ABSTRACT BOOK

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ORAL PRESENTATIONS

O-01

Study on the flow and heat transfer characteristics in the tube side of spiral-wound heat exchanger

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In order to investigate the condensation of heat transfer and pressure drop characteristics in tube-side flow of spiral wound heat exchanger (SWHE), a computational model based on two-fluid multiphase model, k-ε turbulence model and thermal phase change model was established considering the gravity and surface tension. Also, a calculation formula for mean interfacial length between vapor phase and liquid phase was deduced and the wall contact angle was discussed. The modified Silver approach was used to modify the mixed effects of ethane/propane mixture on heat transfer. Based on the above model, numerical simulations were carried out on the condensation flow and heat transfer for propane and hydrocarbon mixture upward flow in a spiral pipe. The heat transfer coefficient and frictional pressure drop are mainly influenced by vapor quality, mass flux and saturation pressure while the heat flux almost does not affect them. These results will provide some constructive instructions for the understanding of condensation heat transfer and pressure drop characteristics in the spiral pipe, as well as the design and prediction of condensation heat transfer and pressure drop performance in SWHE.

O-02

Alternative Energy and Solid Oxide Fuel Cells

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A fuel cell is an electrochemical device that continuously converts chemical energy of fuel directly into electric energy and some heat for as long as fuel and oxidant are supplied. Unlike engines or batteries, a fuel cell does not need recharging and generates only power and water when hydrogen is used as fuel. Thus, it is a so-called “zero emission engine”.

Thermodynamically, the most striking difference between thermal engines and fuel cells is that thermal engines are limited by the Carnot efficiency while fuel cells are not. Fuel cell technology is a very promising potential candidate to replace the hydrocarbon economy with an alternative economy, perhaps based on hydrogen. A major advantage of the hydrogen economy is its similar structure to the hydrocarbon economy with its centralized layout. Fuel cells could provide a means to render power generation more efficient, and a relocation of poisonous exhaust gas emissions could be achieved from urban to rural areas, where they would affect fewer people. Fuel cells are suitable for many different applications. They cause small air pollution (if fossil fuels are used; otherwise none), are quiet or completely silent and minimize maintenance costs, since no or very few moving parts are used.

Solid oxide fuel cells (SOFCs) differ from other types of fuel cells in that the components of the cell materials are solid instead of liquid; especially the electrolyte is ceramic solid oxide. Extensive efforts to develop an SOFC for transportation, power plants, and distributed generation of electric energy are motivated by a need for greater fuel efficiency and reduced air pollution. SOFCs are generally ideal for stationary power applications with an output from 1 kW to MWs. Their working temperatures are typically between 700 and 1000°C, which is much higher than that of other types of fuel cells. The large amount of heat generated by SOFC is usually utilized to drive gas turbine in order to increase the efficiency. This type of hybrid system is expected to reach the efficiency up to 70%.

The unique working temperature and the structure of SOFC give it the following advantages:

1. High efficiency as compared with direct combustion power generator.

2. Suitable for hydrogen fuels as well as hydrocarbon fuels makes it compatible with current energy infrastructure. Hydrogen provides a potential large-scale clean energy solution.

3. Environment friendly: unlike batteries usually containing elements harmful to health, the materials in SOFC have less impact to the environment.

4. There is no liquid electrolyte involved, so it is easy to operate and maintain.

5. The high operating temperatures favour expensive catalysts escape.

6. The working temperature of SOFC is high enough to allow for internal reforming, which means to produce hydrogen from different types of fuel gases within the cell stack itself (without external reformer).

7. There are no moving parts, so no vibration and noise.

8. Suitable both for distributed and large power generation stations.

At the present time great attention is paid to development of SOFCs for self-contained, auxiliary and standby power suppliers (individual houses, farms, cathodic protection of pipelines). The base unit for a development SOFC is a module composed of several electrochemical cells in-series. Variation of module power and quantity of modules in a battery provides the mean power in the range of 10 W and 10 kW and the electrical efficiency up to 60%.

O-03

Study on active and passive integration humidification-dehumidification solar desalination

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Solar desalination is an effective energy saving way to produce freshwater in water shortage area. Humidification-dehumidification (HDH) is the most efficient method of solar desalination, which is suitable for small and medium-sized solar desalination units.

In this paper, a HDH solar desalination process with active and passive air circulation is proposed, in which the latent heat of vapor condensation released in the dehumidification process is recovered by the phase change thermal storage material. Phase change material provides stored heat to the passive HDH process to increase the energy utilization rate of the whole system and produce more fresh water.

The experimental study shows that when the air temperature at the inlet of the dehumidifier is 65℃, the air flow is $5m^3/h$, the initial seawater capacity of the passive humidifier is 1kg, the paraffin wax is 1kg, and its phase transition temperature is 40℃, the fresh water production of the experimental unit is 200mL/h, the cost of it is 23.47 yuan /t, and the gain output ratio (GOR) of the unit is 13.37, which is 84.4% higher than that without phase change material under the same conditions.

The heat transfer between the ordinary paraffin phase change material (I) and heat pipe, the high thermal conductivity paraffin based phase change materials (II) and heat pipe are also studied. It is found that their numerical simulation results are basically consistent with the experimental ones. Under the same conditions, the thermal conductivity of phase change material (I) is lower than that of phase change material (II), therefore, the heat absorbed and phase transition area of phase change material (I) around the heat pipe are larger than that of phase change material (II).

This research provides a reference for the development of HDH solar desalination process unit with condensation latent heat recovery.

O-04

Ordered IR fiber bundles of silver halides for thermography in power engineering

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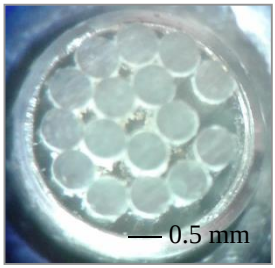
Increasing of heat efficiency is one of the key issues of power engineering. The use of infrared thermography can help to achieve some improvements in this field. In the abstract, we propose the application of silver halide IR fiber bundles (jointly with thermal cameras) as multi-purpose probes for the on-line in-situ investigation of heating networks, thermal power-generating equipment and other units. Earlier, such bundles have been reported about, but other applications have been proposed [1, 2].

We fabricate ordered fiber bundles from silver halide crystals using extrusion technique. The bundles are highly transparent in the spectral range of 2.5–20 μm, nontoxic, nonhygroscopic, and able to transmit temperatures from –130 to +1100 ^{o}C [3]. An example of the bundle is shown in Fig. 1. It consists of 16 unclad single-layer fibers with the diameter of 0.525 mm and with the length of 300 mm; a heat shrink tube is used as a shell. This bundle allows us to transmit thermal images with minimal linear dimensions of 0.5 mm.

(a) 

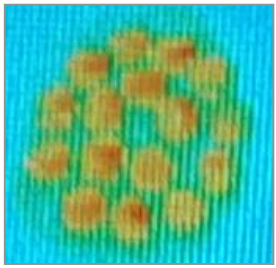
(b) 

Figure 1. Photo of an IR fiber bundle distal end (a), thermal image of a Peltier device transmitted through the bundle (b).

The bundles are suitable for real-time non-destructive multi-point temperature study of the objects such as internal combustion engines, heat exchangers, turbines etc. They make it possible to obtain a thermal field distribution in restricted spaces and in locations where there is no line of sight between the object and thermal camera. The research of heat fluxes in heat transfer media is also possible. Such investigations may be used for the control and optimization of working processes in different mechanisms and systems.

Another possible application of the bundle is as a probe for condition monitoring of thermal power-generating equipment and heat networks including underground pipelines. Commonly, the monitoring is conducted on the outside [4,

5], though there are many units of heat networks and corresponding equipment where the external inspection is impossible. In this case, the probes based on IR fiber bundles may be useful. They will allow gaining thermal images of inner surface of heat pipe and other units in order to identify and localize defects of pipeline insulation, leaks of transferred media, cracks of pipes and so on. This technique will enable to detect defects indiscernible to the naked eye.

In the nearest future, we plan to produce ordered silver halide fiber bundles containing thousands of individual fibers with lower individual fiber diameters (50-100 μm) in order to increase resolution and flexibility, and greater length (up to 3-10 m) for the convenience of practical use in hard-to-reach places.

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O-05

Experience of Ural Federal University in specialists' training for nonpolluting energy on the basis of fast breeder reactors and renewable energy sources

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A significant role in the development of atomic energy in Russia and its' long-term supply of with nuclear fuel is given to the fast breeder reactors which evolve at Beloyarskaya NPP. BN-600 is successfully operating for more than 38 years. The fourth unit with BN-800 reactor was connected to the energy network in 2015. The project of BN-1200 reactor is developed [1]. One of the main conditions of successful realization of this direction of atomic energy is the training of highly qualified personnel on the exploitation and maintenance of NPPs with fast breeder reactors.

The department of Nuclear power plants and renewable energy sources was founded at Ural Federal University in 1962 in connection with the construction of Beloyarskaya NPP. The construction of a power unit with BN-600 reactor required the organization of specialists training for the fast breeder reactors exploitation. The unique technology of sodium-cooled fast reactors demanded the creation of special material and technical facilities.

Unique educational and training facilities were purchased or manufactured. A peculiar role in the operating specialists training has the simulator of BN-800 [2, 3]. It gives the possibility to simulate different operating modes of the power unit including transient modes and emergency conditions (Fig. 1). The tutorials on the operation, maintenance and repair, safety ensuring of NPPs with fast neutron reactors are published. An affiliate of the "Nuclear power plants" department was established at Beloyarskaya NPP in 1981.

The involvement of the students into the implementation of true scientific and research works of experimental and analytical nature, their participation in scientific events and joint development of new technologies helps to speed up the adaptation of the graduates in the team of Beloyarskaya NPP.

The department of Nuclear power plants and renewable energy sources possesses a modern and constantly developing stock of educational and training facilities which gives a possibility to ensure the high-quality training of the specialists in the field of atomic energy with sodium-cooled fast reactors.

Ural Federal University is situated not far from Beloyarskaya NPP (about 50 km), that is why it has the unique possibilities to optimize the process of specialists' training.

Figure 1. Training on BN-800 analytical simulator.

The topics of the diploma works of the students correspond to the future affiliation. It leads to the reduction of adaptation period of graduated students at the place of employment. Nowadays it is developing the practice for the students to take up an entry-level position at the NPP and to take the proficiency examination in terms of the pre-degree apprenticeship.

Since 2012 it is realized the professional retraining course. To date about two hundreds of employees of Beloyarskaya NPP have graduated this course. The efficiency of this training program was confirmed by the results of the partner inspection of Beloyarskaya NPP by Moscow affiliate of World Association of Nuclear Operators (WANO) in September of 2012. It was mentioned the presence of positive dynamics in field of “Training and qualification of personnel” and “Approaches to the training of personnel”.

In 1997 the training of specialists on alternative and renewable energy sources started at UrFU. The peculiarity of this direction is that the students take courses on biogas energy, heat pumps and production of alcohol for energy needs besides the classical courses of wind, solar energy and hydropower. The scientific work of the department is first of all directed to fulfill the demands of Ural region with its sharp continental climate with low-potential winds (3-5 m/s), relatively low solar insolation (250–400 W/m^2) and large amount of little rivers.

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O-06

Thermal performance analysis of high temperature heat transfer process of solar energy

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Volumetric solar receivers (VSR) have become a promising technology for the solar thermal conversion. The absorption of concentrated solar radiation and the heat transfer to the working fluid are the two dominant processes. Some radiative transfer models combining the dish concentrator, solar window and porous absorber are developed. In the present study, the distribution of radiation energy absorbed by the porous absorber and the optical performance of the solar concentrated system are investigated through a Monte Carlo ray tracing simulation. Radiative transfer in the porous media as well as the absorption of the concentrated solar radiation is on the basis of modified P1 approximation model.

Firstly, the effects of two typical modeling approaches of concentrated solar radiation for receiver are compared in view of the porosity and mean cell size. One considers the solar radiation on the front surface of receiver as thermal boundary condition (TBC) and the other as a collimated incident radiation (CIR) beam. Then, the radiation transport within the solar window and porous absorber is fully simulated. The effects of porous structure parameters, slope error of concentrator and the alignment error of receiver are analyzed. The novel concept of dual-layer ceramic foams holds great potential for improving the efficiency. The effects of geometric properties of each porous layer on the thermal performance are considered. Finally, a newly designed volumetric solar receiver filled with cup-shaped Al_2O_3 porous absorber is studied through numerical simulation and experimental verification.

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O-07

Infrared diagnostics of the thermal state of wind power plants

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During operation of windmills, the bearings of the electric motor and lubricating oil warm up. The temperature of these elements increases to 70-100 degrees Celsius, and therefore wind turbines are equipped with an automatic oil and bearing cooling system, which includes two cooling circuits and a device for injecting lubricating and cooling oil into the bearings [1]. For effective operation of automation systems, it is necessary to perform a temperature monitoring of the oil and bearings of the wind generator. Today, control processes are carried out both by classical devices: thermocouples and resistance thermometers, as well as gaining popularity optical fiber temperature sensors (OFTS).

Known monitoring devices are able to perform measurements over a wide range of temperatures, but are subject to electromagnetic generator oscillations and strong vibrations. Fiber-optical sensors made of quartz are able to detect the spectral characteristics of the engine without contact and transmit radiation for tens of kilometers without significant energy losses, but their use for temperature monitoring is possible only in the presence of complex data processing systems due to the limitation of the spectral range by near infrared radiation.

Employees of the "Center for Infrared Fiber Technologies" at the Ural Federal University have developed a new class of photonics materials based on modified silver and thallium halides, transparent in the IR range from 2 to 50 microns [2]. The infrared fibers manufactured on the basis of these materials have high mechanical strength, small optical losses up to 0.5 dB / m, high photostability and radiation resistance [3]. Such infrared light guides are able to transmit thermal radiation from remote and hard-to-reach places and operate under electromagnetic interference and high vibration, so this can be used for thermal monitoring of bearings and oils of wind generators.

Infrared fiber-optic sensors equipped with such infrared light guides allow direct measurement of the temperature of heated objects by a non-contact method by transferring a thermal signal to radiation receivers (for example, bolometer arrays), which subsequently send the temperature data to the controllers of the wind generator. This method of control will significantly reduce the length of the fiber optic line, accelerate and simplify the optical signal processing system, make the temperature measurement more reliable and effective.

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O-08

Hydrogen storage and generation of magnesium based alloys

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The efficient hydrogen production/storage is a major problem facing the development of hydrogen energy. Hydrogen storage and generation of Mg/MgH_2 had received great attention due to its high hydrogen capacity, abundance and mature regeneration technology, and no harm to the environment.

However, pure MgH_2 suffers from sluggish desorption kinetics and a relatively high thermodynamic stability, which results in a large desorption activation energy (~160 kJ/mol) and a high dehydrogenation enthalpy (ΔH = 75 kJ/mol H_2), respectively. The dual-tuning of thermodynamic and kinetic properties of Mg_2Ni and Mg were achieved by the dissolution of In to form a $Mg_2In0.1Ni$ and Mg(In) solid solution. The dehydrogenation enthalpy change of Mg-In-Al-Ti fabricated via dielectric barrier discharge plasma assisted milling (P-milling) reduced to 65.2 kJ/mol and the dehydrogenation activation energy declined to 125.2 kJ/mol.

While the hydrolysis reaction is easily interrupted by the formation of $Mg(OH)_2$ passive film on Mg/MgH_2 surface during hydrolysis process. As a result, the conversion yield is quite low and the kinetics is poor, which limits its practical application. The improved approaches in terms of combination with catalysts and changing solution composition were used to accelerate the hydrolysis reaction of Mg or its hydride. The hydrolysis results demonstrate that small amounts of MoS_2 added could significantly accelerate and enhance the hydrolysis reaction of Mg in seawater. Moreover, flower-like MoS_2 spheres prepared via a hydrothermal method were also confirmed the higher catalytic activity than that of bulk MoS_2 on the hydrolysis of Mg. The effects of Mo and its compounds and transition metal oxides on the hydrolysis properties of Mg were also studied.

Finally, a one-step approach towards hydrogen generation and storage via using Mg/MgH_2 as the new method was also reported.

O-09

Russian experience in development of low-waste nuclear energy on the basis of innovative fast neutron reactors

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Nuclear energy has the biggest potential in easing of negative effects of different technologies of electricity generation with the lesser average costs in energy supply sector in the of estimation intergovernmental group of experts in climate change. On the contrary, the fossil-fueled power plants are the main source of air pollution [1].

Thermal neutron reactors that present the basis of nuclear energy can use about 1% of uranium including fissionable and fertile isotopes. Fast breeder reactors use up to 60% of uranium. World reserves of natural uranium are limited and can't provide the long-run development of atomic energy without fast breeder reactors application.

In 2002 after the analysis of more than 100 projects the experts of GIF (Generation IV International Forum) chose six innovative nuclear systems that give the nuclear energy a possibility to provide sustainable energy need satisfaction in XXI century. One of them is a system with a sodium-cooled fast neutron reactor and closed nuclear fuel cycle that provides the effective actinides treatment and fertile material breeding [2].

The key problems of fundamental advantages of nuclear energy use are the safety ensuring and the reliable waste isolation from the biosphere. Perspective nuclear power must possess guaranteed safety, economic sustainability and competitiveness, prolonged absence of raw material limits, ecological stability.

A NPP with fast neutron reactors has high thermal efficiency, minimal amount of waste, the least radiation loads on the personnel and biosphere, the highest nuclear fuel utilization efficiency and a number of other advantages in comparison with the other types of NPPs [3].

Russia possesses a significant scientific, engineering and design experience in the field of fast sodium-cooled reactors. The third power unit of Beloyarskaya NPP is operating since 1980. The safe technology of sodium treatment is developed. In 2015 it was put into operation a BN-800 reactor with improved technical and economic characteristics and safety features.

It was designed the project of BN-1200 reactor which belongs to the reactor plants of improved safety and can be used in the nuclear energy system of forth generation with closed nuclear fuel cycle. Its sanitary-hygienic zone is in the boundaries of nuclear power plant for any design accident [4].

The closed nuclear fuel cycle on the basis of fast neutron reactors (Fig. 1) minimizes the volume of radioactive waste and optimizes the consumption of

natural resources. The majority of transuranium elements can divide under the influence of fast spectrum neutrons with energy emission. That is why the lower amount of them will pass to high-level radioactive waste.

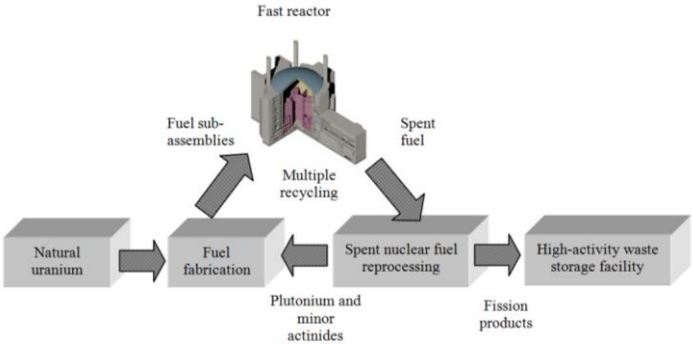

Figure 1. Fast reactor based fuel cycle

The exploitation experience shows that BN-600 and BN-800 are the most environmentally safe nuclear reactors. The thermal efficiency factor of fast neutron reactor NPPs exceeds 40%. That makes the emissions of heat into environment significantly lower than the emissions of conventional NPPs with thermal efficiency factor of about 33%.

According to the data of Public report on the state of environment and the influence of habitat factors on the Sverdlovsk region population health the share of Beloyarskaya NPP in gross volume of pollutants into atmospheric air and water bodies makes up only a 1/100 of 1 percent. The emissions of radioactive substances into atmosphere mainly consist of inert radioactive gases and usually make up less than 1 percent of admissible value.

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O-10

Porous alloying-type Sn/Sb anode materials for superior Li/Na-ion batteries

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Going along with the urgent requirement on rechargeable energy storage devices for electric vehicles (EVs) or hybrid EVs, Li-ion batteries now become one type of the most attractive energy storage technologies.[1-3] As a similar energy storage device, Na-ion batteries re-attracted intensive research attention recently owing to the relatively low cost and infinity of Na resources.[4,5] As one of the important components for the batteries, the anode material plays an important role on improving the comprehensive performance of the batteries. Herein, we summarize our recent progress in the structural design, chemical synthesis, and electrochemical properties of some new alloying-type metal anode materials (e.g. Ni-Sn, Ni-Sb, Sb@C, Sn_4P_3@C) for high performance Li/Na-ion batteries.[6-10] Through well-constructing 3D porous/core-shell/yolk-shell and conductive material-coated structures, the Li/Na-ion storage performances of these anode materials were significantly improved, such as long cycling stability, high rate capability, high specific capacity.

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Ecological and economic advantages of remote heat supply from reactor plant of advanced safety BN-1200

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The objective of this study is the actualization of the problem of long distance transportation of heat from a nuclear power plant (NPP) to big cities. The development of atomic heat supply is important for our northern country with traditional district heating. A nuclear power plant is the most environmentally appropriate source of heat in comparison with conventional fossil-fueled heat sources. It does not consume oxygen, minimizes water consumption, has higher available heat factor.

Heat supply on the basis of combined production of heat and electricity is the basis of rational energy sources use. It makes it possible to increase the efficiency of operating NPPs, to lower significantly the emissions of nitric oxides and greenhouse gases from the fossil fuel burning and to reduce the heat pollution of the atmosphere by cooling towers [1].

The report summarizes the heat supply experience of the enterprises and residential area of Zarechny town from Beloyarskaya NPP. The evolution of heat supply system from Beloyarskaya NPP is described as the power units number 1–4 with reactors AMB-100 (1964), AMB-200 (1967), BN-600 (1980) BN-800 (2015) were started. All the power plants are provided with heating units for heating and hot water supply of Zarechny town [2–4]. The information on foreign experience of atomic power supply is also summarized.

The issue of long distance heat transportation was looked into in eighties by E. Ya. Sokolov, B. V. Yakovlev and other well-known specialists in the sphere of heat supply. The efficiency of heat transportation at 100–150 km distance was proved [5].

To implement the technology of long distance transportation of heat it is required the complex approach to the design of heat supply system. It must include sources of heat, heat delivery pipes, peak sources and networks, heat consumers. Innovative solution of heat supply problem is composed of a set of new technical decisions for all the components of the system which make it possible to reduce the heat transport costs and increase the system reliability. The present day the reasonableness of long distance heat transportation is determined by a complex of technical, economic and ecological factors [6] that are given in the report. The estimation of efficiency of the long distance heat transportation from NPP is made.

It was examined the variant of Ekaterinburg heat supply from Beloyarskaya NPP in terms of the issue of the reduction of emissions to atmosphere when fossil-fueled heat supplying. The layout of heat supply developed in fitness with the

geographical peculiarities of the location and the features of nuclear power plants with sodium-cooled fast neutron reactors (a three-circuit diagram) was taken as a basis (Fig. 1).

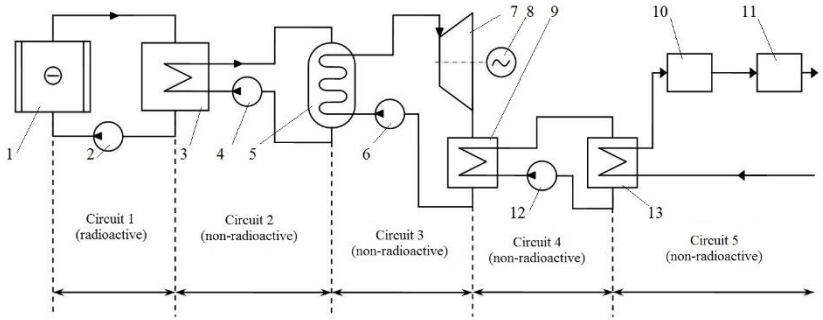

Figure 1. The schematic diagram of Ekaterinburg heat supply from Beloyarskaya NPP: 1 – nuclear reactor; 2 – reactor coolant pump; 3 – sodium to sodium intermedium heat exchanger; 4 – secondary circuit coolant pump; 5 – steam generator; 6, 12 – circulating pump; 7 – steam turbine; 8 – electric generator; 9 – heat exchanger; 10 – peak boiler; 11 – consumers; 13 – heat exchange plant.

The heat supply on the basis of combined production of heat and electric energy is the ground of rational energy sources' use. It gives a possibility to increase the NPP efficiency, significantly reduce the emissions of nitric oxides and greenhouse gases from fossil fuel combustion and the atmosphere heat pollution.

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O-12

Energy harvesting with piezoelectric effect

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High power output of energy harvesting is the key for different applications. Here, we focus the piezoelectric energy harvesting and increase the power output. The piezoelectric materials with different parameters for energy harvesting are carried for the high power output. And, we also display the design and optimization of piezoelectric energy harvesting device.

Harvesting electric energy from mechanical vibration using a mechanically excited piezoelectric circular membrane array is presented especially. The piezoelectric circular diaphragm array is consisted of four plates with series and parallel connection, and the electrical characteristics of the array are examined under dynamic conditions. With an optimal load resistor of 160 kΩ, an output power of 28 mW was generated from the array in series connection at 150 Hz under a pre-stress of 0.8 N and a vibration acceleration of 9.8 m/s^2, while a maximal output power of 27 mW can be obtained from the array in parallel connection through a resistive load of 11 kΩ under the same condition (frequency, pre-stress, acceleration). The results show that using a piezoelectric circular diaphragm array can increase significantly the output of energy compared with the use of a single plate. By choosing an appropriate connection pattern (series or parallel connections) among the plates, the equivalent impedance of the energy harvesting devices can be tailored to meet the matched load of different applications for maximal power output.

The optimization of piezoelectric energy harvesting device is also demonstrated for the high power output with different shape design of mass.

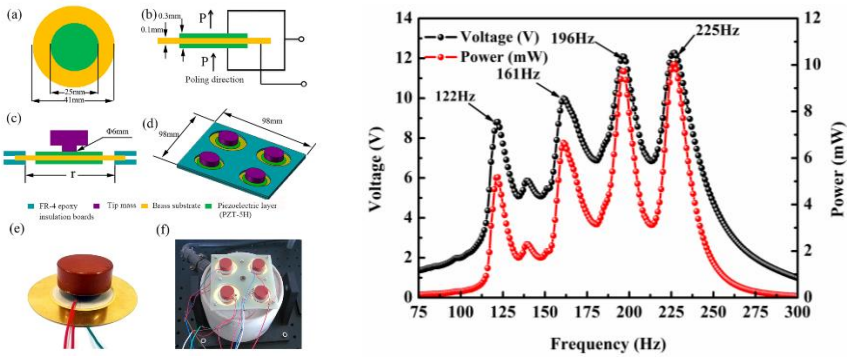

Figure 1. Piezoelectric energy harvesting using piezoelectric array for broadband output.

O-13

Optically active defects induced by electron beam in transparent $MgAl_2O_4$ ceramics

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Utilizing of transparent ceramics for devices operating in fields of ionizing radiation is intensively investigated. Currently, particular attention is drawn to transparent ceramics based on $MgAl_2O_4$. Such materials have increased radiation resistance, 0.2 to 5 μm transparency window and Eg = 7.8 eV band gap, which makes it possible to use them in optoelectronic devices exposed to radiation [1]. However, a number of fundamental questions related to determining of how intrinsic and impurity defects affect optical properties of such ceramics remains. Therefore, the aim of this work was to study the nature and properties of optically active defects in transparent ceramics of aluminum-magnesium spinel (AMS) exposed to fast electrons.

Transparent AMS ceramics were obtained using nanopowders by hot uniaxial pressing in graphite crucible with pressure of 35 GPa at holding temperature of 1550 ° C for 1 hour. Electron irradiation was carried out by “radan-expert” accelerator with 2 ns duration, 130 keV electron energy and 60 A/cm^2 current density.

Optical density spectrum of irradiated samples was recorded with help of Perkin Elmer Lambda 35 spectrophotometer. Optical absorption coefficient was calculated using Bouguer-Lambert formula on the basis of obtained optical density spectrum.

Trace amounts of such impurities as Mn and Ti were discovered according to typical excitation and luminescence bands obtained by optical spectroscopy analysis of studied ceramics.

Figure 1 shows the spectrum of induced optical absorption after transparent ceramics exposure to pulsed electron beam. It can be seen that irradiating by electrons leads to a spectrum shape change. The appearance of new absorption bands is due to intrinsic and impurity defects charge exchange processes. Absorption with maximum in 3 eV is caused by Mn^{3+} to Mn^{2+} impurity ions charge transfer [2]. Extremum in 4.5 eV corresponds to absorption of Ti^{3+} ions in $MgAl_2O_4$ matrix and 5.3 eV maximum is attributed to own F-type defects in AMS (anion vacancy with two trapped electrons) [3, 4]. Additional maximum in 6 eV is observed in 5.5-6.5 eV range. It is presumed that nature of the band is associated with atoms in interstitial positions.

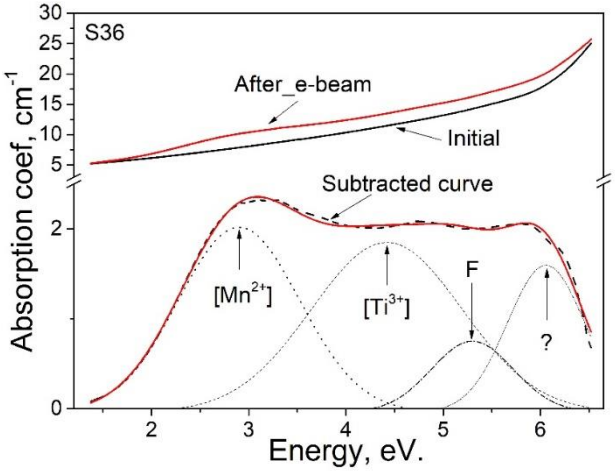

Figure 1. Induced optical absorption spectrum after exposure by pulsed electron beam.

Elementary bands and quantity of optically active defects were estimated using the Smakula-Dexter formula, table 1 based on decomposition of induced optical absorption difference spectrum.

Table 1. Quantity of optically active defects after irradiation by electrons

Mn^{2+}	Ti^{3+}	F	?
1.78×10^{16}	2.06×10^{16}	4.53×10^{15}	9.1×10^{15}

Irradiation by electron beam leads to recharging of cation defects, as well as defects of anion sublattice. Cation defects can be formed due to presence of trace impurities but formation of anionic defects may take place for several reasons. Irradiation by accelerated electrons leads to an oxygen atom shifting from crystal lattice site and formation of anion vacancy. F centers result from electrons localization at such vacancies. Besides, a part of anion vacancies is formed during fabrication of ceramics by hot uniaxial pressing method using graphite crucible according to mechanism described in [5].

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O-14

The influence of solvent additive on P3HT:PCBM bulk heterojunction photovoltaics using TOF-GISANS

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It is generally agreed that processing solvent additives in polymer:fullerene bulk heterojunction solar cells increases power conversion efficiency. However, the understanding of the influence of solvent additive on the BHJ systems is not complete, especially for the quantitative determination of the molecular miscibility of donor and acceptor and the inner morphology changes induced by solvent additive. In the present study, the influence of the solvent additive 1,8-octanedithiol (ODT) on the classic system poly(3-hexylthiophene):[6,6]-phenyl-C61 butyric acid methyl ester (P3HT:PCBM) films are determined. The morphology is investigated via AFM and time-of-flight grazing incidence small angle neutron scattering. The crystalline order is determined using absorption spectroscopy and grazing incidence wide angle X-ray scattering. With solvent additive, an increased crystallinity and prominent phase separation are achieved. Moreover, with a high ODT concentration, a PCBM accumulation layer is found at the top surface.

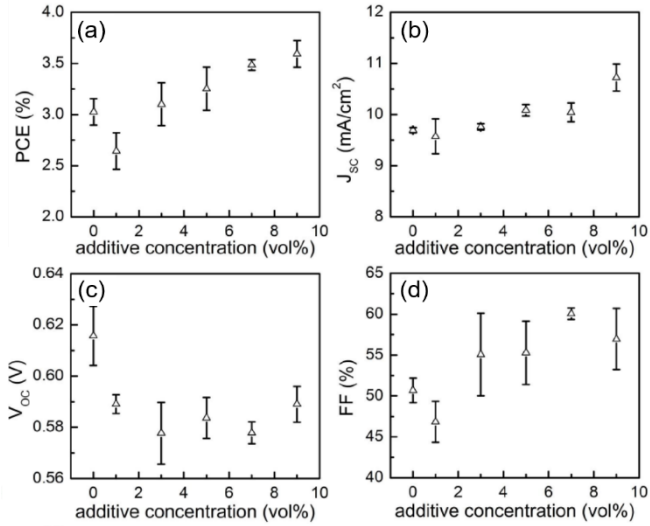

Figure 1. (a) PCE, (b) JSC, (c) VOC, and (d) FF of P3HT:PCBM solar cells with different volume concentrations of ODT.

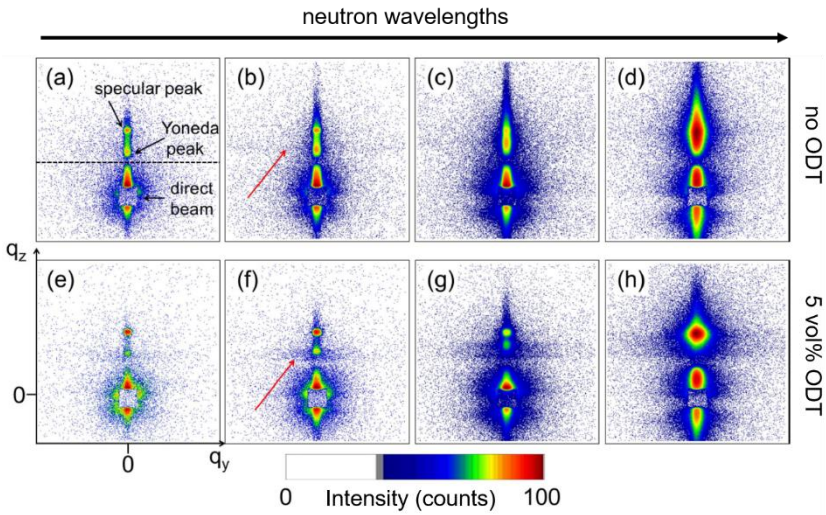

Figure 2. 2D GISANS data of the P3HT:PCBM films (a-d) without ODT and (e-h) with 5 vol% of ODT. The wavelengths are 3.65 Å, 4.92 Å, 6.65 Å, and 9.92 Å, respectively.

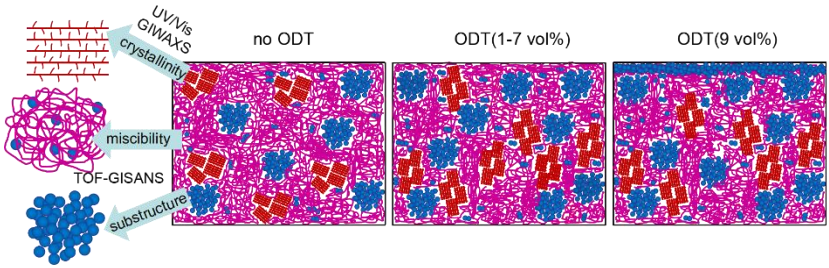

Figure 3. Schematic illustrations of the influence of ODT on P3HT:PCBM solar cells.

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O-15

Domain kinetics in single domain PMN-39PT single crystal during polarization reversal

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The relaxor-PT based $Pb(Mg_{1/3}Nb_{2/3})O_3$– $PbTiO_3$ (PMN-PT) crystals, which can be readily grown by modified Bridgman method with large size, have received considerable attention due to their excellent piezoelectric, electromechanical coupling, acoustic and ferroelectric properties. So that, PMN-PT single crystal has been widely used as energy harvesting devices, medical transducers, acoustic transducers and actuators.

For PMN-PT single crystal, many researchers have adopted the "domain engineering technique" to change the polarization orientation (domain structure) to enhance the intrinsic piezoelectric properties. In order to develop the domain engineering technology and benefit practical applications by using PMN-PT single crystal, studying its domain kinetics and domain structure evolution is essential.

We have systematically studied the domain kinetics during polarization reversal in single-domain tetragonal PMN-PT single crystals by in situ optical visualization of domain kinetics accompanied by analysis of the switching current. At first, the PMN-PT single crystal samples were poled by applying electric field to the original spontaneous polarization direction ([001]) at high temperature to achieve quasi-single domain state for further observation. Then we have studied the domain structure evolution by video recording of instantaneous domain structure patterns obtained during forward and backward switching ad measured the corresponding current data, which allowed us to reveal the three basic processes during the polarization reversal: (1) formation and growth of macroscopic a-domains, (2) formation of small a-domain structures with neutral and charged domain walls at the intersections of macroscopic a-domains, (3) formation and growth of irregularly shaped c-domains. In addition, by comparing the measured and optical currents we have found that the main switching current peak can be attributed to the growth of c-domains and the additional small switching current peak is related to the capacitive input to the switching current induced by charged domain walls. The two orders of magnitude enhancement of dielectric permittivity due to appearance of the charged domain walls was revealed.

O-16

Porous graphitic carbon nitride nanosheets by pre-polymerization for enhanced hydrogen evolution from water splitting under solar light

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A facile and green method was developed to fabricate porous graphitic carbon nitride (g-C_3N_4) nanosheets by simply pre-polymerizing melamine at 350°C for 2 h. A porous structure was formed in the resulted g-C_3N_4 (CN-350). Consequently, the specific surface area and pore volume of CN-350 was greatly enhanced, resulting in superior performance in photocatalytic hydrogen evolution and dye degradation. The hydrogen evolution rate and degradation constant of CN-350 were 11.2 and 8.8 times higher than that of bulk g-C_3N_4 under visible light irradiation. The porous structure not only provided CN-350 with abundant active catalytic sites and cross-plane diffusion channels to facilitate the charge and mass transportation, but also promoted the charge separation in the photocatalytic reaction. This work provided a promising method for mass-production of highly active and stable g-C_3N_4-based photocatalysts to generate hydrogen from water splitting under solar light for environmental and energetic applications.

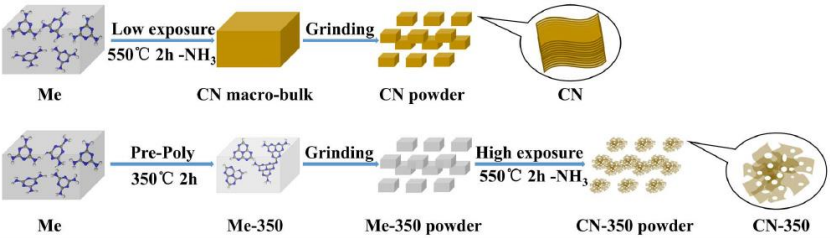

Figure 1. Schematic illustrations of the synthesis process of CN and CN-350.

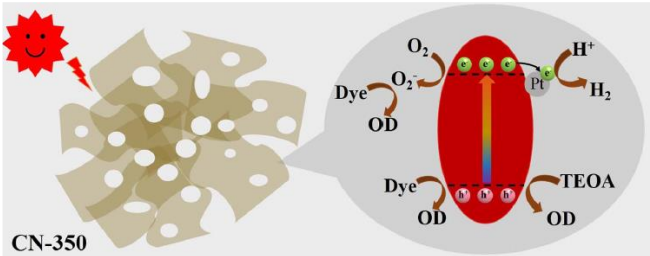

Figure 2. Schematic illustration of the photocatalytic reaction mechanism for CN-350.

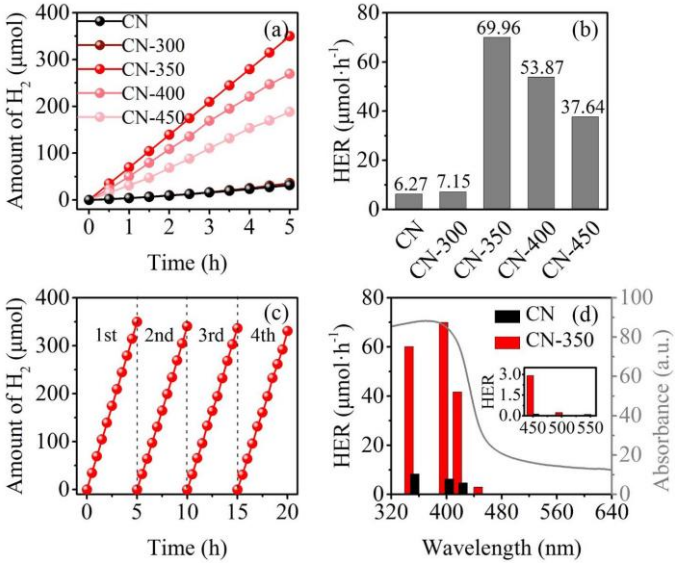

Figure 3. (a) Hydrogen evolution curves, (b) average hydrogen evolution rate of CN and pre-polymerized g-C3N4, (c) stability test of CN-350, (d) wavelength dependence of hydrogen evolution rate of CN and CN-350.

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O-17

Bulk oxygen diffusion and surface exchange limitations in $La_{2-x}Sr_xNi_{1-y}Fe_yO_{4+\delta}$

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The K_2NiF_4-type lanthanum nickelate is one of the promising cathode materials for the intermediate-temperature solid oxide fuel cells (IT-SOFC). This oxide shows fast oxygen-ion transport (via interstitial oxygen) combined with intermediate values of thermal expansion coefficient. However, surface oxygen exchange in La_2NiO_4 was shown to be limited [1,2]. The surface exchange kinetics could be improved by the modification of surface [1] and/or by chemical doping [2]: the surface limitations in La_2NiO_4 were eliminated after simultaneous doping with strontium and iron by increasing the iron content up to y=0.4 at fixed x=0.5 [2]. This work aims to study the effect of higher strontium content on oxygen transport in $La_{2-x}Sr_xNi_{1-y}Fe_yO_{4+\delta}$.

$La_{1.2}Sr_{0.8}Ni_{0.9}Fe_{0.1}O_{4+\delta}$ was synthesized by a citrate-nitrate method as described in [2]. The phase purity of the as-sintered $La_{1.2}Sr_{0.8}Ni_{0.9}Fe_{0.1}O_{4+\delta}$ samples was confirmed by X-ray powder diffraction. The bulk oxygen diffusion and surface oxygen exchange limitations in $La_{1.2}Sr_{0.8}Ni_{0.9}Fe_{0.1}O_{4+\delta}$ were studied by measuring the oxygen permeation flux j through dense ceramic membranes with different thickness (0.8 and 1.2 mm) under various oxygen partial pressure gradients. The oxygen flux was measured at 800, 850, 900, 950 and 1000°C within the oxygen partial pressure gradient interval of $\log(0.21/pO_2)$=0.2-1.8.

The oxygen permeation data allow to estimate the critical membrane thickness, d_c, which corresponds to the change of rate limiting step in oxygen transport. The values of d_c increased from 0-0.5 mm (800-900°C) to 1.6 and 2.3 mm at 950°C and 1000°C, respectively, indicating the change of rate limiting step in the oxygen permeation flux (though 0.8 and 1.2 mm membranes) from bulk oxygen diffusion to surface exchange. One should note that the change of limiting step with temperature correlates with the beginning of active oxygen release at T≈900°C followed by a reduction of Ni^{3+} to Ni^{2+}.

The oxygen-ion conductivity values and oxygen diffusion coefficients for $La_{1.2}Sr_{0.8}Ni_{0.9}Fe_{0.1}O_{4+\delta}$ were calculated at all studied temperatures showing the maximal value of σ_{ion}=0.0023 S/cm and D_{ion}=1.59×10^{-6} cm^2/s at 1000°C, respectively. The bulk oxygen diffusion in the oxygen-deficient (δ<0) $La_{1.2}Sr_{0.8}Ni_{0.9}Fe_{0.1}O_{4+\delta}$ revealed significantly higher activation energy (E_a=195 kJ/mol) compared to that for the oxygen-excessive (δ>0) $La_{2-x}Sr_xNi_{1-y}Fe_yO_{4+\delta}$ [2].

The values of surface exchange coefficients k_{ex} for $La_{1.2}Sr_{0.8}Ni_{0.9}Fe_{0.1}O_{4+\delta}$ were determined at 900, 950 and 1000 °C by fitting the model function based on the modified Wagner equation to the corresponding $\log(j)=f(\log(0.21/pO_2))$

dependencies. Similarly, the k_{ex} values were estimated for the oxygen-excessive $La_{2-x}Sr_xNi_{1-y}Fe_yO_{4+\delta}$ using the data from ref. [2]. The obtained results are shown in Figure 1.

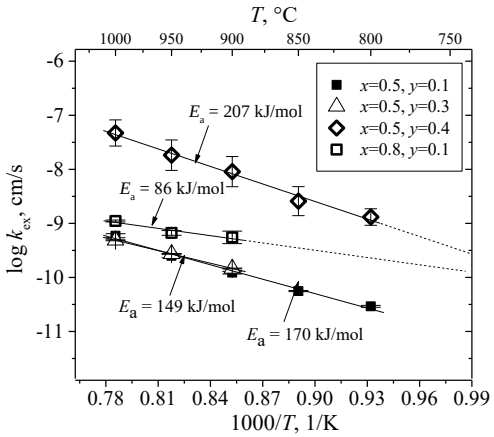

Figure 1. Surface exchange coefficients vs. temperature for $La_{2-x}Sr_xNi_{1-y}Fe_yO_{4+\delta}$.

The activation energy for surface exchange in $La_{1.2}Sr_{0.8}Ni_{0.9}Fe_{0.1}O_{4+\delta}$ was almost twice lower compared to that for the oxygen-excessive $La_{2-x}Sr_xNi_{1-y}Fe_yO_{4+\delta}$ oxides (Fig. 1). The obtained results also indicated that the surface oxygen exchange kinetics for $La_{1.2}Sr_{0.8}Ni_{0.9}Fe_{0.1}O_{4+\delta}$ should be similar to $La_{1.5}Sr_{0.5}Ni_{0.6}Fe_{0.4}O_{4+\delta}$ in the intermediate temperature range (see the dashed lines in Fig. 1).

The aforementioned observation allows concluding that $La_{1.5}Sr_{0.5}Ni_{0.6}Fe_{0.4}O_{4+\delta}$ can be considered as a superior cathode material compared to the strontium-rich $La_{1.2}Sr_{0.8}Ni_{0.9}Fe_{0.1}O_{4+\delta}$: although both exhibited comparable surface exchange kinetics the latter showed significantly lower oxygen-ion conductivity values in the intermediate temperature range.

The research was supported by the Ministry of Education and Science of the Russian Federation Agreement no. 02.A03.21.0006.

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O-18

Research on energy utilization in recovery of CO_2 from boiler flue gas

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With the rapid development of the society and the improvement of the people's living standards, it is more valuable to save energy and reduce emissions and turn waste into treasure. In this paper, according to 14% CO_2 in the 2×40 t/h heating boiler flue gas in Xi'an, China, ethanolamine is used for chemical absorption as the same time formative carbamate is used to desorption. the solar energy is used to provide the pump-driver to drive the entire system to save energy more. On the one hand, carbon emissions are reduced by absorption. On the other hand, CO_2 as a new product is made for resource. The waste heated boiler flue gas is used to heat the absorption and the desorption. The results showed that the best absorption rate was 82.28% when the ethanolamine concentration was 40% and the absorption temperature was 40°C. The energy consumption was 59.82 KJ/mol. The best desorption temperature of carbamate is 115 °C, the desorption rate is 55%, and its energy consumption is 694.3 KJ/mol. Two pump need 1.49 KJ/h.

An actual production process is designed to use the waste heated boiler flue gas energy 4.3 × 108 KJ / year and solar energy 4351 KJ / year. reduce CO_2 42.8 t/year and regenerate CO_2 23.54 t/year. The effect of energy conservation and emission reduction is remarkable.

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O-19

The analysis of the possibility of use of nanofluid as the heat carrier for increase in efficiency of heat supply systems

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The article is about the possibility of applying nanofluids in heat supply systems as a coolant. The most effective nanofluids were selected by analyzing the thermal conductivity, concentration, size, mass, and velocity of nanoparticles. It is presented the dependences of the heat transfer coefficient of a nanofluid on the Reynolds number and the heat transfer coefficient on the volume concentration. According to calculations, with the addition of 1% vol. of nanotubes to the coolant path that gives heat in the evaporating section of the heat pump, the heat transfer coefficient of a nanofluid increases by 100%.

POSTER PRESENTATIONS

P-01

The effect of simultaneous homo- and heterogeneous doping on transport properties of $Ba_2In_2O_5$

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One of the key positions of modern materials science is the development and research of solid oxide fuel cells and their components, including electrolytic membrane materials. By this way there is the task of finding inexpensive and technological solid electrolyte with high conductivity and stability at high temperature, in oxidizing and reducing atmosphere. Medium temperatures are the most optimal region in terms of energy costs. Prospective ionic conductors for this temperature range are proton electrolytes based on the complex oxides.

The most studied method for modification of their structure and optimization of physicochemical properties is a homogeneous cationic doping. However, the homogeneous anionic doping is new promising way for the obtaining of new materials with improved properties. Earlier, we have reported a new route for increasing oxygen-ion and proton conductivities by F^--doping of brownmillerite $Ba_2In_2O_5$. It was proved that small F^--concentrations can improve the oxide-ion (mixed anion effect) and the proton conductivities. The other prospective method of improving transport properties is a heterogeneous doping. The composites based on $Ba_2In_2O_5$ with chemically inert Ba_2InNbO_6 oxide phase as a heterogeneous dopant demonstrate significantly increasing of conductivity level. The maximum conductivity corresponds to the ratio of the components 0.7:0.3. In this work the possibility of application of simultaneous homogeneous and heterogeneous doping has being described for the first time. The composite $0.7Ba_{1.95}In_2O_{4.9}F_{0.1}\cdot 0.3\ Ba_2InNbO_6$ has been chosen for the investigation.

The synthesis was carried out by solid state method. According to XRD analysis sample contained two phase – cubic perovskite type Ba_2InNbO_6 phase and brownmillerite type $Ba_{1.95}In_2O_{4.9}F_{0.1}$ phase with partial disordering of oxygen vacancies.

Thermal analyses of composite system showed the composites reversibly changed their mass at temperatures 300-500ºC in wet atmosphere ($pH_2O=2\cdot 10^{-2}$ atm), which corresponds to processes of intercalation and removal of water molecules. The maximal water uptake for composite system is proportional to the content of the phase $Ba_{1.95}In_2O_{4.9}F_{0.1}$ with incompletion in the oxygen sublattice and is 0.60 mole H_2O per formula $0.7Ba_{1.95}In_2O_{4.9}F_{0.1}\cdot 0.3\ Ba_2InNbO_6$. The Ba_2InNbO_6 phase is nominally complete in the oxygen sublattice and is capable of absorbing only small amounts of water due to an insignificant change in stoichiometry during the synthesis. Thus, the main amounts of proton defects are concentrated in the grains of the phase $Ba_{1.95}In_2O_{4.9}F_{0.1}$, as well as in the covering layer.

The conductivity measurements were carried out under dry ($pH_2O=3.5\cdot10^{-5}$ atm) and wet ($pH_2O=2\cdot10^{-2}$ atm) air by varying the temperature (250-1000ºC). The conductivity values of composite system $0.7Ba_{1.95}In_2O_{4.9}F_{0.1}\cdot0.3\ Ba_2InNbO_6$ are significantly higher that values for both undoped $Ba_2In_2O_5$ and F-doped $Ba_{1.95}In_2O_{4.9}F_{0.1}$ compositions in whole temperature range. The increasing in conductivity under wet air for composite proves the ability of sample to the proton transfer.

P-02

Effects of $La_2Mo_3O_{12}$ doping on properties of $La_2Mo_2O_9$ oxide-ion conductor

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Complex oxides of the LAMOX-family were first studied by Lacorre et al. [1] and show comparable to YSZ values of oxygen-ion conductivity – 10^{-2} S/cm at 800 ºC for $La_2Mo_2O_9$ which creates the prerequisites for their using as solid electrolytes of SOFCs.

Heterogeneous doping with an inert additional phase $La_2Mo_3O_{12}$ (is adjacent phase to $La_2Mo_2O_9$ in the phase diagram) was used to modify the functional properties of lanthanum molybdate $La_2Mo_2O_9$. It should be noted that conductivity of $La_2Mo_3O_{12}$ is 2-3 orders of magnitude lower than conductivity of the matrix phase.

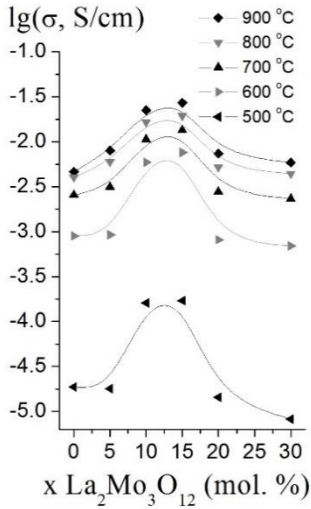

Figure 1. Concentration dependences of bulk conductivity of composites.

Polycrystalline samples $La_2Mo_2O_9$, $La_2Mo_3O_{12}$ and the composites {(100-x)$La_2Mo_2O_9$ – $x$$La_2Mo_3O_{12}$}, where x = 5; 10; 15; 20; 30 mol. % were obtained by solid state synthesis and were checked by X-ray diffraction analysis. The conductivity was measured by AC impedance method in cooling mode and the frequency range 500 Hz-3 MHz. An increase in bulk conductivity of composites with x = 10 and 15 mol. % (Fig. 1) by approximately 1 orders of magnitude is associated with appearance of a composite effect in studied system. It should also be noted that addition of inert phase does not suppress the phase transition α-

$La_2Mo_2O_9 \leftrightarrow \beta$-$La_2Mo_2O_9$ and doesn`t stabilize high-conductivity phase β-$La_2Mo_2O_9$ at room temperature, as occurs in some cases of homogeneous doping. The dominant ionic conductivity is maintained both for matrix phase and for composites in the wide range of oxygen partial pressures. The ion transport numbers calculated from conductivity dependences are 0.93-0.98.

This study was carried out within the framework of the state task of the Ministry of Education and Science of Russian Federation No. 4.2288.2017/4.6.

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P-03

Bismuth molybdate based oxygen ion conductors: synthesis and properties

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The present research is devoted to the synthesis and investigation of properties and structure of substituted $Bi_{26}Mo_{10}O_{69}$ (also named as $Bi_{13}Mo_5O_{34.5-d}$). The $Bi_{26}Mo_{10}O_{69}$ has unique structure what contains columns $[Bi_{12}O_{14}]_n$, $[MoO_m]$ polyhedra and "isolated" Bi ions. The $Bi_{26}Mo_{10}O_{69}$ -based solid solutions show one-dimensional oxygen-ionic conductivity at mediate temperatures. The $Bi_{26}Mo_{10}O_{69}$-based solid solutions crystallize in monoclinic symmetry at the temperatures above ~310°C, below this temperature they have a triclinic distortion. Ordinary substitution in $Bi_{26}Mo_{10}O_{69}$ can be realized by doping molybdenum sublattice or "isolated" bismuth positions resulting to the general formula $Bi_{26-2x}Me_{2x}Mo_{10-2y}Me'_{2y}O_{69-d}$.

In this work the several solid solutions $Bi_{26-2x}Me_{2x}Mo_{10-2y}Me'_{2y}O_{69-d}$ were researched. Mono- and double substituted complex oxides were synthesized. The following elements were chosen as dopants: Me= Ba, Mn, Me'=S, P. The complex oxide samples have been synthesized using conventional and co-precipitation methods. The phase composition was defined by XRPD. The dopant concentration homogeneity ranges and ranges of stabilization of the monoclinic form were determined. The details of structure were researched with the IR FT spetroscopy and Rietveld full profile structure refinement at XRPD data. The laser diffraction and SEM were used for investigation of morphology of powder samples. Porosity of samples was examined by hydrostatic weighting and was determined to be less then 5%, dense ceramic samples were observed. Magnetic measurements were carried out for Mn-doped samples and show Mn^{2+} oxidation state of Mn. Photocatalytic properties were investigated at RhB oxidation undo UV irradiation. Electrical conductivity was studied with impedance spectroscopy. The characteristic Arrhenius plots have linear shape and activation energy values are typical for oxygen-ion conductors. As a result, the best samples of $Bi_{26-2x}Me_{2x}Mo_{10-2y}Me'_{2y}O_{69-d}$, Me= Ba, Mn, Me'=S, P series can be recommended as a high ionic conductive material.

This study was supported RFBR, project №16-33-60026.

P-04

BIFEVOX-based composites: synthesis and investigation of electrophysical characteristics

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Over a period of several decades, oxygen-ion conductors, based on the bismuth vanadate family (BIMEVOX), have been studied as electrolytes for solid oxide fuel cells (SOFCs). It was found out that the doping of bismuth vanadate by metal oxides with a different oxidation state stabilizes the high-conducting γ-phase in the range of average temperatures (500-700 °C) and increases the ionic conductivity of the samples. A promising direction in studying the conductivity of materials is the synthesis of composites based on them for use in various electrochemical devices. It was shown that in this way it is possible to improve the quality of the material and get rid of the drawbacks inherent in other electrolytes. Bismuth niobate doped with iron was chosen as a composite additive because it is similar in composition to the matrix part of the composite.

Samples of compositions of the family BIMEVOX with the general formula $Bi_4V_{2-x}Fe_xO_{11-\delta}$ (BIFEVOX), where x = 0.25 - 0.35 (Δx = 0.05) and bismuth niobates with the general formula $Bi_3Nb_{1-y}Fe_yO_{7-\delta}$, where y = 0.01-0.06 ($\Delta$y = 0.01) were synthesized by the standard ceramic technology. Phase composition characterization of powder samples was carried out with XRPD method. The iron concentrations in compounds of the composition $Bi_3Nb_{1-y}Fe_yO_{7-\delta}$ were chosen in accordance with the homogeneity range (0-6%), the iron concentrations in the compounds of the $Bi_4V_{2-x}Fe_xO_{11-\delta}$ composition were chosen, because γ-modification of these concentrations is formed, and the samples show better electrophysical characteristics. Studies have shown that reflexes on the X-ray patterns of the BIFEVOX samples can be well described in a tetragonal unit cell with a space group I4/*mmm*, i.e. they correspond to the high-temperature γ-modification of the solid solution; and the reflections of the $Bi_3Nb_{1-y}Fe_yO_{7-\delta}$ samples can be described in a cubic setup with the space group *Fm*3*m*. The unit cell parameters of the composites phases were determined. As a supplementary method for estimating the phase and element composition of composites the scanning electron microscopy (SEM) method was used. The particle size was determined by the laser diffraction method. Dylatometric analysis was used to establish possible phase transitions and to determine the linear thermal expansion coefficient (LTEC). An additional condition for the survey was a change of the gas environment to a reducing cycle at 700 °C with a subsequent cooling-heating cycle and a further change in the atmosphere to the room atmosphere also at 700 °C. Curves, which show the change in LTEC, were plotted. The LTEC values of BIFEVOX before and after the oxidation-reduction cycles did not change significantly and remained in the range $17–19\cdot10^{-6}$ K^{-1}. Composite materials based

on $Bi_4V_{2-x}Fe_xO_{11-\delta}/Bi_3Nb_{1-y}FeyO_{7-\delta}$ bismuth vanadate were obtained by mechanical mixing of solid solutions. It was confirmed that no chemical interaction occurs when mixing the BIFEVOX and $Bi_3Nb_{1-x}Fe_xO_{7-\delta}$ materials.

The electrophysical characteristics of bismuth niobates and vanadates, as well as composites based on them, were studied. The electrical conductivity of bismuth vanadate samples as a function of temperature was studied in the temperature range 800-200°C in the cooling regime, samples of bismuth niobates in the range 850-200 °C in the cooling regime by impedance spectroscopy. The Cole-Cole diagrams were obtained and the dependence of the conductivity on the temperature for different compositions was plotted (Fig. 1). The general form of the dependencies for the samples studied has a rectilinear descending relation with possible fractures corresponding to the transition from one modification to another and characteristic for perovskite-like compounds.

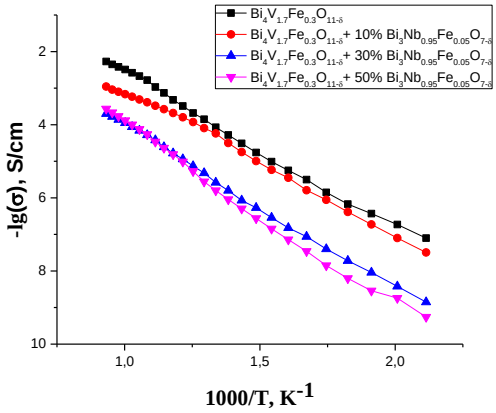

Figure 1. Temperature dependence of electrical conductivity of samples $Bi_4V_{1.7}Fe_{0.3}O_{11-\delta}/xBi_3Nb_{0.95}Fe_{0.05}O_{7-\delta}$

This work was supported by the Russian Foundation for Basic Research, Grant No. 17-53-04098 and President's scholarship (SP-3376.2016.1).

P-05

Solid solution films $Cd_xPb_{1-x}S$ AS materials for solar energy

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It is known that cadmium sulphide approved itself as a suitable material for using as a window layer in solar radiation converters: CdTe/CdS [1] и CIGS/CdS [2]. Lead sulphide is effectively used as an absorbing material [3]. Therefore, recently it has been observed the increased interest to getting and investigating of thin film heterostructures with *p – n* transition in the system CdS-PbS for production of solar cells. The solar cell with the structure ITO/CdS/PbS, covered with transparent conductive layer of ITO (indium tin oxide) exceeds by its conversion ratio other similar structures in this system. In work [4] the possibility of increasing of radiation conversion efficiency for thin film solar cells PbS/CdS without considering the contribution of quantum dots is noted.

For the absorbing semiconducting layer in solar cells the optimum bandgap width is 1.5 eV, which can be achieved by production of solid solutions in the form of ternary compounds $Cd_{1-x}Pb_xS$. Varying their composition, the optical and semiconducting properties can be optimized, providing more than 40% of efficiency coefficient of conversion.

In most publications, it is noted that to provide suitable functional properties their sensibilization is necessary made by thermal annealing of as-deposited solid solution layers $Cd_xPb_{1-x}S$ in the presence of oxygen. However, in monograph [5] it is shown that the chemical bath deposition of enriched solid solution films $Cd_xPb_{1-x}S$ can be predicted. Cadmium content in solid solution $Cd_xPb_{1-x}S$ in the conditions of metastable structure formation at low temperature hydrochemical synthesis is influenced by cadmium salt.

Therefore, the purpose of this research is a chemical bath synthesis of films $Cd_xPb_{1-x}S$ on sitall substrates, study spectral characteristics of it depending on the cadmium acetate content in the reaction bath.

For investigation of composition and optical properties of solid solutions in PbS-CdS system thin films of this compound was obtained from citrated-ammonium reaction mixture at temperature 353 K during 120-140 minutes, where the concentration of cadmium acetate $Cd(CH_3COO)_2$ was varied from 0.01 to 0.1 mol/L.

In solid solution films $Cd_xPb_{1-x}S$ ($0.01 \leq x \leq 0.24$) synthesized by chemical deposition there is a crystal state with lattice NaCl (*B*1) type. They don't require sensabilization after their removing from the reaction mixture and are ready to their practical use. The range of spectral sensitivity of substitutional alloys $Cd_xPb_{1-x}S$ depends on their composition. With the increasing of cadmium content (x) in solid solution structure gradual shift of spectral characteristic into short-wave region occur. As it is shown in Fig., with the rise of cadmium fractional concentration in solid solution $Cd_xPb_{1-x}S$ critical frequency and maximum of photoresponse moves in the short-wave region from c 3.1 to 1.6 μm and from 2.5 to 1.2 μm correspondently.

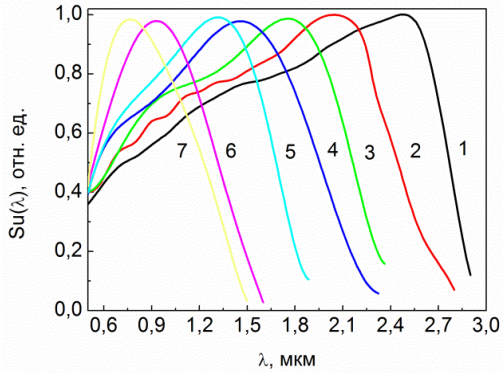

Figure 1. Plots of relative spectral photosensitivity of films based on PbS (1) and solid solutions $Cd_xPb_{1-x}S$ of various composition: $Cd_{0.03}Pb_{0.97}S$ (2), $Cd_{0.06}Pb_{0.94}S$ (3), $Cd_{0.09}Pb_{0.91}S$ (4), $Cd_{0.12}Pb_{0.88}S$ (5),$Cd_{0.20}Pb_{0.80}S$ (6),$Cd_{0.22}Pb_{0.78}S$ (7).

The obtained results create a base for the purposely chemical bath deposition synthesis of solid solution films $Cd_xPb_{1-x}S$ with the ordered composition to make semiconductive materials for solar radiation transducers with variable spectral characteristics.

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P-06

Precursor compounds for Cu_2ZnSe_2 structure

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Here we describe precursors compounds for Cu_2ZnSe_2 structure.

One of the typical representatives of $A^{II}B^{VI}$ compounds is ZnSe which can be used in creation of semiconductor electronics devices and information display systems, as active laser medium, color TV displays, optical light modulators and other optoelectronics devices. In ecological point of view, it's very important that ZnSe is nontoxic material due to absence of heavy metals in its compound.

The thin filmed copper (I) selenide is under increased attention of specialists in solar energy, micro- and optoelectronics because it can express wide specter of semiconductor and specific electrophysical properties due to its elemental composition and microstructure. In particular, band gap of copper (I) selenide thin films with nonstoichometric compound $Cu_{2-x}Se$ is 1.1–2.3 eV. These values are optimal for use $Cu_{2-x}Se$ films as absorbing layer and as precursor for multicomponent kesterite $Cu_2ZnSnSe_4$ structure.

According to many researchers, the most perspective method of thin films obtaining is chemical bath deposition of ZnSe and Cu_2Se semiconductor layers. This method is characterized by simplicity of process, economy, ecological safety, process control flexibility and wide possibilities in variation of composition and functional properties [1], [2]. However, the main difficulties of ZnSe and Cu_2Se chemical bath deposition from aqueous mediums process are determination of optimal synthesis conditions and determination of recipe.

Authors of this work obtained ZnSe from the reaction system "$ZnCl_2$ – $Na_3C_6H_5O_7$ – $NH_2OH{\cdot}HCl$ – NaOH – $Na_2Se_SO_3$" and Cu_2Se from the reaction systems "$CuCl_2$ – $NH_2OH{\cdot}HCl$ – Na_2SeSO_3" and "$CuCl_2$ – $NH_2OH{\cdot}HCl$ – Na_2SeSO_3 – KSCN".

As a result, 100-500 nm thickness Cu_2Se films and 100–800 nm thickness ZnSe films were obtained on sitall substrates. All films have good adhesion to substrate. The morphologies of Cu_2Se and ZnSe are given on Fig. 1 and Fig. 2, respectively.

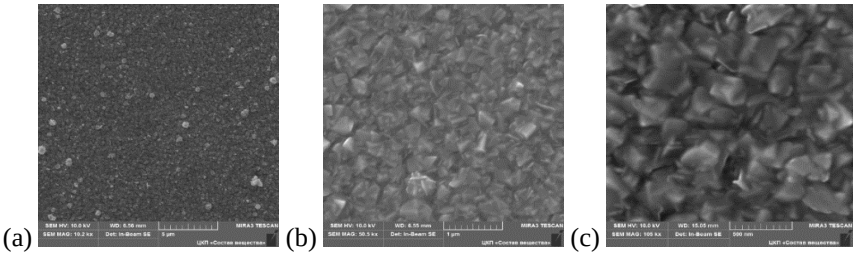

Figure 1. Electron microscope images of Cu_2Se film obtained from reaction system containing potassium thiocyanate. Duration of the synthesis 120 min at the temperature 343 K. Magnification: 10000 (*a*), 50000 (*b*) and 100000 (*c*).

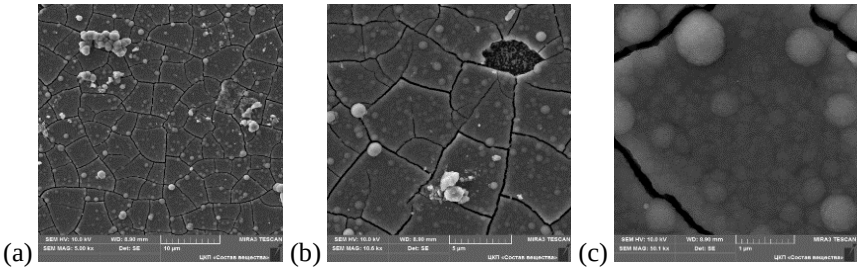

Figure 2. Electron microscope image of ZnSe film obtained from the reaction system "$ZnCl_2$ – $Na_3C_6H_5O_7$ – $NH_2OH{\cdot}HCl$ – Na_2SeSO_3" at the temperature of 353 K and duration of the synthesis — 120 min. Magnification: 5000 (*a*), 10000 (*b*) and 50000 (*c*).

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P-07

Optical properties of Cu_2S/SnS precursor layers for the preparation of kesterite Cu_2SnS_3 photovoltaic absorber

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Thin film solar cells attract much attention due to their low cost, high stability and efficiency. Research is mainly focused on *p*-type semiconductor Cu(In,Ga)(S/Se) and CdTe absorber layers, However, Cu_2SnS_3 (CTS) consisting of non-toxic and abundant elements has been also offered as a possible candidate for photovoltaic applications in recent years. The band gap of this semiconductor depends on the crystal structure and varies from 0.93 to 1.51 eV [1-4]. The Cu_2SnS_3 film can be fabricated by sequential deposition of Cu_2S and SnS precursor layers. In this report, the crystal structure, morphology and optical properties of Cu_2S and SnS thin films have been studied.

The Cu_2S and SnS layers have been prepared by chemical bath deposition method. In the case of Cu_2S, the solution of $CuCl_2$, Na_2SO_3 has been used, the wine acid ($C_4H_6O_6$) and hydroxylamine hydrochloride (NH_2OH HCl) have been added for providing of slightly acid and recovery environment. In the case of SnS the synthesis has been carried out from the solutions of tin chloride ($SnCl_2$) and sodium thiosulphate ($Na_2S_2O_3$). Sodium citrate used as the reagent regulating the content of active Sn^{2+} ions in the reactor. The films have been deposited on the fat-free glass substrates during 2 hours at 353 K.

The results of the SEM and EDX analysis confirm a high stoichiometric of the synthesized semiconductor layers of Cu_2S and SnS. In the first case the contents of copper and sulfur are 62.86±1.0 and 31.43±1.0 at. %. For the latter films that of tin and sulfur are 50.43±1.0 and 49.57±1.0 at. %. The films are formed from the particles with sizes of several hundred nanometers.

Fig. 1 shows the spectral transmittance curves of Cu_2S and SnS thin films; the onsets of fundamental absorption are situated at 420–800 nm and 800–1500 nm, respectively, that coincides with the reported values for these phases. The optical absorption data were analyzed using the Tauc relation [5] for determination of the value of the optical bandgaps. The E_g value for Cu_2S film calculated for direct allowed transitions is 2.25 eV. Since there is a discrepancy concerning with the type of transition in SnS compound, we estimated E_g taking into account a direct and indirect allowed transitions and the two functions $[\alpha h\nu]^{1/n}$ versus $h\nu$ have been plotted. In both cases the curves characterizing the two types of transitions have the wide linear regions, indicating that the direct as well as indirect bandgap

relations are applicable. The calculated E_g value for SnS thin film is equal to 1.21 eV and 1.17 eV for direct and indirect transition type, respectively.

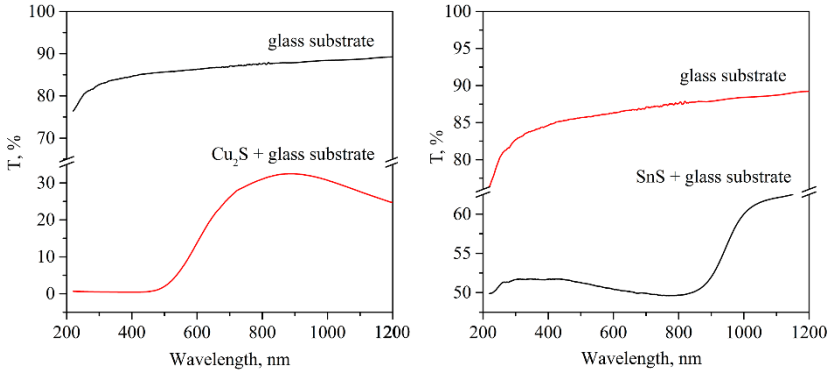

Figure 1. Transmittance spectra of Cu_2S, SnS thin films and glass substrate.

The work was financially supported by the program 211 of the Government of the Russian Federation № 02.A03.21.0006 and by the FASO program No. AAAA-A16-116122810218-7.

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P-08

Magnetic force driven noncontact triboelectric nanogenerator based on Fe_3O_4 NPs embedded PVDF nanofibres

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A novel magnetic force driven noncontact triboelectric nanogenerator for scavenging biomechanical energy to sustainably power portable electrics is presented. Based on the electrospun Fe_3O_4 nanoparticles embedded PVDF fibers membrane employed as triboelectric layer. A magnet is utilized as the trigger to non-contactly drive contact-separation mode TENG due to the magnetic responsiveness of triboelectric materials. The triboelectric nanogenerator with a small dimension has a peak output power of 0.23 mW under a load resistance of 25 MΩ. Furthermore, the hybrid nanogenerator exhibits a good stability for the output performance and charging performance, so it can be utilized to charge energy storage devices and sustainably power some portable electronics. This work demonstrates a novel prototype of nanogenerators toward harvesting human biomechanical energy and its potential applications in building up self-powered systems.

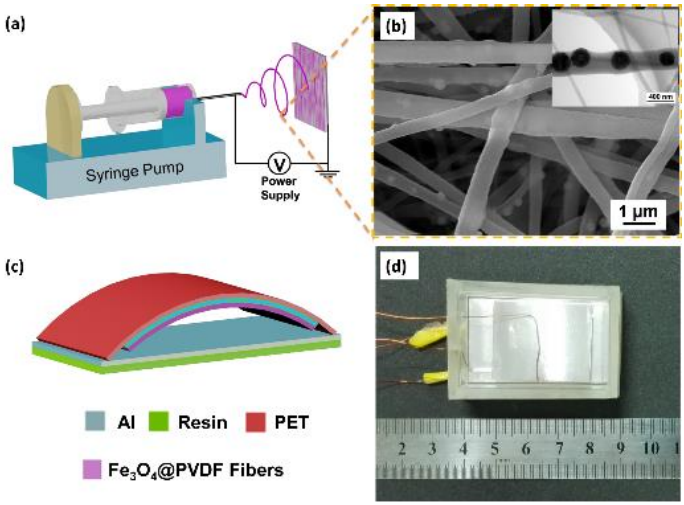

Figure 1. (a) Schematic illustration of preparing Fe_3O_4 NPs embedded PVDF fibres. (b) SEM and TEM image of Fe_3O_4 NPs embedded PVDF fibres. (c) Schematic illustration and (d) photograph of the magnetically driven triboelectric nanogenerator.

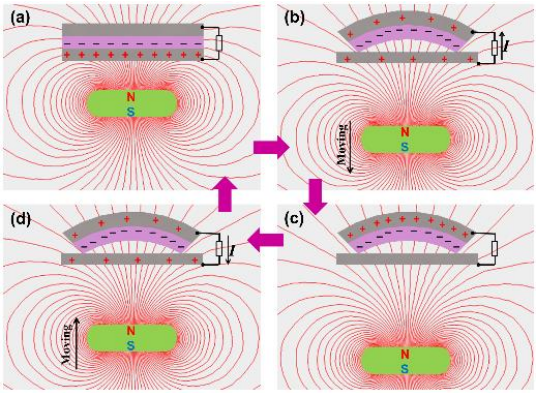

Figure 2. Schematic diagrams of the working principle of the magnetically driven triboelectric nanogenerator.

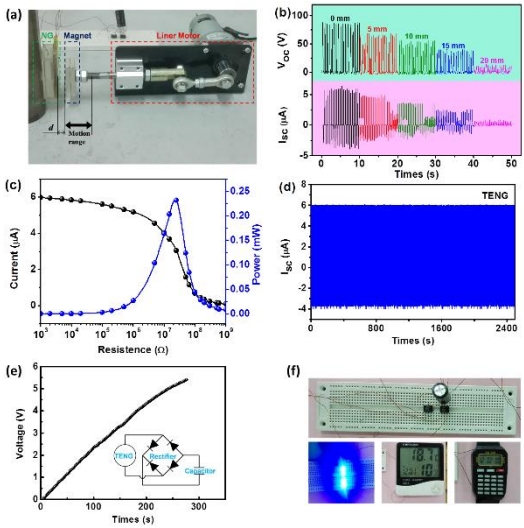

Figure 3. (a) Photograph of the setup for measuring the output performance. (b) The V_{OC} and I_{SC} versus time of TENG with different distances between the generator and the magnet. (c) The output power on the external loading resistance of the TENG. (d) The durability of the TENG. (e) The charging voltage curve of the commercial capacitor by TENG. (f) Demonstration of the self-powered electronic devices.

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P-09

The new application of metal hydrides in energetic materials: advantages and difficulties

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Metal hydrides are regarded as a series of promising hydrogen-supplying fuel for solid rocket propellants. The application research of metal hydrides additives in solid rocket propellants were introduced systematically, the application advantages and existing problems of metal hydrogen-storage materials in solid rocket propellants were analyzed simultaneously, the solutions of existing problems were analyzed and compared, which were based on metal hydrogen-storage materials of physical and chemical properties, dehydrogenation thermodynamics and kinetics characteristic, synthesis and modification methods in this paper. It is pointed out that the above-mentioned metal hydrogen-storage materials can promote the decomposition of components of propellants, improve its combustion properties and enhance its energy performances[1,2,3]. Moreover, the prospects and limitations of applications of all kinds hydrogen-storage materials in solid rocket propellants were analyzed. It is proposed that metal hydrides and metal complex hydrides are promising candidates as additives in solid rocket propellant. Much attention should be paid to the possible limitations that hamper the utilization of hydrogen-storage materials in propellants, such as the high sensitivity of hydrogen-storage materials to oxygen and moisture and their potentially poor compatibility with the present propellants.

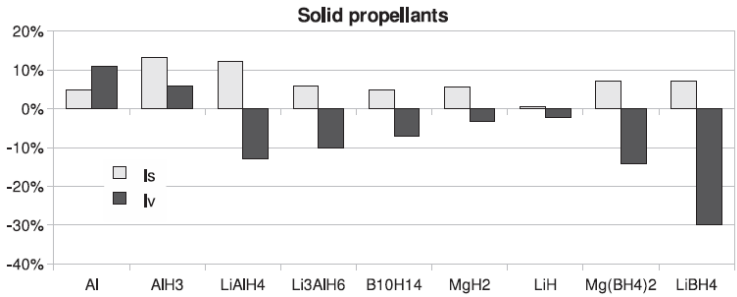

Figure 1. Solid propellant performance comparison. Optimal Is and Iv normalized to nonmetalized baseline formulation (AP/HTPB mass fraction 89/11).

In addition to that synthesis is also the difficult and challenge, for example in the phases of AlH_3 (α-, β-, γ-, δ-, ε-, ζ-AlH_3) α-AlH_3 is the steadiest phase but it is so difficult to be synthesized. There are many properties modified methods

beneficial to hydrogen-storage materials application in propellants, for example the nanosizing not only adjust dehydrogenation thermodynamics and kinetics of various metal hydrogen-storage materials[4], but also the nanoscale chemical-physical hydrogen-storage materials can be adopted as both hydrogen sources and combustion catalysts for propellants.

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P-10

Hydrogen-induced crystallization of amorphous phase: A new mechanism for the electrochemical capacity decay in Mg-Ni alloys

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To explore the origin of the electrochemical capacity and its decay for milled Mg-Ni alloys as negative electrode of Ni-MH battery, nanocrystalline Mg_2Ni and amorphous Mg-Ni alloys were prepared by combining the magnetic levitation melting with ball milling method. Their hydrogen storage properties and the microstructure evolution were systematically investigated in relating to electrochemical performance. The results reveal that the discharge capacity mainly originates from the hydrogen desorbed from Mg-Ni amorphous phase in milled alloys. And different to the general understanding of past 20 years, in addition to the electrochemical corrosion, hydrogen-induced crystallization is also, even dominating, intrinsic reason responsible for capacity decaying in amorphous Mg-Ni anode.

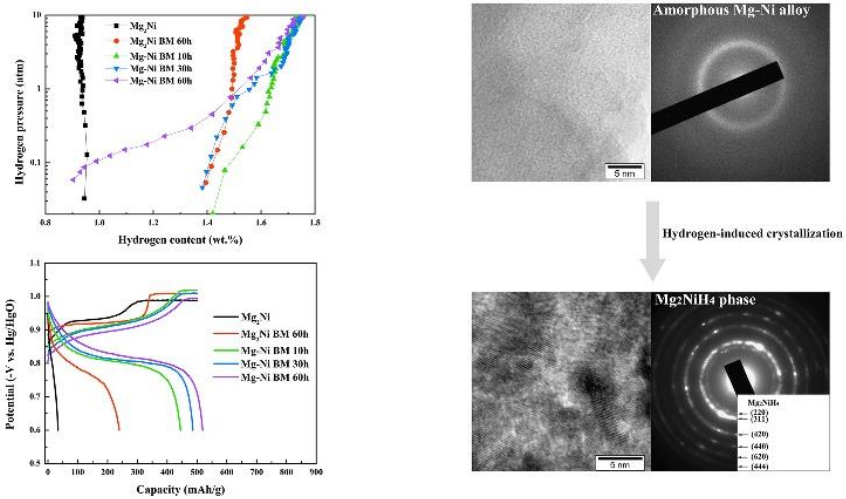

Figure 1. The hydrogen desorption pressure-composition-isothermals, first charge/ discharge curves and microstructure evolution of ball milled Mg-Ni alloys.

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P-11

Novel metal phosphides as anode materials for lithium-ion and sodium-ion batteries

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Lithium-ion batteries have been widely used in portable intelligent devices due to their high energy density and long service life, while sodium-ion batteries have promising applications in large energy storage devices due to the abundant reserve and economical supply of Na in the earth [1]. However, the capacity, stability and rate performance of these two types of batteries still need to be improved for the further application and development of these devices. Red phosphorus has received significant attention because of its high theoretical specific capacity (2596 mA h g^{-1}) for both lithium storage and sodium storage [2, 3]. However, its poor electron conductivity and huge volume changes during electrochemical reaction processes lead to low reversible capacity and poor cycle stability for both lithium-ion and sodium-ion batteries.

To overcome the disadvantages of phosphorus-based anodes, one feasible method is to introduce metal elements into phosphorus to form metal phosphide anodes. The intermediate products that form *in situ* during the charge/discharge processes can provide sufficient electrical conductivity and buffer the large volume changes of phosphorus during the electrochemical reaction processes. In this, we first synthesized AgP_2 by simply mechanical-chemical reaction of highly conductive Ag and high capacity P, by further compositing AgP_2 with carbon black, a new AgP_2/C composite was obtained. When served as anode material for lithium-ion batteries, the composite anode delivers a high discharge capacity of 790 mA h g^{-1} at 0.5 A g^{-1} after 100 cycles and excellent rate capability with a reversible capacity of 605 mA h g^{-1} at 10 A g^{-1} in half cells. However, it delivers a poor electrochemical performance for sodium-ion batteries, this is attributed to Ag particles cannot efficiently refining P particles, causing the difficulty to maintain structural stability during sodiation/desodiation processes. Thus we further synthesized $ZnGeP_2$/C composite with smaller particle size, when served as an anode material, it delivers a high reversible capacity of 807 mA h g^{-1} at 0.2 A g^{-1} after 100 cycles for lithium-ion batteries and 584 mA h g^{-1} at 0.1 A g^{-1} after 50 cycles for sodium-ion batteries.

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P-12

Synthesis, structure and investigation of bismuth niobate substituted by alkaline-earth elements

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At the present time there is an active search of suitable electrolyte materials for new ecological resources of energy such as solid oxide fuel cells (SOFCs). The most important requirements for solid complex oxide electrolytes are high oxide-ion conductivity values, ability to form dense sintered ceramics, good compatibility with other components of electrochemical devices. δ-Bi_2O_3 is one of the most perspective solid electrolytes with electroconductivity value 1-1.5 S×cm^{-1} [1]. However, it exists only at high temperatures (730-830 °C). So there is necessity to stabilize δ-phase at room temperature, using, for example, substitution by such cations as Nb^{5+}, W^{6+}, Mo^{6+} etc. The bismuth niobate Bi3NbO7 remains fluorite-like cubic structure of δ-Bi_2O_3, but one has lower conductivity than the bismuth oxide. In our present work, we tried to increase electroconductivity values of Bi_3NbO_7 by doping by alkaline-earth ions Ba^{2+}, Ca^{2+}, Mg^{2+}, and Sr^{2+}.

The samples with general formula $Bi_{2.9}M_{0.1}NbO_7$ (M=Ba, Ca, Mg, Sr) were obtained via solid state method at 600 - 1000 °C with slow cooling at furnace and intermediate regrinding. As the initial compounds the Bi_2O_3, Nb_2O_5, $CaCO_3$, $BaCO_3$, $MgCO_3$, $SrCO_3$ were taken. The results of X-ray diffraction analysis (DRON-3 diffractometer, $Cu_{K\alpha}$-radiation, Russia) showed samples had tetragonal structure (S.G. *I*-4*m*2) after annealing at 850 °C and cubic structure (S.G. *Fm*3*m*) after 1000 °C. Further investigations were performed with the samples sintered into briquettes. The images (Fig.1) obtained using scanning electron microscopy (SEM) (scanning electron microscope JEOL JSM 6390LA, Japan) of the $Bi_{2.9}Ca_{0.1}NbO_7$ showed ceramics had high density after sintering at 1000 °C.

The electroconductivity was measured by impedance spectroscopy (impedance meter Z-3000 “Elins”, Russia) using two-probe method with platinum electrodes in temperature range 850-200 °C at cooling regime. Plotted temperature dependences of electroconductivity had linear type with activation energy *ca.* ~ 1 eV. It was found that there were no large differences in the electroconductivity values between the samples of one series (it depended on sintering temperature

850 °C or 1000 °C). And the electroconductivity of the substituted bismuth niobates with tetragonal structure was higher than the other.

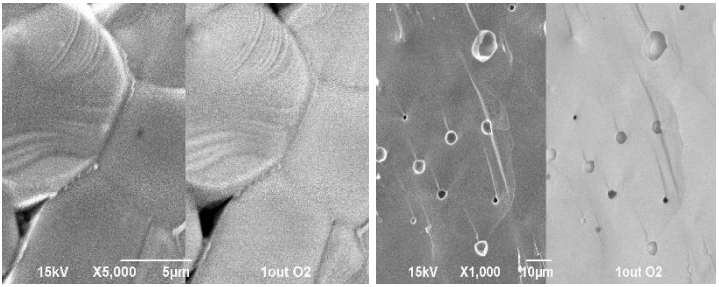

Figure 1. SEM images of the briquette Bi2.9Ca0.1NbO7 sintered at 1000 °C: surface (left) and chip (right).

The work was carried out within the framework of the state task of the Ministry of education and science of the Russian Federation № 4.2288.2017/PCh.

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P-13

Temperature dependence of phase composition in Ca-Bi-Nb-M-O and Ca-La-Nb-M-O (M = Mo or W) systems

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The development of Solid Oxide Fuel Cells (SOFCs) is one of the available technologies that best addresses the worldwide energy issues. Nowadays the objective of the discovery and optimization of highly performing oxide ion conductors is being solved by material scientists.

Only a limited number of efficient electrolyte materials are used today. The current technology employs well established materials such as YSZ and ScZO (yttria-stabilized zirconia and scandia-stabilized zirconia), doped CeO_2 systems (SDC, GDC), and doped lanthanum gallate perovskites (LSGM) with highly symmetric structure [1]. More recently, it has been demonstrated that fast oxygen ion conduction can be achieved in lower symmetry structures, involving the presence of interstitial oxygen species, both for purely ionic and mixed conductors. The scheelite ABO_4 class of ternary oxides is a wide family of materials with several fields of applications, ranging from solid state scintillators to laser materials and catalysts. One of the key features of this class of compounds is the possibility of doping on both the A and B sites with a wide range of aliovalent elements, leading to the formation of oxygen vacancies or interstitial oxygen ions, making them versatile ionic conductors [2]. Examples of such compounds are $LaNbO_4$ [3], $La_2Mo_2O_9$ [4], and solid solutions based on them.

The present work reflects the results of the investigation of phase formation processes in the systems Ca-La(Bi)-Nb-Mo-O and Ca-La(Bi)-Nb-WO with the purpose of establishing the mechanisms of formation, composition and structural features of previously discovered and new complex oxides and solid solutions based on them, as well as evaluating the composition and properties of the intermediate phases.

The powder samples were prepared by solid-state reaction technique by using stoichiometric amounts of $CaCO_3$, La_2O_3, Bi_2O_3, Nb_2O_5, MoO_3 and WO_3 in accordance with the specified composition of the system. The starting powders were mixed in an agate mortar with the addition of ethyl alcohol as a homogenizer. The obtained mixtures were calcined at 500ºC, 600ºC, 700ºC, 800ºC, 900ºC, and 1000ºC for 8 h per each stage in air. The composition of the final products after each step was controlled by the XRD.

Based on the XRD patterns, the temperature dependence of the phase composition of the samples was investigated. In each system, compounds based on complex oxides with the general formula ABO_4 ($LaNbO_4$, $BiNbO_4$, $CaMoO_4$,

$CaWO_4$) are predominantly formed. In smaller quantities La_2MO_6, $La_2M_2O_9$, Bi_2MO_6, $Bi_{38}M_7O_{78}$ (M-Mo, W) and others were detected.

In the future, a selective synthesis of the detected phases and solid solutions based on them is planned to refine the areas of existence and study the electrochemical properties.

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P-14

Oxygen-conducting composites based on $Me_2(WO_4)_3$ (Me=Sm, Al)

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Composites $Sm_2(WO_4)_3$-WO_3, $Al_2(WO_4)_3$-WO_3 and $Al_2(WO_4)_3$-Al_2O_3 were obtained and composite effect was studied in this work.

Samarium and aluminum tungstates have different structures: $Sm_2(WO_4)_3$ has monoclinic 'defective scheelite' structure whereas $Al_2(WO_4)_3$ crystallizes in the $Sc_2(WO_4)_3$ structural type. Both of these tungstates are oxygen-ion conductors.

In order to increase the ion conductivity heterogeneous doping of these tungstates with WO_3 (a semiconductor of n-type) and Al_2O_3 was produced.

Electrical conductivity of $Sm_2(WO_4)_3$-WO_3, $Al_2(WO_4)_3$-WO_3 and $Al_2(WO_4)_3$-Al_2O_3 samples was measured by using impedance spectroscopy method. Concentration dependences of electrical conductivity are shown in Fig. 1.

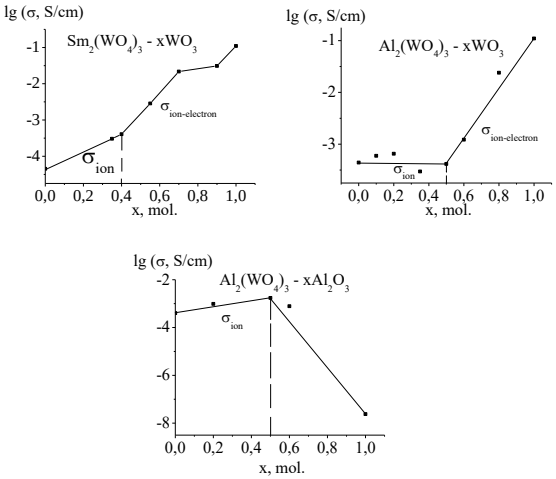

Figure 1. Concentration dependences of electrical conductivity of $Sm_2(WO_4)_3$-WO_3, $Al_2(WO_4)_3$-WO_3 and $Al_2(WO_4)_3$-Al_2O_3 samples at T=900°C.

As seen, a sharp increase in the electrical conductivity is observed in the $Sm_2(WO_4)_3$-WO_3 system with an increase in the concentration of the additive of tungsten oxide. This phenomenon can be explained by the fact that tungsten oxide has a lower surface energy, which leads to its spreading along the grain boundaries of samarium tungstate and formation of a statistically distributed composite.

There is no composite effect in the $Al_2(WO_4)_3$-WO_3 system: the introduction of up to 50 mol% of WO_3 does not lead to a change in the electrical conductivity.

This is probably due to the negative thermal expansion coefficient of $Al_2(WO_4)_3$. When WO_3 content is more then 50 mol. % the individual WO_3 grains crystallize; the composite conductivity increases, gradually approaching the conductivity of the WO_3 semiconductor.

A composite effect was observed in the $Al_2(WO_4)_3$-Al_2O_3 system: the introduction of 50 mol. % Al_2O_3 leads to increasing of O^{2-}conductivity by 0.6 orders of magnitude. When WO_3 content is more then > 50 mol. % the electrical conductivity decreases due to the formation of ensembles of low-conductivity Al_2O_3 grains, which gives a blocking effect. The obtained results are well interpreted in terms of the block-layer model.

Thus one may conclude that $Sm_2(WO_4)_3$ and $Al_2(WO_4)_3$ are the perspective matrixes for creation new oxygen conducting composite solid electrolytes.

P-15

Statistical Raman spectroscopy as a quality control tool for carbon coated electrode materials

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Lithium battery plays the crucial role in the emerging transportation and energy systems decarbonization. Global battery industry has shifted its focus from portable electronics towards electric vehicles and energy generation/grids, thus changing topical issues for battery research society. Ramping up battery production, battery manufacturing cost decreasing and lithium battery recycling raise the importance of the battery materials quality control and decrease the importance of specific capacity growth.

X-Ray diffraction (XRD) is still the main quality control tool for the material research community and Raman Spectroscopy has been always considering as an alternative tool for structural characterization. Unfortunately, while the Raman Spectroscopy (RS) is developing very fast, and, for example, Surface Enhanced Raman Spectroscopy (SERS) have already became popular tool for the detection of small amounts of different forms of matter, RS usage by battery research community still have plenty room to growth.

In this work, we present that so-called statistical RS can be successfully used for structural characterization of electrode materials, namely $Li_4Ti_5O_{12}$ (LTO) and $LiFePO_4$ (LFP), both pristine and composites with small fraction of conductive carbon additive (LTO/C and LFP/C). The idea of using statistical RS for quality control of electrode materials is not something new and we can mention the early paper of Panitz and Novak [1] for $LiCoO_2$. In this work, we propose to use more advanced both statistical and correlational analysis approach [2].

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P-16

Thermal annealing and single–domain preparation in tetragonal relaxor–PbTiO3 crystals for linear and non–linear optical applications

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Relaxor-$PbTiO_3$ ferroelectric single crystals have been widely used in the energy harvesting, industrial nondestructive evaluations, underwater acoustics, medical ultrasonics, electro-optic devices and so on [1,2]. Preparation of single–domain crystal as a critical process for applying in electro–optic and non–linear optical devices. However, the crystals always suffer from serious and inevitable cracking during the poling process because of giant strain generated by ferroelastic domain walls switching. Therefore, we have proposed a pre-poling thermal annealing process which can successful reduce the chance of cracking by releasing residual stress from crystal growth and the ferroelectric–paraelectric phase transition. The effects of the thermal annealing on strain behavior, dielectric properties and domain configuration have been studied. As a result, the annealed single crystal demonstrated lower and sharper strain peak at coercive field (Ec) compared to the unannealed one. The permittivity of the thinner sample has increased significantly up to the values for single a-domain crystal after annealing, while the permittivity of the thicker one has decreased down to the values of the single c-domain crystal. It indicates that polarization direction of annealed crystals can be associated with depolarization factor. After annealing, ferroelastic domain walls vanished almost completely which was verified by optical microscopy. As a result, crack-free single–domain relaxor-PT crystals were successfully prepared. Domain switching in single-domain crystal under an antiparallel electric field has been studied using the polarized light microscopy. During polarization reversal of c-domains under electrical field without mechanical stresses, 90° domain switching was observed to occur at certain positions, instead of uniform 180° domain switching. In addition, we have shown that the relaxor-PT single crystals have high transmittance of about 70% in visible and near infrared regions. The refractive indices were fitted by the sellmeier equations according to the data measured by an auto-collimation method. Moreover, the large values of 2nd order non-linear coefficients in relaxor-$PbTiO_3$ single crystals were obtained by estimation of the frequency doubling effect in powder, making them a promising candidates for applications in electro–optic and non–linear optical devices.

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Influence of charge compensation methods on ferroelectric domain formation upon focused ion beam irradiation in lithium niobate crystals

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The crystals of lithium niobate (LiNbO3, LN) family are used for wide range of applications such as energy harvesting, light frequency conversion, signal modulation due to its outstanding piezoelectric, nonlinear-optical and electro-optical properties. The charged particles beams (electron and ion) are utilized for studying and modification of various properties of such crystals. However, the surface charging limits the using of these techniques.

In this work, the methods of a surface charge control upon focused ion beam (i-beam) irradiation have been devised and its influence on ferroelectric domain formation by i-beam [1] has been studied in lithium niobate crystals.

The samples were represented by 0.5-mm-thick Z-cut LN wafers. Before irradiation the Z+ polar surface was carefully cleaned. The opposite Z- polar surface was covered by solid 100-nm-thick Cu electrode. The irradiations by electrons and Ga+ ions were performed by dual-beam workstation Auriga Crossbeam (Carl Zeiss) attached with i-beam lithography system Elphy Multibeam (Raith). The created domain structures were visualized at the polar surfaces by optical and scanning electron microscoies after selective chemical etching in pure HF and by confocal Raman microscopy in the bulk of crystal.

The method for charging control using simultaneous electron (e-beam) and i-beam irradiation has been developed [2]. It was shown that the efficiency of charging suppression can be adjusted by varying of e-beam current. The optimal ratio of the e- and i-beam currents have been obtained.

Charging control method based on simultaneous co-illumination with a deep-UV (275-310 nm) light-emitting diode (LED) has been developed [3]. It was demonstrated that UV LED co-illumination during i-beam irradiation leads to effective removal of surface charge and improvement of periodical 1D and 2D structures homogeneity (period, random displacement of elements). Moreover, the method efficiency can be adaptively controlled by the intensity of the UV LED. The charging suppression was attributed to photo-effect, namely to photo-ionization of electrons trapped at the sub-surface defects to the free vacuum state and, hence, the efficiency of method was depended on wavelength.

It has been found that UV irradiation leads to a change in the shape of isolated domains upon point irradiation and to a decrease in the domain depth. The UV LED co-illumination during 1D periodical poling resulted in uniform nucleation of domains within the irradiated area and an increase in the total switched area.

The equipment of the Ural Center for Shared Use “Modern nanotechnology” Ural Federal University was used. The research was made possible by the Russian Science Foundation (grant № 17-72-10152).

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P-18

Synthesis, crystal structure and properties of NdNi0.5Mn0.5O3-δ – a promising cathode material for IT-SOFCs

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The reduction of operating temperature of solid oxide fuel cells (SOFCs) down to the intermediate temperature range (600–800°) is one of the main challenges for materials scientists today, which facilitates the development of new materials with improved performance. The efficiency of standard SOFC cathode material based on $LaMnO_3$ can be noticeably enhanced when lanthanum is substituted by neodymium [1]. Moreover, B-site doping of $LaMnO_3$ with nickel was shown to improve its catalytic properties [2]. Therefore, the aim of this work was to synthesize the $NdNi_{0.5}Mn_{0.5}O_{3-\delta}$ complex oxide and determine its properties in the temperature range of 25–1000 °C in air.

Polycrystalline $NdNi_{0.5}Mn_{0.5}O_{3-\delta}$ was synthesized by decomposition of citrate-nitrate precursors. Prior to synthesis the amount of absorbed H_2O in Nd_2O_3 had been determined by TGA. The starting materials Nd_2O_3, $Mn(CH_3COO)_2{\times}4H_2O$ and $Ni(CH_3COO)_2$ were mixed in the appropriate molar ratio with an addition of nitric acid and crystalline citric acid monohydrate $C_6H_8O_7{\times}H_2O$. The resultant powder was calcined at 1100°C for 20 h and finally pressed and sintered at 1200°C for 15 h in air.

The phase composition and crystal structure of the prepared sample were determined by X-ray diffraction (XRD). The impurity of NiO was found to be <1%. XRD profile of $NdNi_{0.5}Mn_{0.5}O_{3-\delta}$ was refined using the Rietveld method. The studied sample showed monoclinic structure with P21/n space group at room temperature.

The high-temperature XRD (HTXRD) was performed in air within the temperature range of 30–1000°C using XRD-7000 Maxima instrument with installed HT-chamber HTK 1200N (Anton Paar). It was difficult to understand whether it crystalized as monoclinic (sp. gr. P21/n) or orthorhombic (sp. gr. Pbnm) in the studied temperature range. The refinement was performed separately using monoclinic, orthorhombic and two-phase model. The best refinement results were obtained for monoclinic unit cell (sp. gr. P21/n) at all studied temperatures.

The thermal expansion of $NdNi_{0.5}Mn_{0.5}O_{3-\delta}$ was investigated by HTXRD. The TEC value was equal to $9.82{\times}10^{-6}$ K^{-1} within the temperature range of 25-1000 °C. The calculated TEC value is slightly lower than that for Pr_2NiMnO_6, which was reported as a promising material for IT-SOFCs [3].

Temperature dependence of oxygen non-stoichiometry was determined by thermogravimetric analysis using Netzsch STA 409 PC instrument. The absolute values of oxygen content (3–δ) in the $NdNi_{0.5}Mn_{0.5}O_{3-\delta}$ sample were calculated

using the results of iodometric titration. The δ value was found to be 0.30±0.02 at room temperature.

Temperature dependence of electrical conductivity in $NdNi_{0.5}Mn_{0.5}O_{3-\delta}$ was measured by a DC 4-probe method over the temperature range of 30°C-1000°C in air. The studied sample behaved like a semiconductor in the whole temperature range studied. The maximum value of conductivity (≈15 S/cm) was obtained at 1000ºC, which is higher compared to that for Pr_2NiMnO_6 [3]. The Seebeck coefficient for $NdNi_{0.5}Mn_{0.5}O_{3-\delta}$ increased within the temperature intervals of 25-300°C and 600-1000°C possessing almost constant values in the intermediate range of 300-600°C. The minimum and maximum values of the Seebeck coefficient were equal to -85 μV/K and -32 μV/K at 150ºC and 1000ºC, respectively, indicating that electrons were predominant charge carriers in the studied oxide.

In this way, $NdNi_{0.5}Mn_{0.5}O_{3-\delta}$ can be considered as promising cathode material for IT-SOFCs. This material exhibits higher conductivity and slightly lower TEC value than that for Pr_2NiMnO_6 [3]; the latter is still comparable with that for well-known electrolytes like $La_{0.9}Sr_{0.1}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ (10.1×10^{-6}) in the temperature range of 600-800ºC.

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Method of improving performance of automobile gas engine

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Depletion of crude oil resources leads to the need for large-scale use of alternative raw materials. Natural gas is the most widely used of these alternative resources. Natural gas is considered to be relatively cheap and environmentally friendly motor fuel in comparison to oil fuels. This is due to the light fractional composition of natural gas that mainly contains methane and absence of polycyclic aromatic hydrocarbons and sulfur in its composition in comparison to liquid oil fuels. Currently in the United States and Western Europe there are some restrictions stipulating the maximum allowable engine mass emissions of the following toxic substances as: nitrogen oxides NOx, carbon monoxide CO, unburned hydrocarbons CHx, particulates. Separate toxicity and smoke checks of EG are used in different regions of the World. In Europe truck diesel engines with the payload of more than 3.5 tons (for buses with No of seats over 9) used to be checked based on steady running conditions corresponding to the 13-mode cycle of the ECE R49 (Fig. 1).

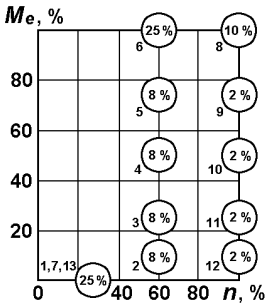

Figure 1. European Stationary 13-mode cycle (ECE R49 standards) used to assess the toxicity of exhaust gases of truck diesel engines in bench conditions. The circles indicate the share of the engine operation time in each mode, next to the mode number.

The most preferred alternative fuels cannot be identified clearly based on published characteristics of different diesel engines running on diesel and alternative fuels and based on the developed methods for assessing their environmental safety. This is because the assessment of the efficiency of using of these fuels in diesel engines should be checked in accordance with the toxicity of exhaust gases and the fuel efficiency. In this regard, it is necessary to carry out some researches of environmental parameters of natural gas fuel engines together with appropriate ways of improving these parameters. Such researches were made based on experimental data of gas fuel engine rebuilt from KAMAZ-type diesel engine. The ignition of natural gas in the combustion chambers is provided by spark plugs in this mono-fuel RGK.EC.820 type natural gas engine.

The engine integral performance of fuel efficiency and toxicity of exhaust gases during its operation in accordance with the 13-mode cycle ECE R49 (Fig. 1) are calculated based on the multi-parameter characteristics of this engine running on natural gas (for example, the characteristics on Fig. 2).

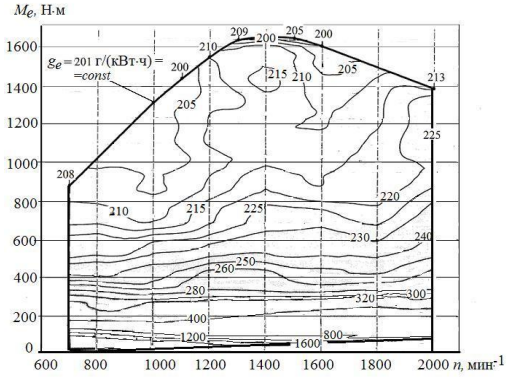

Figure 2. Universal (multi-parameter) characteristic of natural gas RGK-family KAMAZ engine by specific effective fuel consumption.

Multi-parameter characteristics of the RGK-family engine were converted using the following method. The fixed speed modes of the engine operation in the range from the nominal speed mode of nnom (n=2000 min^{-1}) to the minimum speed mode n=0,4 nnom (n=800 min^{-1}) were considered. For each of these high-speed modes, the load characteristics are drawn so that the dependence of its performance on engine load (its torque Me). Different load modes are shown: from full capacity (relative time equal Me max=1) mode to partial load mode (Me =0,3 Me max). All obtained characteristics of the engine are shown in Fig. 3.

Presented in Fig. 3 load characteristics confirm the effectiveness of the method of switching off a part of the cylinders at the modes with incomplete load to reduce fuel consumption and emissions of toxic components of the exhaust gases. According to these figures, we can note a significant trend in reducing the specific effective fuel consumption ge, specific mass emissions of carbon monoxide eCO, total unburned hydrocarbons eCHx and non-methane hydrocarbons enmcn together with increasing load. In particular, at the nominal speed of n=2000 min-1, the increase of the relative torque of the engine Me from 0.3 to 1.0 is accompanied by decrease of: the specific effective fuel consumption ge from 265 to 213 g/(kW·h), eCO – from 3.4 to 1.9 g/(kW·h), eCHx – from 6.6 to 3.0 g/(kW·h), enmcn – from 1.3 to 0.5 g/(kW·h). So if the load of the engine is reduced (with a decrease of Me), it is good practice to reduce the number of active (working) cylinders. Then the remained active cylinders work with full load (at Me=1) or close to it. As we see, the emissions of nitrogen oxides eNOx increase from 2.0 to 4.4 g/(kW·h) at n=2000 min^{-1} and changing of the relative torque of

the engine Me from 0.3 to 1.0 (Fig. 4). Therefore, by implementing of this cylinder switching-off method a simultaneous implementation of some NOx reducing methods should be involved. They are the follows: adjustment of ignition advance angle, installation of EGR, fitting of NOx neutralization systems.

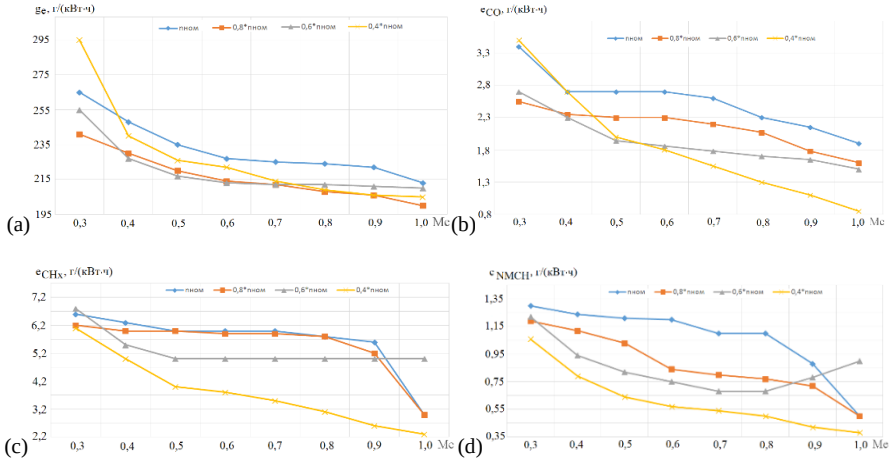

Figure 3. Dependence of the specific effective fuel consumption of ge (a), specific mass emission of carbon monoxide ECO(b), total unburned hydrocarbons e CHx (c), non-methane hydrocarbons enmcn (d) of the exhaust gases of RGK-family KAMAZ engine on its speed and different load modes.

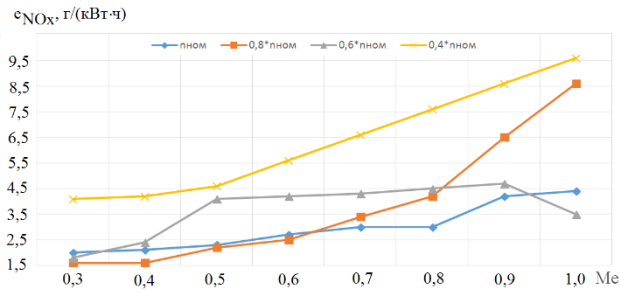

Figure 4. The dependence of the specific mass emission of nitrogen oxides eNOx with exhaust gases in terms of the speed and load modes of RGK-family KAMAZ engine.

The best performance of fuel efficiency and toxicity of exhaust gases of the investigated automobile gas engine is achieved at the external speed characteristic modes. In this regard, to achieve the best performance of the investigated automobile gas engine is advisable to ensure its operation at full load. This performance improvement in fuel efficiency and exhaust emissions of the studied vehicle gas engine can be achieved by switching-off some of its cylinders to let the remained cylinders at full load. Implementation of this method should be accompanied together with NOx reducing methods.

P-20

Project development of an underground nuclear power plant on the basis of the integrated ship reactor, KN-3

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In this study we focused on the development of device module along with the fabrication process in search of alternative energy sources. At present, the power supply of remote areas is carried out mainly through gasoline and diesel generators and this leads to high fuel costs and negative impact on the environment. In addition, when using only diesel and gasoline generators, it is not possible to optimize the schedule of their load in order to reduce fuel consumption. One of the solutions to the above problems can be the use of modular super low power (50-100 MW) integrated ship reactors.

The idea of underground placement of nuclear reactors is not new. Underground nuclear power plants have not become a rarity since the very beginning of nuclear power development. In the Soviet Union underground blocks of industrial reactors were built in Krasnoyarsk. A number of such power units were built in a land layout. The period of rapid growth in the number of such reactors was abruptly cut off after the accident at the TMI NPP in the USA and especially, after the Chernobyl catastrophe in the USSR. Many countries of the world there is a large number of territories that do not have connections with centralized electric networks. Energy supply of such areas is one of the most difficult tasks.

According to the opinion of Russian scientists, the construction of a 900 MW underground station is three times shorter than that of a similar nuclear power plant hence the construction requires much less capital investment. This is due to the peculiarities of the technological solution of their operation. FNPP is a series of energetically connected reactors-modules, which are produced entirely in the plant. Such factories exist in Russia, for example, in St. Petersburg, before they specialized in producing reactors for nuclear submarines. Some changes in the reactor, which are necessary for peaceful operation, are made quite easily. Reactor modules are delivered to the site of operation and simply drop below ground to a depth of about 70 meters. To operate the floating NPP, an area of less than 25 hectares is needed, which allows them to be installed almost anywhere. When the impact on the FNPP of 32 standard extreme factors was calculated, it turned out that 19 of them (58%) had no influence on the mode of its operation. Among them, hurricanes, tornadoes, earthquakes, explosions outside the station. The station withstand even of a direct hit of an atomic bomb with a capacity of up to 50 kilotons.

At present, nuclear power plants are used throughout the world as base capacities (varying during the day and depending on the time of the year,

electricity needs are provided by other types of power plants). The specificity of the operation of nuclear power plants lies in the fact that their production cycle is practically continuous and does not allow to regulate the amount of electricity that is supplied to the country's power system.

The design of the reactors allows reliability in sustainable energy consumption. The sluggishness of modern nuclear power plants does not allow reacting quickly to changes in energy consumption during peak hours. The downtimes of VVER stations are explained by the fuel reset, as well as by routine maintenance to check the reliability of the power units. In case of FNPP installed from several reactor modules, the need for shutdown is eliminated because one module is always in reserve. Recharging and testing of reactors are performed in turn, so that the required power can always be maintained. This allows the underground station with a capacity of 900 MW to produce in the year up to 6 billion kWh.

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P-21

Experiment on focal flux distribution of a solar concentrator by infrared and thermal measurement

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The concentrating performance of solar energy plays an important role in its application at high temperature. To evaluate the focal flux distribution of a solar concentrator, one kind of measurement system was established, in which an infrared camera and several thermocouples along with a heat flow meter were employed.

Under working conditions, the solar energy was usually higher than the emission energy of common objects such as the steel target. The thermocouples were exposed to the concentrated solar energy. The energy loss of thermocouples was through hemispheric radiation according to Planck's law. These thermocouples, at the same time received the local concentrated energy and finally reached thermal equilibrium. An energy formula was used to get the real focal flux value of the fixed position according to the complexly practical conditions. The flux density distribution can be then acquired by the real thermal parameters of the steel target and the infrared images.

A 60 kW High-times Concentrating Directional Transmission System (CDTS) was built, including primary heliostat and secondary dish concentrator. Several key factors were obtained through the experiment: i) the concentrated heat flux of central area, ii) the diameter of focal planes, and iii) the average temperature of focal spot. Compared with the traditional method, some errors were corrected. The experiment showed that the present technique was an effective approach to acquire more refined heat flux distribution on the focal planes of solar energy.

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P-22

Thermal stress analysis of solar thermochemical reactor using concentrated solar radiation

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Due to the increasing demand for clean energy, the application of solar energy has become an indispensable form of alternative energy use in modern society [1-2]. Nowadays, a solar-driven thermochemical reaction system using concentrated solar radiation for hydrogen and syngas (mainly H_2 and CO) production has been an effective alternative to traditional fossil fuels to solve energy problems and climate change, which has attracted tremendous interests worldwide [3-4]. In reaction process, the concentrated solar energy is transmitted into the reactor inner cavity through a transparent quartz glass window installed on the front surface of reactor, which provides the necessary energy for reaction process. However, the processes of cracking and reforming would not happen until the operating temperature reaches at least 1000 K [5]. During the experiment, we found a significant problem that the quartz glass window might break due to high heat flux. In the meanwhile, the Al_2O_3 ceramic insulation cavity also has the possibility of fragmentation as a result of thermal expansion. In view of the above problems, the thermal stress of solar thermochemical reactor using concentrated solar radiation will be investigated to find out the broken conditions and provide useful references for further study.

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P-23

Analysis of characteristics and feasibility of high pressure and low temperature water jet method exploit marine natural gas hydrate

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Marine natural gas hydrate (MNGH) account for 99% of the global hydrate resources, of which 90% are deposit in marine clayey silt sediments. Because of its enormous reserves, hydrate in clayey silt sediments has great economic benefits and development prospects. However, Current methods for MNGH exploitation are mainly used for hydrate in sand sediments, which have certain limitations and cannot meet commercial production requirements. Therefore, in order to meet the need of the hydrate in clayey silt sediments exploitation and improve efficiency of hydrate in sand sediments production, some scholars proposed the solid exploitation method. In 2016, Jilin university proposed the high pressure and low temperature water jet method, which is one kind of solid exploitation method. This paper analyze the characteristics of solid exploitation method based on the assessment of research progress in MNGH exploitation method, MNGH trials exploitation project, and project termination reason. Combining the characteristics of hydrate in clayey silt sediment, we design the high pressure and low temperature water jet experiment, and the critical velocity was determined by laboratory experiment. Results show that high pressure and low temperature water jet is feasible for hydrate exploitation, and the present study can provide reference for subsequent MNGH exploitation research and engineering applications.

P-24

Effect of hydrological parameters on gas production from hydrate-bearing sediments by depressurization

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The Shenhu area, the location of China's first pilot production, is located in the northern continental slope of the South China Sea, and also is considered as one of the most promising fields for gas hydrate exploitation. A 2D radially symmetric system is used in this article, and numerical simulations of SH2 site in Shenhu area evaluated the influence of bottom hole pressure and hydrological parameters such as irreducible fluid saturation and gas entry pressure on gas production potential from marine gas hydrate deposits. The results show that reducing the pressure of the production well will help to improve the gas production, and irreducible water saturation and irreducible gas saturation have significant effects on water and gas production, and the effect of irreducible gas saturation is more obvious. In addition, although the increase of gas entry pressure increase capillary pressure obviously, the effect on water production and gas production is negligible. In conclusion, hydrological parameters such as irreducible fluid saturation and gas entry pressure have an important effect on the exploitation of hydrate.

P-25

Guest-exchange behaviors of different hydrocarbons with CO_2 + N_2 occurring in sII mixed hydrates

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Natural gas hydrates have recently received considerable attention as a promising future energy source because of the large amounts of massive hydrate reservoirs. The CO_2 replacement method has recently emerged as a promising method of recovering hydrocarbons without hydrate dissociation and sequestering CO_2 into natural gas hydrate reservoirs, simultaneously. Considering that multiple guests engaged into small and large cages of sII natural gas hydrates, the replacement occurring in sII hydrates may follow a unique pattern. The replacement of CH_4 + C_2H_6 + C_3H_8 mixed hydrates by use of CO_2 and CO_2 + N_2 are studied under different pressure of replacement gas in this work. The guest-exchange behaviors of different hydrocarbons with CO_2 + N_2 were examined though the composition analysis of the hydrate and vapor phases during replacement, primarily focusing on the possible replacement mechanisms and the evolution of preferential exchange behaviors during replacement. In order to examine the difference in exchange behaviors of different layers within the replaced hydrate particles, the heterogeneous composition of the final replaced hydrates caused by solid state diffusion during replacement was indirect measured using replaced hydrate decomposition method. Furthermore, the replacement efficiencies of different hydrocarbons were calculated based on the final compositions of the replaced hydrates to identify the relationship between the extent of replacement and the replacement mechanisms. The present study will help in figuring out the precise mechanism of guest exchange in sII gas hydrates and selecting the favorable condition for enhancing replacement efficiency in field production tests.

P-26

Reliable power supply with the use of microgeneration on the basis of alternative and renewable in arctic conditions

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The cold climate of the Arctic has always a priori created the illusion of the impossibility of using solar energy for a number of reasons: a long polar night, a low angle of inclination of the Sun to the horizon, the traditional hope for Northern delivery to provide organic fuel diesel generators in the vast expanses of the polar region and Siberia [1]. For example, 95% of the energy of Kamchatka works on imported fuel. The responsibility for the delivery of goods via the Northern delivery is vested in the Executive bodies of the constituent entities of the Russian Federation who make applications, enter into contracts and Finance the importation of own-account and provide them with the borrowed funds.

In recent years, both in Russia and in the world, the understanding of the need to develop the Arctic zone is growing due to the discovery of new oil and gas fields, as well as the release of ice from coastal areas and their potential use for year-round navigation [2]. There was a need for a thorough analysis of the solar and wind potential of the polar and Arctic zones [3]. The study of the available insolation data showed that the Northern latitudes have significant energy potential when using solar photovoltaic power plants. For Fig. 1 the duration of the solstice at latitudes from 400 to 900 p.s. is presented [4].

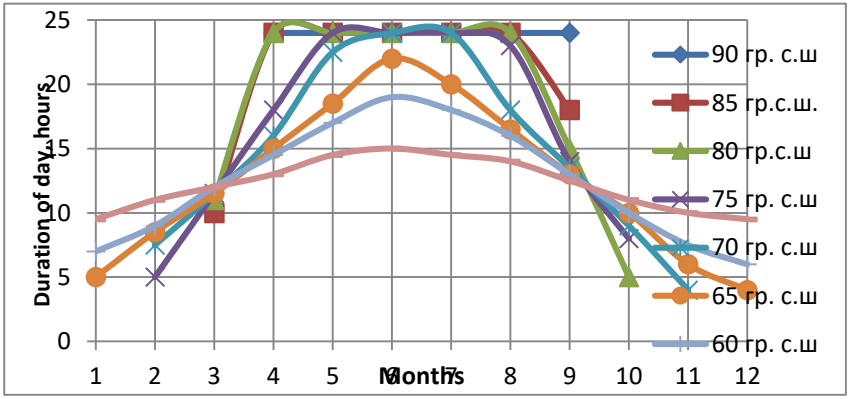

Figure 1. Duration of sun exposure in the Arctic region.

It is necessary to understand that one way or another, the existence in the Arctic region implies the provision of heating on the object stay of people. In this case use of the complex system [5] consisting of FEP (round – the-clock in the summer period), VEU (year-round, stochastic stipulated period), TEG (thermoelectric generator) - year-round from a heat source and DG (diesel

generator), as a reserve risk-free energy source is required. Severity of climatic conditions of the region can be integrally described by indicator of GSOP (degree-days of the heating period) and is presented [6].

One of the options for generating electricity from waste heat is the use of a thermoelectric generator [7]. On the heated objects located in the Arctic region, a thermoelectric generator can be used for this purpose, the scheme of which is shown in Fig. 2. As a real installation, the thermoelectric furnace Indigirka and its main elements are presented in [8]. Low electric efficiency of thermoelectric furnace is caused by extremely low usage of heating surface by thermoelements, which can be taken into account in further developments. At the same time, to meet the minimum requirements (lighting, communication, charging microsecondary generators) this option can be used effectively.

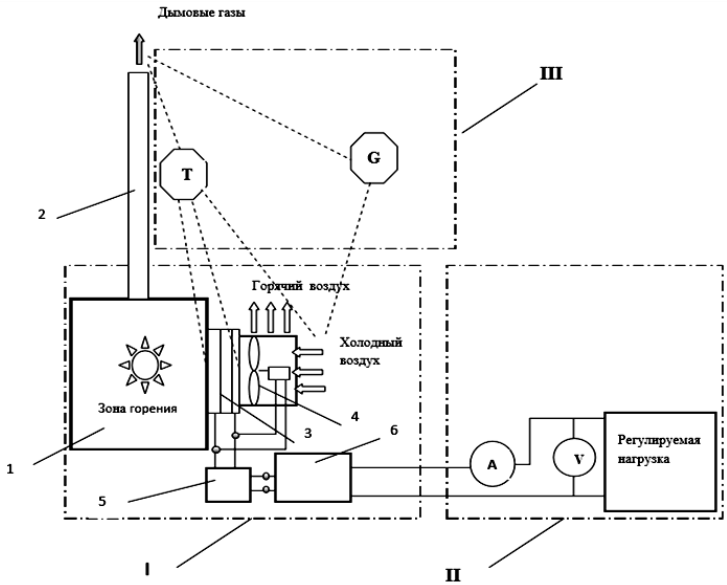

Figure 2. Scheme of using the furnace for power generation. I – a thermoelectric furnace, a II – unit of measurement of electrical characteristics, III-thermal hydrodynamic characteristics measuring unit; 1-furnace, 2-chimney, 3-thermoelectric generator, 4-TEG cooling fan, 5-charge controller, 6-accumulator battery.

It follows from the graph that the total electricity production for an Autonomous facility at the expense of solar energy (on a polar day) and a thermoelectric generator (on a polar night) exceeds the social limit, i.e. the minimum required level of energy supply to the consumer.

The amount of thermal energy required for full-fledged functioning in the Northern climatic conditions in the winter period is large enough and allows to raise the question of the creation of cogeneration thermoelectric plants that

generate electric energy on the heating load. In the summer, the arrival of solar energy in most regions of the country is sufficient to use modern photoelectric converters. For realization of possibilities of thermoelectric power supply of Autonomous consumer development of the specialized furnace systems providing during all period of burning of fuel constant level of temperature of TEG and the maximum receipt to them of the thermal energy released at burning of fuel is necessary.

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P-27

On improving the energy efficiency of buildings in severe climatic conditions through the use of renewable energy sources

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A mathematical model was developed and optimization algorithms of building energy consumption for districts without connection to energy and gas supply systems were created. The model takes into account the features of weather conditions typical for strongly continental climate with high seasonal and daily temperature differences and extremely low temperatures during winter.

The model of co-use of energy supply system based on renewable energy sources (wind turbines, solar collecting panels, photoelectric converters and heat pump) with cogeneration diesel-generator source of electricity and heat was developed based on the performed calculations and optimization.

The calculation data was taken as a basis of the project of energy-efficient cottage which was built in the Sverdlovsk region, settlement “Rastushchij”. In 2009 the project was granted the V. I. Vernadsky National Environmental Award.

The purpose to build an energy-efficient building is inspired by a desire to create a healthy living environment against the insufficiency and increase in the cost of energy resources (countries of European Community) or their considerable expenses in severe weather conditions (Russian Federation) which also leads to rising of building maintenance costs. One of the global trends aimed to reduce expenses for energy power supply is to provide a considerable proportion of buildings supply by means of renewable energy sources. However not only conservative skepticism but also an unwarranted optimism of potential consumers of energy sources prevent the widespread implementation of renewable energy in severe weather conditions typical for many regions of the Russian Federation.

In this work an independent cottage with no connection to the central electric power and gas supply systems is considered, total floor area is 200 square meters, located at the Ural climatic zone. Building heat insulation and cold and hot water consumption rates correspond to the accepted construction and community regulations for energy-efficient buildings in Russia [3, 4].

In year cycle is simulated an energy supply of the building with optimization of the structure of systems on minimization criterion of organic fuel consumption for closing DPS [6].

The comparison between received optimal structures and traditional methods of building energy supply by steam generating units (heat supply) and DPS (energy supply) is made. Efficiency of energy circuit with renewable energy sources depends on numbers of various factors: value of calculated electrical and thermal loads; climatic factors; units and types of equipment. Public-utility requirements of energy have an integrated nature and are the combination of

household requirements of electric energy, heat energy necessary for hot water supply (HWS) and heating. The heating load depends on climatic factors and thermotechnical parameters of a building. Final optimum choice is based on the determination of integral economic impact presented.

The mathematical model for calculation of efficiency indices and reliability of the system under investigation is based on the daily calculation of load value, temperature curves of external air, wind speed and energy of solar radiation with the following determination of basic power equipment capacity and parameters of system conditions (charge level of energy storages). Integral annual rates of energy production are determined by combining results of daily indices.

The methodology for reasoning of local systems of heat and energy supply with integrated use of renewable and traditional energy sources is developed. In contrast to the known methodologies, the developed methodology gives the possibility to optimize the projects based on the combination of RES and traditional electric power installations for the integrated energy supply of local objects. The implemented as software code methodology makes it possible to analyze the alternatives optionally of the most practical equipment units for the local systems of integrated energy supply according to efficiency and reliability. The researches of system of energy supply of public-utility consumers, based on the methodology mentioned above and for required conditions, showed the possibility to considerably reduce the annual fuel consumption using RES for the Russian climatic conditions.

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Development of the heat supplying project for UrFU educational laboratory campus with the use of solar collectors

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The project of heat supply of the educational and laboratory building through the integrated use of renewable and non-traditional energy sources is considered. To implement this project, a number of studies were carried out, such as thermal imaging building monitoring. As a research task, the authors determined an attempt to evaluate the heat loses reducing possibility as well as the implementation of this event in the Ural region.

The UrFU educational laboratory campus was chosen as the subject of studying where is planned to implement heating and hot water supply system through the integrated use of renewable and unconventional energy sources (solar collectors and heat pump). The use of solar heat supply is planned in the spring-autumn period. This combined system is necessary, since the heat pump cools the groundwater in the process of constant operation.

Tasks of the project are: 1) To carry out research of using solar energy possibility to meet the energy needs of the educational and laboratory building in the Ural region conditions; 2) To carry out thermal imaging monitoring in order to identify the main sources of heat losses in the building and make a decision how to eliminate them; 3) To provide thermal protection of the building's enclosing structures not worst than the required SP 50.13330.2012 [1] during the entire lifetime of the building; 4) To develop a solar heat supply scheme of this research object as part of a combined system.

The shooting took place on January 25, 2018 at night, outside the room, and in daylight - inside in a sunny day. That is why the sunlight on the wall of the building gives a small error during the television survey. The survey carried out in the absence of precipitation, with slight gusts of wind up to 6 m/s, the wind was from southeast, with air temperature about 19 °C and relative humidity of 64%. The average temperature on the five floors of the building was 25 °C, also the temperature of the last floor of the building is 13 °C. The surface of the walls was thermographed perpendicular to the wall, or deviating from this direction to the left, to the right, up and down, not exceeding 30°.

In installation (Fig. 1) the heat carrier is cooled, thereby heating the water going on hot water supply. The heat carrier, cooled in the storage tank, is sent back to the solar collector. The minimum temperature of the heat carrier at the input of the solar collector (in autumn and spring) is 5-70℃, at the output is 25-85℃ depending on the season and insolation [2].

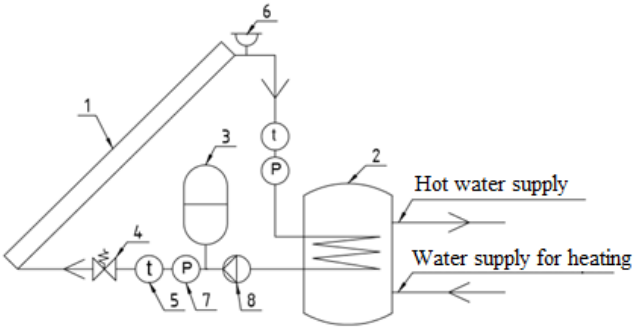

Figure 1. Solar plant scheme: 1 - flat solar collector; 2 - accumulator tank; 3 - expansion tank; 4 - safety relief valve; 5 - thermometer; 6 - automatic air valve; 7 - manometer; 8 - circulating pump.

It should be emphasized that in the conditions of the Ural region with sharply continental climate it is difficult to carry out heat supply of this building only with use of solar power throughout the year. Therefore, such a scheme of heat supply should be combined with an unconventional energy source – a heat pump. In this project, the load cover with the help of solar collectors in the summer will contribute to the regeneration of the warmth of groundwater in the well, because in the process of operation, the potential heat of the groundwater is constantly decreasing and you need to renew the resource.

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P-29

Optical fibers based on modified silver halide crystals for nuclear power

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In Russia, the generation of electricity using nuclear power plants is steadily growing. Various chemical reactions taking place in radioactive waste tank cubicles, hot cells, special force main sewage and other high radiation environments should be monitored using FTIR spectroscopy. Due to this method, one can evaluate media composition qualitatively and quantitatively, and observe kinetics of various processes. However, there is a technical problem of employment of online FTIR spectroscopy under conditions of increased ionizing radiation. Nowadays, FTIR spectrometers are placed directly in high radiation environments. This leads to breaking the electronics of the spectrometers after approximately half a year of such use, and they have to be replaced with new ones. To avoid this, one can use ionizing radiation resistant optical fibers able to transmit data from a spectrometer, placed in lower radiation environment to a high radiation zone and vice versa.

At present, two-layer IR fibers made by extrusion from AgCl-AgBr crystals are well-known. They are transparent from 2.5 to 18.0 μm, and used as probes for IR Fourier Transform spectrometers of various companies, such as Mettler Toledo, Art Photonics, Bruker, and others [1]. Nevertheless, silver halide fibers are photosensitive, especially to ultraviolet and ionizing radiation. One of the possible solutions to this problem is the use of a two-layer crystalline IR fiber fabricating by extrusion technique. The fiber comprises a core and a cladding made of silver bromide crystals containing different percentage of $TlBr_{0.46}I_{0.54}$ solid solution; the core diameter is 900 ± 10 μm, the total fiber diameter is 1100 ± 15 μm. These fibers are transparent in the spectral range of 4.0 - 26.0 μm, photo- and radiation-resistant, and the prolonged exposure to ultraviolet or ionizing radiation (β and γ) does not cause a translucence effect in the fibers [2]. The use of the fibers (jointly with a FTIR spectrometer) allows controlling the composition of reaction products and the kinetics of the processes occurring at isolated nuclear facilities.

Thus, two-layer crystalline IR fibers made of AgBr-$TlBr_{0.46}I_{0.54}$ crystals, transparent in the spectral range of 4-26 μm and compatible with FTIR spectrometers, may be used in high radiation environments. Firstly, they allow to determine chemical composition of various substances (including D_2O) in real-time with a detection limit of 10^{-3}-10^{-4} mol/l, under conditions of high ionizing radiation with a dose of up to 1500 kGy. Secondly, the core diameter of these fibers is 900 ± 10 μm; that simplifies their connecting with a FTIR spectrometer.

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P-30

Improvements of biogas production monitoring during methanogenesis by using computer vision system

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The article presents results and approbation of distance continuous estimation methodology for biogas production during methanogenesis. The biogas production level was monitored by fully independent and automated video-based monitoring system. The results show much lower errors of gas monitoring evaluation than permissible error obtained by manual data registration. Thus, the system improves accuracy of reaction rate changes determination which allows to evaluate changes in general patterns and detect even minor deviations during methanogenesis for long-time period (up-to 2 months). Presented solution is non-contact and cheap, it allows to digitize pointer indication of analog measuring systems and include them in intellectual factory networks.

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Designing a wind farm using simulation software PSCAD

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Interest in alternative energy is growing every year all over the world, in particular, in wind energy, as a renewable energy source. Wind power farms have as advantages and as disadvantages, which certainly should be considered in the design and construction.

The main problem of wind power farms is the unstable nature of the wind. Therefore, the power capacity of wind plants at each moment of time is variable. Consequently, it is impossible to obtain a stable amount of electricity to ensure an uninterrupted electricity supply to the consumer.

Energy storage systems (e.g. industrial batteries) are actively used as a solution to this problem. One more solution is connecting wind generators to electric networks and systems that have sources of energy of other types, such as gas-turbine arrangements and solar power plants. Or if it's possible, it can be connected to distribution networks of a unified system of traditional energy.

However, this way has some nuances too. For example, the problems of synchronization with external networks by voltage and frequency levels, the need to introduce smart energy metering systems, solving stability issues of distributed generation systems.

The correct choice of types and operating parameters of electrical apparatus is a very important issue for the stable functioning of electric power systems and power supply systems.

This paper shows one of the ways to simulate and design the wind generation farms. It includes the measurement of parameters for the calculation and subsequent choosing of electric apparatus, simulation, analysis and optimization of different operating modes of the power plant being developed. The project was developed using the PSCAD software package for simulating electric power systems.

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Energy-efficient lighting with the help of mechanical power accumulators

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The purpose of the research to study the possibility of conversing the mechanical power derived from doors opening/closing to electrical power. The object of our research is the system of interaction between a person and a device within the university premises. The subject being analyzed is the process of opening and closing the doors from the point of view of energy generation.

Before we started our research, we have set the following tasks: 1) to observe the process of doors opening/closing; determine its duration and recurrence; 2) to design a device, which will converse the mechanical (oscillating) motions power to electrical power; 3) to develop the scheme of mechanical power conversion to electrical power; 4) to calculate the amount of generated electrical power with the help of the designed device and examine the possibility of this power use for after-hours lighting of lyceum premises; 5) to analyze cost-effectiveness and ecological expediency of this device use.

We suggest the following hypothesis: recurrent door motions during its opening/closing can be transformed into electrical signals, [1] and their accumulated power can be sufficient for providing after-hours lighting of premises at night. Scientific novelty of this research consists in employing the recurrent door motions during its opening/closing as a source of alternative and environmentally safe energy. Practical relevance of our study consists in the possibility of using the derived electrical signals, which were accumulated in the form of energy, for powering the energy receivers of low capacity (for example, for after-hours.

Analysis of related professional and scientific literature, video recording and mathematical processing of the obtained results, building the model of the device which converse the motion energy to electrical signals.

According to our estimations, 100 LED lamps with current consumption of 2 A can work for 12 hours taking the power from the storage battery with capacity of 24 Ah (in this case it necessary to avoid full battery discharge). This is quite enough for lighting the university corridor at night. [2] The payback period of the 12-generator set will be around 5 months.

The process of doors opening/closing can be a potential energy source and is accompanied by recurrent motions, which can be transformed into electrical signals. Conversion of mechanical kinetic energy to electrical power is performed with the help of electrical power generator installed into the door profile. The calculated amount of electrical power, which was generated by the designed device, proves the device usefulness and efficiency. Use of LED lamps for after-hours university lighting allows significant energy saving. The designed device is

environmentally safe, because energy saving contributes to decreasing the greenhouse gas emissions. [3]

Based on the conclusions above, we drew the practical recommendations. We observed the device operation on only one object (one door in the university). Taking into consideration the total number of doors, it is possible to estimate the prospective of using such devices in other universities from the point of view of implementing the energy saving technologies in social sphere. Similar energy, ecological and economic effect can be obtained at other popular places where lots of people pass (supermarkets, cinemas, cafés, etc.). The implementation of such devices in these places will allow significant energy saving in the city, our region and the whole country.

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P-33

Investigations of dynamic models of the wind turbine based on a magnetic gearbox with a magnetic continuously variable transmission

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Nowadays, wind power engineering is one of the most dynamically developing branches of alternative energy in the world. Note that the modern development of wind power is carried out in two independent directions. On the one hand, it is scaling to increase the unit capacity to the detriment of energy efficiency. On the other hand, it is the improvement of energy efficiency and mass and dimensions parameters. However, as investigations of the wind turbines show, an improvement in energy efficiency with a possible increase in energy conservation facilities [1]. It should also be noted that the expanded overall dimensions of wind power plants guarantee a small speed of rotation of the turbine. The electric generator and its transmission are the heart of the wind power system. There are two basic concepts for constructing wind turbines [1]. The first is a classical reducer system based on an asynchronous double-supply machine or a synchronous machine with permanent magnets. The second is the direct drive concept of a synchronous multipolar machine with permanent magnets. The advantages of the reduction gear concept include comparative cheapness, shortcomings - significant losses of mechanical energy in the generator and in the transmission. The main advantage of the gearbox system is relative cheapness, as for the disadvantages; there are considerable losses of mechanical energy in a generator and a gearbox. Moreover, field experience of mechanical gearboxes showed high wear at overloading and shock impacts' damages caused by a wind turbine. Frequent wear and failures of mechanical gearboxes result in considerable maintenance costs. It should be emphasized, that the presence of lubricants inside the mechanical gearbox is one of the main causes of ignition of a wind turbine nacelle. Advantages of the concept of direct drive include high energy efficiency and the absence of a reducer with oil-containing substances. Unfortunately, large dimensions and mass make this arrangement expensive [2]. The purpose of this study is to assess the voltage quality at the faked direct drive outputs and compare it to a generator without an integrated magnetic gearbox. This study reflects an analysis of the output characteristics of the faked direct drive, which is based on combining in one machine a magnetic reducer and a synchronous generator on permanent magnets. Studies carried out by a number of foreign teams claim that dynamic performance may be improved compared to direct drive [2]. The physical principle of the operation of the magnetic reducer is described in studies [2-3]. The effect of magnetic reduction is based on the principle of magnetic field modulation produced by the high-speed rotor with permanent magnets and ferromagnetic segments of the low-speed rotor with harmonics generation, which are divisible by the number of pole pairs of permanent magnets at the outer stator

that provides conditions for torque transformation. The specified ratio of the number of pole pairs of permanent magnets of the high-speed rotor and the number of ferromagnetic segments of the low-speed rotor determines the gear ratio. The development of a faked direct drive is the possibility of using an electromagnetic variable speed ration to provide electromechanical compatibility in parallel operation with an autonomous electric power system of wind turbines based on synchronous generators with permanent magnets.

In the study, the results of a comparative analysis of the voltage quality in the steady state of the ideology of a faked direct drive and a classical generator were presented. Dynamic models of the faked direct drive, and an electromagnetic variable speed ration, that based on it, are also presented for the purpose of replacing the mechanical gearbox in the layout of the wind turbine. The results of transient processes are shown at a sudden load shedding and in case of a short circuit in an autonomous electric power system where implementation of such systems is proposed.

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Band-like Investigation of CO_2 geologic sequestration and the density-driven convection process

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In this work we outline the process and a brief review of CO2 geologic sequestration, accompanied with some study results of the density-driven convection, which is a significant phenomenon in the CO2 geologic sequestration process. At first, a simple introduction of the steps of CO2 geologic sequestration is provided. Then, some CO2 geologic sequestration projects are listed and the comments are discussed. At last, some results of our research work are introduced on density-driven convection. Specifically, the density-driven convection flow in porous media is numerically investigated with a stream-function-vorticity system, combining with high accuracy pseudo-spectral method and sixth order compact finite difference. Some significate results are presented and discussed.

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Development of a system for monitoring the effectiveness of renewable energy installations in harsh climate conditions

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While solving the renewable energy tasks, problems with the calculation of some statistical changes, important for the development of their structure and practical application may arise. The following factors are stochastic:

- Energy reception (solar, wind, water resources, etc.)
- Energy consumption (domestic, municipal and industrial areas)
- Changes in ambient temperature.

These factors have a wide range of time changes, periodic and random components.

It is obvious that these groups of causes are correlated, the growth of the solar energy reception leads to the increase in temperature and illumination, which in turn reduces the need for heat and electricity consumption.

In order to fulfill the detailed analysis of the connection between climatic factors, their influence on the efficiency of the existing renewable energy equipment in the UrFU, a high-speed multi-channel monitoring system for climate and energy characteristic has been developed and put into operation. The system includes a distributed network of local devices connected to the central server that collects, accumulates and processes data of more than 100 measured parameters gathered every second.

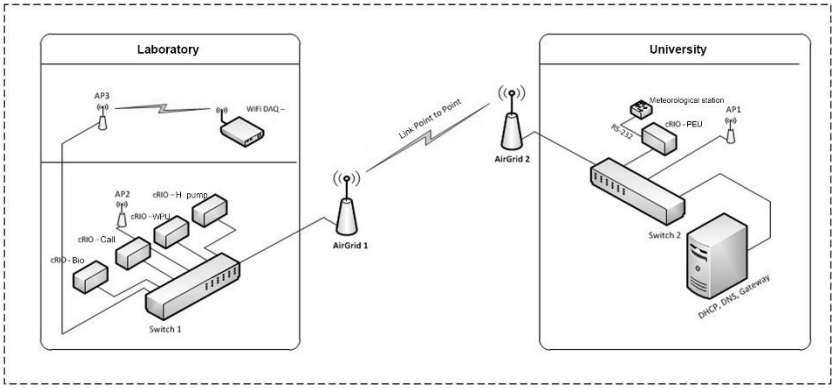

Figure 1. Stands location on the UrFU territory.

Based on the long series of observations, the system allowed an assessment of renewable energy productivity in the conditions of variable ambient temperatures, typical for the region with extreme continental climate.

The system provides the constant collection of the information from more than primary transducers and 6 fast-acting video cameras that control the parameters and images of wind power, photoelectric, biogas, and other renewable energy research stands on the territory of the UrFU (Figure 1); it collects and transmits the information via Wi-Fi channels to the server and periphery users' workstations for the following analysis and processing. To provide fast monitoring of the units' characteristics special processing software was created in LabVIEW.

The system allows to solve the following tasks: 1) the multi-channel, multi-parameter, high-speed, distributed in space computer monitoring system for energy reception from different renewable sources was developed and put into operation; 2) experimental studies of the solar energy reception, ambient air temperature, heat and electricity consumption during long-term, monthly and daily cycles.

The experimental results indicate the possibility of power supply, in climatic zones with an extreme continental climate, without the traditional energy sources usage during summer.

The principal importance of the small discretization periods and sufficient sample volume usage for the acquisition of probabilistic estimates of studied statistical parameters was shown.

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P-36

The best available technologies as a carbon regulatory system in Russian Federation

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The requirements for carbon intensity are contained in the legislation of many countries. There are international standards of estimating emissions as well as national standards, including Russian state standards. More and more companies in the world are beginning to report direct emissions of greenhouse gases as well as disclose data on the carbon footprint of their products throughout the supply chain - from raw material extraction to the disposal of the product at the end of its life cycle. [1] The company's commitments to reduce greenhouse gas emissions is caused both economic advantages and by the desire to provide objective information to ensure reputation in the eyes of investors and consumers, noting the stability and competitiveness in the market.

The issues of climate change are relevant nowadays. The task of this study is study the system of carbon regulation, designed to stimulate business and cooperation with it, and current system of applying the best available technologies, which involves the exemption of enterprises, which use similar technologies, from pollution charges.

An important task of this study is to identify the compliance of existing legislative and regulatory practices with regard standardization of permissible impact on the environment. And also, to make changes in the legislation for the implementation of the provisions of carbon regulation in Russian Federation.

Application the administrative methods of influence. The technology standard is used in the format of the best available technologies, when the regulator forms reference books the best available technologies in different industries, and these technologies are gradually becoming mandatory for using by all companies. [2]

Standards of efficiency. A single technology is not set as mandatory, any technology can be used, but these technologies must meet the requirements that are set within the standard of efficiency. [3] The upper limit of emissions - a certain limit of greenhouse gas emissions is set for each company and this company should not exceed it.

Requirements for developing standards for permissible emissions / discharges of substances and microorganisms into the environment, standards for permissible physical impacts on the environment, standards of waste generation and consumption, which must ensure environmental quality standards. [4]

There are four categories of objects that have a negative impact on the environment. For each category, a set of government regulation measures is established, including mandatory accounting of emissions, as well as planning actions to improve the situation, including by introducing the best available

technologies, which provide reducing emissions and pollutions. It was decided to economically stimulate the introduction of the best available technology by business entities.

There are all basic prerequisites for the introduction the system of rationing based on the best available technologies in Russia. It is necessary to eliminate the contradictions between the provisions of the current legislation and the practice of regulation in rationing of the permissible environmental impact. The inclusion of renewable energy technologies in the list of the best available technologies for the implementation Federal Law No 219-FL can be one of the effective steps to stimulate the renewable energy development in Russia in real, economically justified and efficient projects.

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