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Poster session

В первый день семинара параллельно пленарным докладам свои работы участники представили в виде традиционных плакатов.

Хроника некоторых представленных докладов

The Reduction of Graphene from Graphene Oxide

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I. INTRODUCTION
 Graphene has a surprising combination of properties: exceptional strength, excellent peak mobility of charge carriers (free electron, fermions), and high thermal conductivity. It is elastic and impermeable with respect to molecules of the other substance. The way of obtaining graphene today is to use graphene oxide produced in the form of flakes by oxidizing graphite with oxidizing reagents. The material can be considered graphite intercalated with oxygen-containing carbon groups that give it the ability to be intercalated in water and hydrophilic oxygen atoms. When intercalating with different oxidizing agents, graphene oxide is converted into different states of low structural quality [1-4] due to the additional degradation of oxygen. Graphene oxide is converted into different states of low structural quality and various intercalation agents were used to obtain different structural conditions. In addition, graphene materials of different structural quality and various sizes were used to obtain graphene oxide [5, 6].

In this work, we therefore study the effect of the reducing agent used in [1, 4-7] on the structure and chemical composition of graphene oxide in order to assess the prospects for using it to obtain graphene. In all reduction processes, graphene oxide was derived from graphite with the same chemical composition, structure, and structure. Such research methods or 3D array deposition spectroscopy (3DAS), Raman spectroscopy (Raman spectra), and scanning electron microscopy (SEM) were used to assess the quantitative and qualitative composition of the initial and final materials, and their structural features.

II. PRIMARY HEADER
 Graphene oxide was synthesized according to the Hummer method [8] from graphite powder treated with a half tablet of potassium dichromate (K₂Cr₂O₇) and sulfuric acid (H₂SO₄) and potassium persulfate, used also for this purpose. The reduction of graphene from graphene oxide was conducted in hydrochloric, hydrofluoric, hydrobromic, and hydroiodic acids. The process was conducted with hydrochloric acid using the original method described in [1].

The reduction of graphene from graphene oxide to ethylene glycol was conducted as described in [7]. Graphene was also reduced from graphene oxide with hydrogen sulfide (H₂S) solution (1:10, 20% and 100%) [9].

The quantitative and qualitative composition of the investigated materials were studied by 3DAS in three locations on an array. The Raman spectra were obtained at a laser excitation wavelength of 532 nm using a 4-fiber spectrometer (Duke Tech Technology), while SEM images were recorded with an S-4000 (Hitachi). The Raman spectra of the investigated materials are presented in Table 1 and Fig. 1.

Sample	GO, wt. %	GO, wt. %	GO, wt. %	GO, wt. %	GO, wt. %	GO, wt. %	GO, wt. %	GO, wt. %	GO, wt. %	GO, wt. %
1	93.00 ± 0.40	1.70 ± 0.30	0.00 ± 0.00	0.00	0.00	0.00	0.00	463.3 ± 0.9	11	
2	77.00 ± 0.20	20.70 ± 0.30	0.00	0.00 ± 0.00	0.20 ± 0.00	1.00 ± 0.00	1.00 ± 0.00	1.0 ± 0.2	33	
3	68.00 ± 0.40	27.00 ± 0.40	0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	1.0 ± 0.1	57	
4	47.00 ± 0.40	30.00 ± 0.40	0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	1.0 ± 0.1	34	
5	18.00 ± 0.40	30.00 ± 0.40	0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	1.7 ± 0.1	128	
6	18.00 ± 0.30	5.00 ± 0.30	0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	21.0 ± 0.4	126	

GO - oxidized graphite; GO - graphene oxide; GO - after reduction with method 1; GO - after reduction with method 2; GO - after reduction with method 3; GO - after reduction with method 4; GO - after reduction with method 5; GO - after reduction with method 6.

The area of 3DAS method indicates the graphene oxide contains small amounts of the precursor used to produce it, to produce, by mass, 100%, 10%, of precursor, 10% of water, and 10% of impurities. Overall, these data show the graphene oxide and the materials reduced from it had almost no impurities.

Analysis of these data shows that graphene oxide had substantially higher I_D and lower I_G and I_D/I_G values than the reduced samples. The reduction from water was a more severe effect of water leads to its structure [14].

III. CONCLUSIONS
 Our study of the reduction of graphene from graphene oxide at different temperatures and in various media indicates that this process is possible only upon high-temperature treatment in an inert atmosphere containing hydrogen. This results in 10-100% complete removal of physically adsorbed water from the precursor in a graphene oxide were used to determine the distribution of hydroxyl functional groups in the structure of films, thereby enhancing the effect of hydrogen reduction on them. This leads to drastic changes in the structural composition and structure of the material, producing large-scale graphene flakes.

REFERENCES
 1. Wang, G., Li, X., Liu, J., Piner, I., Park, J., Park, S., et al. (2009).
 2. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 3. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 4. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 5. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 6. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 7. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 8. Hummer, W. A., Dai, J., Bonnell, A. J., et al. (2000).
 9. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 10. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 11. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 12. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 13. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).
 14. Park, S., Han, S., Park, S., Park, S., Park, S., Park, S., et al. (2009).

Solution-based Hot-casting Technique to Receive a Micrometer-scale Crystalline grains of Perovskite

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Abstract The possibility of obtaining perovskite microfilm films by the method of applying a precursor solution onto a hot substrate has been experimentally proven.

Introduction The use of organometallic halogen perovskites as an absorbing layer of photovoltaic cells (PV) made it possible to increase the efficiency from 7% to 20%, which corresponds to the level of the traditional cells in silicon. At present, the main requirements for the development and fabrication of a PV based on perovskites are an increase in the efficiency of solar cells, reduction in their cost, as well as an increase in their service life and stability in severe atmospheric conditions (high humidity, temperature extremes, UV radiation). One of the solutions of these problems is the development, investigation and modification of methods for the formation of perovskite films.

The purpose of this work is to research perovskite films obtained by applying a precursor solution to a hot substrate at different substrate temperatures.

Method of the process of depositing organometallic perovskite halide films on a hot substrate

As in the experiments, a hot (~80 °C) mixture of lead iodide solution (PbI₂) and methyl ammonium iodide (CH₃NH₃I). The mixture was applied to the substrate at a specified temperature (120 °C, 200 °C). Then centrifuging for 15 seconds to obtain a homogeneous film.

Scheme of the process of depositing organometallic halide films of perovskite on a hot substrate

The structure of the perovskite film obtained by the method of deposition on a hot substrate

The film obtained at 120 °C consists of nanocrystallites with sizes from 1 to 50 nm. Nanocrystallites are densely packed, holes and punctures are absent. Films obtained at a substrate temperature of 200 °C have the same dense structure, but consist of microcrystalline grains with sizes from 100 nm to 500 nm.

The dense nature of the structure is confirmed by micrographs obtained by scanning electron microscopy.

The perovskite film has a thickness of 1.47 μm for 120 °C and about 2.5 μm for 200 °C.

Achievements of colleagues from the National Laboratory of Los Alamos

The composition of the precursor solution is identical to ours.

The mixture of precursor solution was heated by 10 °C.

The substrate temperature was maintained at 120 °C and 170 °C.

SEM images of perovskite films obtained by applying to a hot substrate

Conclusion It is established that the temperature of the substrate directly affects the size of microcrystallites in the perovskite film deposited on the hot substrate. With increasing temperature, fine crystallites coalesce and form crystallites of much larger size. The resulting crystallites have a leaf-shaped structure. It is also found that the size of microcrystallites when deposited on a hot substrate varies from 1 μm to 50 μm (at a substrate temperature of 120 °C) and 100 μm to 500 μm (at 200 °C).

It has been established that as a result of experimental studies, the method of depositing a layer of perovskite on a hot substrate is very promising. Since the substrate temperature is maintained at the boiling point of the precursor solution with this method of deposition, the solvent evaporates very rapidly, which makes it possible to obtain large crystalline grains. From these data, it can be concluded that the use of high-boiling solvents can provide ideal conditions for the growth of large crystalline grains.

Literature

- Wang, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 2. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 3. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 4. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 5. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 6. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 7. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 8. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 9. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 10. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 11. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 12. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 13. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 14. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).
 15. Han, H., Han, H., Han, H., Han, H., Han, H., Han, H., et al. (2015).

NANOSTRUCTURED THIN FILM OF HALIDE PEROVSKITES VIA TWO-STEP SOLVENT-SOLVENT EXTRACTION

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Annotation An improved method for obtaining nanostructured films of halide perovskites for creating photovoltaic cells is described. The results of researches of the obtained nanostructures with a scanning electron microscope are presented.

Introduction The combination of electrical properties and absorption characteristics of hybrid perovskites made it possible to increase the efficiency of energy conversion of solar cells on their basis during 2012-2013 from 7.2% to 20% [1]. It can be used in solar cells instead of silicon or as an upper-layer of silicon solar cells to increase energy production by absorbing light from a part of the spectrum, that silicon can not absorb.

The key problems of the perovskite solar cells (PSCs):

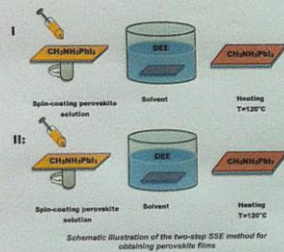
- the uniformity of the films,
- the lack of stability,
- the durability of perovskite solar cells, which are directly related to the methods of film formation on the substrate.

Among the methods of obtaining perovskite films, an interesting method is the solvent-solvent extraction from solution (SSE) [2]. The advantages of the SSE method:

- room-temperature process,
- rapid crystallization,
- uniform application,
- film-thickness control,
- film smoothness,
- compounds versatility.

However, there are a number of disadvantages in this method. There are through holes between the individual crystals of the film, the materials of hole-transporting and electron-transporting layers meet, forming parasitic contacts, which are shorting the organometallic perovskite and reducing the open-circuit voltages of the solar cell. And a small grain size, which reduces the effectiveness of PSCs.

In this article we proposed and researched a two-step SSE method with following thermal annealing.

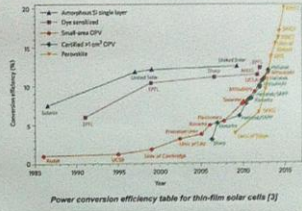


- Results:**
- The film thickness is 615 nm.
 - A nanoporous structure with a pore size in the range of 20 + 200 nm.
 - A microcrystallite size of about 200 nm.

Pores of a through nature are lack, which excludes the possibility of closing the functional layers of the photovoltaic cell.

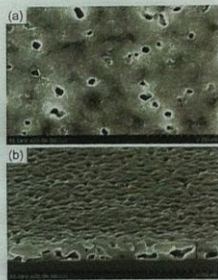
Conclusions Thus, it was found that, in contrast to the one-step application of the perovskite precursor and drying of the perovskite film at room temperature, the two-step SSE method makes it possible to improve the crystal structure of thin perovskite films. Due to overlapping of the two layers of the film, porosity is reduced and there are no through holes that short-circuit the functional layers of the photovoltaic cell. Moreover, the annealing promotes consolidation and packing of film grains.

References:
 1. Park N.G. Organometallic perovskite light absorbers toward a 20% efficiency low-cost solid-state mesoporous solar cell // J. Phys. Chem. Lett. - 2013. - Vol. 4. - P. 5623-5628.
 2. Zhao Y., Yang M., Wu Y., Zhao K., Patra N. P. Room-Temperature Crystallization of Hybrid Perovskite Thin Films via Solvent-Solvent Extraction for High-Performance Solar Cells // J. Mater. Chem. A - 2015. - Vol. 3. - P. 7374-7378.
 3. K. Lee Sign of stability // Nat. Nanotechnol. - 2015. - Vol. 10. - P. 774-775.



Process:

1. The perovskite solution was obtained by mixing CH₃NH₃I and PbI₂ in an organic solvent of N-methylpyrrolidone.
2. Spin-coating of the precursor solution to a previously applied ITO template on a glass substrate.
3. Immersion of the substrate in a bath of diethyl ether (DEE).
4. Oven drying T₁220°C.
5. Reiteration of 1-4 stages.



Microphotographs of a perovskite film obtained by a two-step SSE method

Unrelaxed InAs_{1-x}Sb_x alloys grown on compositionally graded buffers with molecular-beam epitaxy.

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INTRODUCTION

Antimonide-based materials that can absorb and emit light in the technologically important spectral region from below 2 to over 12 μm are promising for infrared technology. In particular, the solid solutions InAs_{1-x}Sb_x (x=0-1) with energy gap about 150 meV, which is less than that in nitride compounds InAs (415 meV) and InSb (236 meV) are suitable for development of the infrared devices with operating wavelength over 5 μm. GaSb substrates are suitable only for solid solution with x=0.1 and lattice mismatch constraints arising during heteroepitaxial growth of the lowest device structures can be overcome by using compositionally graded metamorphic buffer layers.

In this work unrelaxed layers of InAs_{1-x}Sb_x (x=0.43 x ± 0.03) solid alloys were obtained by the molecular-beam epitaxial method by using the well graded buffer GaIn_{0.5}Sb_{0.5} layers and characterized using X-ray diffraction, scanning electron and atom force microscopy, optical laser microscopy techniques and etc.