# **Scientific Report**

**INTELBIOMAT Short Visit Grant 3538** 

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#### Title: Chalcogenide glasses as potential thermoelectric materials

#### 1- Background

Thermoelectric devices are heat engines that convert thermal energy into electricity and reversibly electricity into heat. Recent approaches to improve performance of bulk thermoelectric (TE) materials show that they should have complex structures, include inclusions and impurities, possess mass fluctuations, disorder and be based on heavy elements. Glasses can possess these properties. In order to identify glasses with interesting TE potential, attention should be focused on small gap semiconducting or semimetallic glasses. Interesting results have already been obtained in the Ge-Te-Cu system in which a huge increase in the power factor is observed, up to a maximum value of 60 mWK<sup>-2</sup>m<sup>-1</sup> for the Cu<sub>27.5</sub>Ge<sub>2.5</sub>Te<sub>70</sub> glass at T=300 K [1]. The first stay in ITN granted by ESF (Short grant 3342) permits to investigate new glassy compositions as potential materials for thermoelectric applications. The most important result was obtained in the system  $Te_{55}Cu_xAs_{45-x}$  (20<x<35) where the power factor has been doubled for the composition Te<sub>55</sub>Cu<sub>30</sub>As<sub>15</sub> in comparison with the Ge-Te-Cu system [2]. During this second stay we investigated sulfur-based compositions instead of tellurium based-composition for safety, environment and cost reasons. As for tellurium, the effect of germanium (4-fold coordinated) and arsenic (3-fold coordinated) has been investigated.

#### 2- Systems investigated

The glassy systems investigated during this short stay were:

-  $xCu_2S-(1-x)GeS_2(50 < x < 90)$ 

-  $xCu_2S-(1-x)As_2S_3(50 < x < 90)$ 

## **3- Preparation of glasses**

Glasses were first prepared by melting the appropriate amount of each element in a vacuumed silica tube at 1000°C (batch of 3g). After quenching in water, the different glass compositions, mostly unstable against crystallization, were then melt-spinned to obtain small pieces of glass.

# 4- Characterizations

All the samples were characterized by X-Ray Diffraction and thermal analysis (DSC). The electrical properties (Seebeck coefficient, resistivity, etc) were also measured. These measurements are still in progress.

## 5- Conclusion

This second short stay allows us to investigate new glassy systems as potential thermoelectric materials at room temperature. The thermoelectric properties of sulfur-based systems are still in progress and therefore we need more time to conclude about these systems.

[1] "Conducting glasses as new potential thermoelectric materials: the Cu–Ge–Te case", A. Pereira Goncalves, E. Branco Lopes, O. Rouleau and C. Godart, J. Mater. Chem., 2010, 20, 1516–1521

[2] "Enhanced thermoelectric properties in the Te-As-Cu chalcogenide glassy system: from ribbons to glass bulk", G. Delaizir, A. Pereira Gonçalves, E. Branco Lopes, J. Noudem, C. Godart, J. Mater. Chem., submitted