ABSTRACT

If we consider the fact that 2/3 of energy production from fuels is disposed as heat, improving the production methods through thermoelectric technologies is very crucial. This combined with the already industrialized applications, in cooling and power generating systems, has led in a rapid increase in research on thermoelectric materials. Research on high-performance materials focuses on low thermal conductivity semiconductors. The presence of structure alterations in nanoscale, structure defects and interfaces are considered to be the main factors affecting the thermoelectric properties. The above tend to scatter the phonons in the crystal allowing the passage of electric carriers. For this reason, the structural characterization of the interfaces is of the utmost importance for the understanding of the thermoelectric properties.

In this study we investigate the structural characteristics and interfaces of the nanostructured, thermoelectric system, $AgPb_{18}SbSe_{20}$ with HRTEM electron microscopy. Initially the theoretical scientific background is presented in order to understand the forthcoming study. The phenomena of thermoelectric materials are presented, as well as the connection of the structural characteristics with the thermoelectric characteristics. Connection that also reflects the purpose of the particular work. There follows an introduction to electron microscopy with an emphasis on transmission electron microscopy (TEM). A description of the TEM electron microscope, as well as its imaging modes, is made. It is followed by a preface on Geormetric Phase Analysis (GPA), which is a method for measuring and mapping displacement and strain fields from periodic lattices.

In our experimental main part of this work, we first mention the materials and the computational packages used. The following is the GPA analysis for the occurring phases of the nanocrystals that have been examined. The GPA confirms the three phases of the material, the phase boundaries and the morphology of the interfaces. Following are the simulations of the first two phases, the matrix and the B phase based on the models that are already known. The simulations were performed using the JEMS software. Afterwards a revision of the C phase of our system is taking place, changing the one we know today. We construct structural models that are simulated to compare with our experimental image. By choosing the most appropriate **one**, we proceed to model the interface of the two nanocrystalline phases B and C. Four models are proposed where the HRTEM image simulations show the validity of these models. Finally, we choose what best illustrates our experimental image.

Key words: Thermoelectric materials, Transmission Electron Microscopy (TEM), Geometric Phase Analysis (GPA), High Resolution Transmission Electron Microscopy (HRTEM) micrographs, structure modeling, crystal structure simulations with JEMS.