectrum of high optical absorption ratio provides important potential applications of silicon-based photo-electric devices, such as infrared detectors and solar cells. But the causes of these characteristics also lead to great conjectures and controversy. Problems mainly focus on the following three aspects [1–7]:

1. The cause of multiple reflections of incident light. The special surface structure can lead the incident light to go around it, which makes it possible to enhance the light absorption. The absorption has closely link with the geometry and size of the structure. It is well known that the surface of the material has anti-reflective property when it being treated with microstructure [8–11]. The problem is what the influence degree is between the structure and the light absorption. Even though no light will be reflected, the absorption can only reach to nearly 50% rather than 90% for silicon?
2. The cause of measurement. The absorption of black silicon sample is calculated using the formula from $1-T-R$ where T means transmittance and R means reflectance. The reflectance of black silicon is measured in integrating sphere. During the measurement of diffuse reflection, the micro-structured surface gets in touch with integrating sphere sample port in Fig. 1. So there maybe two reasons for misreading of the measurement. First of all, light may travel along the bottom of the peak and, ultimately, goes out from other peaks which are out of integrating sphere. Secondly, some of them may go out in the form of surface wave though the unmicrostructured part of silicon. Each of them will lead to lower reflectance than precept, and then the absorption will be enhanced by this reason. The first part may be neglected for its lower area ratio, but the surface wave may be not.
3. Other two causes. One is the sulfur [3,4]. For the preparation of the black silicon samples should be under SF_6 environment, the surface of sample contains many sulfur atoms whose maximum proportion reaches to 0.7%. Although the ratio is not very high, the light absorption of sulfur may have a greater contribution.The other important one is the impurity energy band. Light can be absorbed when the energy of the incident photon is greater than the band gap energy in silicon. In the preparing of black silicon, high temperature in a short time generated by femtosecond laser may cause deviations from periodicity within the crystal lattice. Moreover, the doped sulfur and fluorine atoms may also lead the energy band structure changed, reducing the black silicon conduction band, thus increasing the absorption of black silicon.

These three reasons will be analyzed to estimate each contribution to the high absorption.

2. The estimate effect of multiple reflections

To get the relationship between the structure and absorption of material, an ideal model was set up which is based on pure

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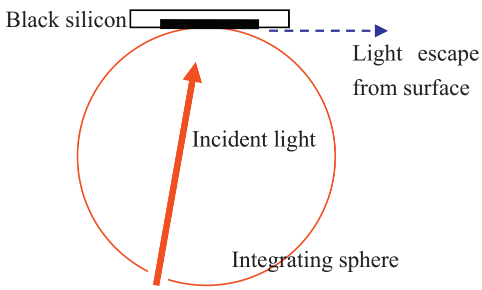

Fig. 1. The diffuse reflection measurement for black silicon.

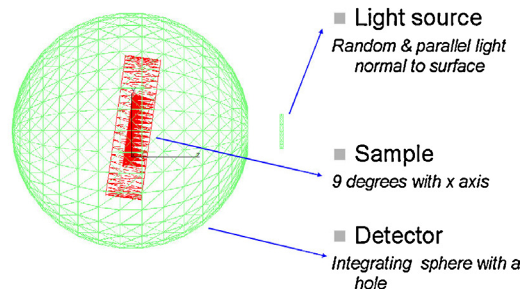

Fig. 3. Model for simulation.

crystal silicon so that the affection of impurity atoms and deviations from periodicity within the crystal lattice can be avoided. Simulation software, named Tracepro Version 50, from Lambda Research Corp., is used for calculation about the absorption characterization between light and substance with complex surface.

2.1. Preparations for simulated virtual sample

In SEM figure of sample, the surface of black silicon was covered with hundreds of the melon-shaped peaks that are in size of micrometers, closer with each other and mutual independence. Taking into account the difficulty of modeling and computer simulation speed, in our virtual sample, we simplify the melon-shaped peaks to a conical one. Refer to the scale of the melon-shaped peaks, the ratio of the slope and bottom radius of cone was set to 5:1. Then let 255 such cones arrayed in 15 rows and 15 columns to form a nearly square shape and the bottom of each cone should be a litter overlap mutual to get close together without any space. In Fig. 2, these cones are put in excavated rectangular vacant of the silicon to ensure that the vertex of the cone and the top surface of silicon wafers are in the same plane. The surface properties of this virtual sample are set to the average of ideal mirror and diffuse.

2.2. Parameters of silicon for simulation

For simulation, it is necessary to know the refractive index of materials and absorption coefficient under a specific wavelength. For the transparent plate bulk material, NIST gives the relevant formula under normal incident condition [1],

$$\tau = \frac{(1-r)^2\tau_i}{1-r^2\tau_i^2}\left(\tau_i = e^{-\alpha t},\quad r = \left|\frac{n-1}{n+1}\right|^2\right)$$

$$\rho = 1 - \frac{(1-r)(1-\tau_i)}{1-\tau_i r} - \tau$$

where τ means transmittance, ρ means reflectance, τ_i means normal internal transmittance, r is the reflectance of the surface, α is the absorption coefficient and n is refractive index of the material. Therefore, the refractive index and absorption coefficient of the material can be solved out by measured transmittance and reflectance. After all, it is necessary to simulate the reflection and transmittance of plate virtual sample to make sure the correctness of relative parameters.

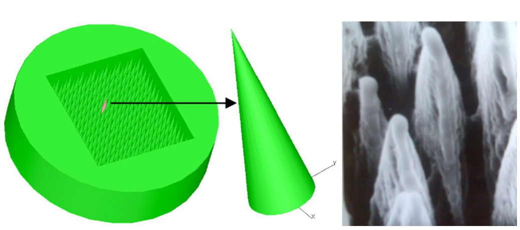

Fig. 2. Simulated sample and real sample.

2.3. Model for simulation

In Fig. 3, an integrating sphere is used for simulation. To maximize realistic, there is an angle with 9° between incident light and normal direction of the sample. The virtual light source emits large parallel light to the sample randomly; the reflected and transmittance light is received by the sphere.

Simulation is based on Monte Carlo method. The light source has a number of 200,000 parallel rays with certain energy. Everyone interacts with the surface of materials follow Fresnel laws. While rays transfer in the material, energy attenuation (A) accords to formula $A = e^{-\alpha t}$, where α is the absorption coefficient, t is the distance that light has traversed. (More details and the relationship between shape and absorption will be described in another paper.)

2.4. Simulation result

Simulation result shows that the reflectance and transmittance of micro-structured silicon do get lower comparing to flat silicon wafer in Fig. 4. Comparing to unmicrostructured silicon, the trend of the reflectance and transmittance is basically the same. From the simulation data, when the wavelength is more than 1.3 μm, the simulated reflectance is about 0.15, which is 0.10 higher than that measured. For transmittance, the simulated transmittance is nearly the same with the actual measured data. For absorption, it

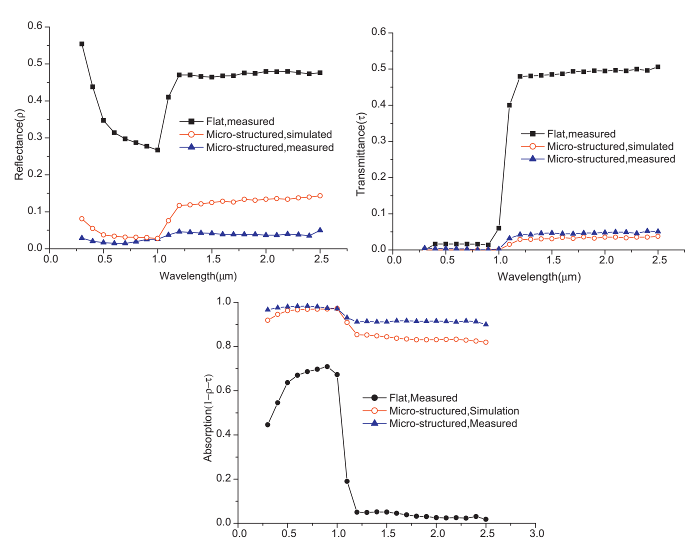

Fig. 4. Simulated results of transmittance, reflectance, and absorption of micro-structured materials compared with measured results.