Final Report

Project acronym: *THERMOSS*

Project number*: 4299*

M-ERA.NET Call 20*16*

Period covered: 1/6/2017 to 31/8/2020

Publishable project summary

In recent years, increasing concerns on global warming and depletion of fossil fuels have renewed the interest in academia and industry to develop technologies for directly generating electrical power from waste heat (e.g. cement industry, glass industry or car exhaust) and natural heat sources (e.g. solar or geo thermal energy exploitation) with thermoelectric (TE) generators. Their performance is related to the materials figure-of-merit $ZT=\alpha^2\sigma T/\kappa$, where α: Seebeck coefficient, σ: electrical conductivity, κ: thermal conductivity at temperature T. Due to the interdependence of these physical parameters, designing efficient materials being at the same time stable in all working temperature range and inexpensive is challenging.

The core concept of the **THERMOSS Project** was to develop and deliver new energy harvesting TE materials and modules, based on *n*-Mg_2X(X:Si,Sn) (n-silicide) and *p*-$Cu_{12-x}(Mn,Ni)_xSb_4S_{13}$ (p-tetrahedrite) systems. These TE systems are advantageous since they exhibit many attractive characteristics, such as: (i) high ZT, (ii) operational in a medium temperature range, important for waste heat recovery, (iii) made from widely-available pure materials with very large EU supply chains, (iv) low raw material cost (cost target for thermoelectric generation is less than €1/W), (v) are nontoxic. Commercial generators are mainly based on materials such as Bi_2Te_3 and PbTe, making the technology expensive and environmentally unfriendly (toxic).

THERMOSS project delivered prototype TE modules based on *n*-type Bi-doped $Mg_2Si_{0.6}Sn_{0.4}$ (n-silicide) and $Cu_{11}Mn_1Sb_4S_{13}$ / $Cu_{10,5}Ni_{1,5}Sb_4S_{13}$ (p-tetrahedrites) as cheap and nontoxic materials for medium temperature range applications. Emphasis was given on the design/synthesis, optimization, properties and characterization of materials/modules as well as the investigation of possible applications.

The main activites of THERMOSS Project were:

- **Synthesis of n-silicides and p-tetrahedrites** with high TE figure-of-merit working at 350˚C.
- Development of **scalable methodologies** for the synthesis/processing of n-silicides and p-tetrahedrites.
- Investigation of the relationship between composition / process / structure / properties of the materials via advanced and complementary characterization techniques.
- **Development of advanced models using MATLAB programming and Finite Element / multi-physics tools** for the design and optimization of TE modules. The optimum features of the modules consisting of the best compositions of n-silicides and p-tetrahedrites were selected. A parametric optimization of conventional general purpose module, as well as large-scale custom module geometry, was also done.
- **Development and characterization of prototype modules** under various required operating parameters.
- **Stability studies** using various coatings for working conditions in argon and air were investigated. Suitable coatings were selected (i.e. BN, silicone pastes)
- **Prediction of the module performance** via finite element analysis for specific waste energy harvesting applications at intermediate temperatures up to 350˚C; mainly cement industry as well as automotive.
- **Simulations for the application in cement industry** aiming to maximize electrical output power were carried out. The generators including heat exchangers as well as their integration in a cement waste heat recovery system were investigated. Numerical techniques along with ANOVA and Taguchi optimization method to design segmented TEGs were applied.

- **Potential application in automotive** via simulations aiming maximum electrical output power were also investigated. The concepts developed seem to be able to surpass the conventional (non temperature-controlled) automotive TEG concepts in terms of average power in highly variable driving cycles. A thermosiphon-assisted generator working with the exhaust gas heat as well as a new generator concept which used heat pipes instead of thermosiphons, allowing for a more compact and suitable installation for vehicles were proposed.
- A systematic framework for the environmental assessment of TEG electricity system in cement plant was provided. **Life-cycle analysis (LCA)** showed that the most obvious outcome of improvement in cement plant efficiency is the reduction in greenhouse gas emissions.
- A cost performance has been applied to thermoelectric generator for waste heat recovery in cement industry. The **Cost-benefit (CBA)** study showed an acceptable payback period of just over 6 years (for new technology anything under 7 years payback period is acceptable).
- **Dissemination** of the THERMOSS results as well as the application of thermoelectrics for waste energy harvesting via publications / conferences / website / presentations.