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Application of 3D modeling, micro and nano computed tomography and machine learning to optimization an energy-saving and ecological method of producing and improvement of properties of materials for energy conversion

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In the forthcoming era of sustainable development, industry will need to switch to eco-friendly, highly energy-saving, and low-waste new technologies. Recently, within the frame of search for efficient thermoelectric materials used for waste heat recovery, some promising compositions have been identified among semiconducting silicides, selenides or antimonides, which could be produced by the so-called *Self-propagating High-temperature Synthesis* (SHS). Materials belonging to this group can find application in the construction of thermoelectric coolers or thermoelectric generators which convert waste heat into electrical energy. Moreover, some of them have properties which make them useful in other areas, such as coolers of microprocessors or sensors in microelectronic devices, light absorbers for ultrathin solar cells, light emitters in photothermal therapy of cancerous tissues, hydrogen storage systems or electrodes in electrochemical cells. In contrast to traditional manufacturing, which is generally time and energy consuming, SHS has several advantages. It is very quick, like flame propagation after ignition of combustible materials. Once initiated by spark or resistance heater, the reaction goes by itself without any external source of heat. It produces no wastes and overall can be classified as green technology. Moreover, in SHS, impurities are continually removed from the reaction front, which improves quality of the obtained material. However, in spite of many advantages of SHS, there are still open questions and problems to be solved, in particular troublesome upscaling, difficulties in securing adiabatic conditions or sufficient propagation velocity and attainment of complete conversion of reactants in the entire volume of compressed powders.

In this project we will focus on comprehensive description and optimization of thermoelectric materials manufacturing by SHS. We are convinced that in order to find the most economically efficient fabrication conditions, a three-dimensional (3D) physicochemical model must be used, which takes into account energy transfer (in the form of heat, radiation and convection), reaction kinetics, microstructure of reactants mixture, and fluid dynamics in the reaction chamber. The 3D model will be used to optimize the SHS parameters by means of standard optimization methods and artificial neuron networks.

The expected outcome of the project is an improvement of the SHS process design so as to overcome possible limitations, e.g. troublesome upscaling. This may open a new way of ultra-fast, low-cost, large-scale production of TE materials and provide new insights into combustion process, with a possibility of broadening the range of materials that can be successfully synthesized by this technique.

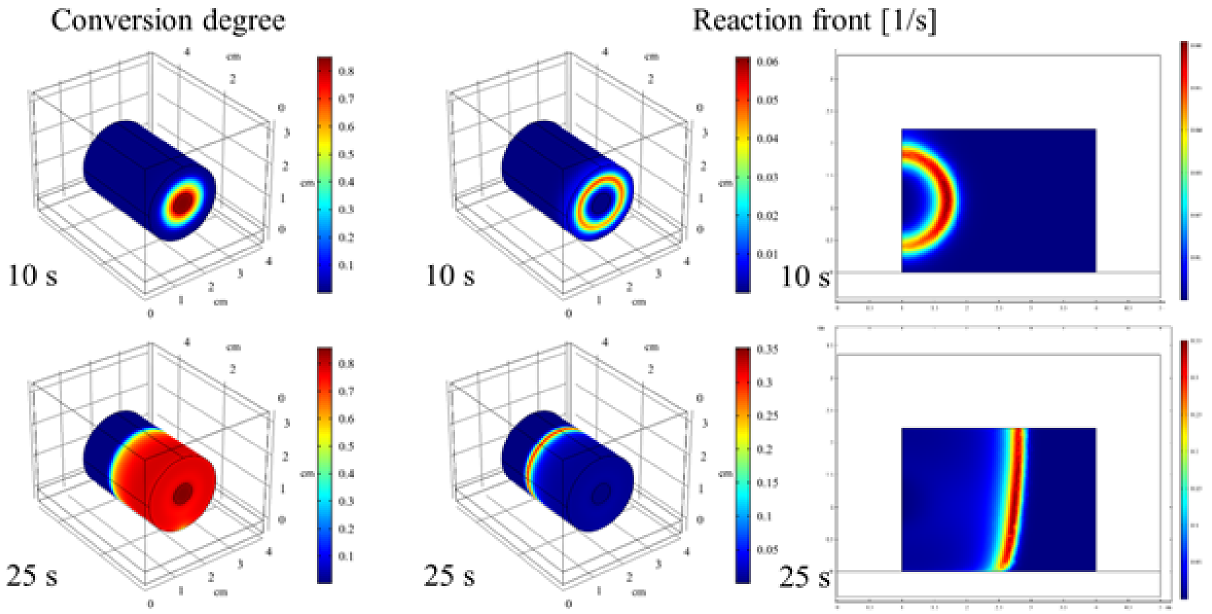

Fig. 1 Example results of 3D Self-propagating High-temperature Synthesis model simulations after 10s and 25 after ignition. Pictures present conversion degree of reactants and location of reaction front.