DESCRIPTION FOR THE GENERAL PUBLIC (IN ENGLISH)

In the era of growing demand for energy, which causes an increase of fuel and energy prices, finding of new sources of energy, including the recovery of waste heat, is of great importance. Our civilization produces huge quantities of wasted heat, *e.g.* using combustion engines, in which only about 2/3 of the energy is converted into useful kinetic energy, and the rest is mostly dissipated as a heat. One of the potential technologies that could allow the recovery of such wasted energy and convert it into useful electrical energy are thermoelectric generators TEG. They utilize thermoelectric phenomena exhibited particularly strong in a group of semiconductor compounds, which allow direct conversion between thermal energy and electricity. Thanks to the simplicity and maintenance-free construction of TEG they are used primarily in mobile and miniature cooling devices and thermoelectric generators operating in extreme conditions, such as space. Limitation to an extensive use of TEG is their efficiency, directly related to the effectiveness of the thermoelectric materials, reaching nowadays about 5%. However, in the last fifteen years new materials with much improved properties have been developed, which use allows for theoretical increase of the TEG efficiency up to 18%. One of the main obstacles to the construction of such a device is to provide protection against oxidation and degradation of thermoelectric materials operating at high temperatures, which are necessary to obtain high efficiency of the generator. Therefore, the objective of the proposal is to develop a comprehensive method for increasing the chemical stability of selected modern thermoelectric materials. The comprehensiveness of the proposed solutions applies to both, methods of protection, which include the development of coatings protecting against oxidation and simultaneous appropriate modification of thermoelectric material, and specific approach to the problem combining advanced quantum methods for numerical modeling of materials using high performance supercomputers with sophisticated experimental methods for creating theoretical models and their verification.

The thermoelectric materials selected for this study are based on relatively new but well known and simultaneously showing excellent thermoelectric properties $CoSb_3$ and Mg_2Si, materials and on Cu_2S – a compound which recently gained huge attention for its exceptional thermoelectric properties. All of these compounds undergoes oxidation in the air at the TEG operating temperatures.

As the protective layer a use of the so-called black glasses is planned. These are modern amorphous materials obtained by sol-gel process resulting from hydrolysis of the appropriately selected organosilicon compounds. Because of presence of the Si-C bonds in their structure, they possess very good mechanical and chemical properties. Our preliminary studies have shown that application of such coatings is possible for thermoelectric materials including the selected ones. It is also planned to produce layers compatible chemically and physically with the selected thermoelectric materials ensuring creation of a stable passivation coating on their surface. The durability of coatings and protective efficacy will be evaluated by characterization of the structure and properties of the thermoelectric materials before and after prolonged annealing in air.

A wide range of advanced methods will be used in the synthesis and characterization of the prepared materials and coatings. The extensive experience of our team in the field of thermoelectric materials, amorphous coatings and in the research on high temperature corrosion will, in addition to receiving the assumed materials and layers, allow to analyze the obtained results and create appropriate structural models of the studied materials and simulated phenomena for simultaneous computer simulations. The results of these calculations will be repetitively used in the modification of materials (selection of the amount of dopant) and coatings which will significantly speed up and reduce the cost of developing effective ways to improve the durability of the thermoelectric materials.

These studies will allow a significant development in the fields of materials research such as thermoelectric materials and glassy coatings, understanding the mechanisms that affect the chemical stability of thermoelectric materials and a better explanation of the processes of their high temperature oxidation. Finding effective ways to protect high-performance thermoelectric materials against corrosion will also enable the creation of thermoelectric generators with higher efficiency and their practical application leading to the reduction of global energy consumption.