**Formation and optical properties of BaSi2 films on Si (111) –   
a promising nanomaterial for solar cells**

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Nowadays, scientists investigate new more efficient materials for creating solar cells. One of such materials is thin films of barium disilicide. In this paper, we describe formation of BaSi2 films on Si(111) by layer-by-layer solid phase epitaxy and study their optical properties in visible and infrared range.

**Keywords**: silicon, barium, barium disilicide, thin film, solar cell.

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**1. Introduction**

Nowadays, investigating materials for photovoltaic converters is one of the important areas of research in the surface physics. One of such materials is thin films of barium disilicide [1]. Different groups of authors are studying the optimal conditions for the formation BaSi2 on Si [2-4].

**2. Methods**

We prepared the samples in the UHV-chamber model PHI-590 with a base pressure of 10-10 Torr. The substrate of 5×15 mm2 size were cut from the standard FZN100 washer with surface orientation (111) and resistance 50-85 Ohm∙cm. Then it was cleaned in acetone and isopropyl in ultrasonic bath for 5 minutes in each substance. After that it was placed in the chamber where it was degassed for 6 hours at a temperature of 600°C; immediately prior to forming a sample it was subjected to high-temperature cleaning performed at 1250°C for 3 seconds with intervals of 10 minutes in order to remove the silicon oxide layer.

Deposition of barium was conducted from a standard thermal source performed of tantalum tube with a puncture. Before being placed in the chamber, barium was purified in acetone to remove the mineral oil and the top oxide layer, and subjected to prolonged degassing chamber for final purification of the oxygen. Deposition of silicon was carried out with the same plate as the substrate samples and they were subjected to the same pre-treatment procedures. The rate of deposition was determined by quartz sensor production Sycon Instrument, and varied in the range of Ba 0,5-2 nm/min and Si 1-1,5 nm/min.

As a result, three samples of thin films on silicon barium disilicide were formed by method of layer-by-layer solid phase epitaxy (Ba = 15 nm, Si = 10 nm), followed by recrystallization at different temperatures (sample #1 – 800°C, sample #2 – 850°C, sample #3 – 900°C) during 15 minutes.

These samples were examined by optical spectroscopy in the visible and infrared range.

**3. Results**

According to the optical reflection spectra in the visible range (Figs. 1-3), barium disilicide thin films formed on samples #1 (800°C) and #2 (850°C), and the spectrum of the sample #3 (900°C) does not differ from the spectrum of clean silicon. Diffusion spectra of samples indirectly indicate a greater roughness of sample #2, than those of #1 and #3 ones.

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Analysis of IR spectra of samples #1 and #2 (Figs. 4-5) revealed the formation of a thin film on a substrate of barium disilicide: positions of the peaks corresponded to the peaks defined previously in another study [5]. Absorption peaks for the sample #2 are bigger that indicates that larger quantities of BaSi2 were formed in the film.

**4. Discussion**

Analysis of IR spectra of samples #1 and #2 (Figs. 4-5) revealed the formation of a thin film on a substrate of barium disilicide: positions of the peaks corresponded to the peaks defined previously in another study [5]. Absorption peaks for the sample #2 are bigger that indicates that larger quantities of BaSi2 were formed in the film.

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**5. Conclusion**

Thus, for layer-by-layer solid phase epitaxy (based on the article data and our earlier work) recrystallization temperature optimum lays in the range 800-850°C. At higher temperatures substantial desorption from the surface is observed, which leads to a lack of film. At lower temperatures BaSi2 is formed in smaller quantities, possibly due to the low coefficient of inter diffusion of barium and silicon atoms. However, the surface roughness in this temperature range is considerable, which makes it impossible to use a layer deposition method for film formation of barium disilicide for subsequent use in creating solar cell.

We believe that the solution of this problem lies in codeposition of barium and silicon and recrystallization at lower temperatures, thereby reducing the surface roughness. The results of these investigations will be published elsewhere.

**Acknowledgement**

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**Figure captions**

**Figure 1.** Optical reflection spectra in the visible range of the sample #1 and clean silicon.

**Figure 2.** Optical reflection spectra in the visible range of the sample #2 and clean silicon.

**Figure 3.** Optical reflection spectra in the visible range of the sample #3 and clean silicon.

**Figure 4.** Optical absorption spectrum of the sample #1 in the infrared range.

**Figure 5.** Optical absorption spectrum of the sample #2 in the infrared range.