An electron crystallography study of the existing nano-phases in the thermoelectric composite PbTe+25%$PbSnS_2$

Abstract

The scope of this thesis is the structural characterization of the thermoelectric system PbTe+25% $PbSnS_2$. Different methods for solving crystal structure and investigating phases with nano-dimensions were performed. The present work is divided into two parts. The first part contains the theoretical scientific background. Emphasis is given to the electron microscope and the process of data collection. Further analysis of the double diffraction problem and the techniques used to reduce it are noted, followed by a description of thermoelectric materials and the materials used. The second part is a detailed description of the experiments and data processing. Low Magnification Images, Electron Diffraction patterns as well as High Resolution Transmission Electron Microscopy Images were recorded. Low-magnification images prove that the system is nanostructured. The presence of $PbSnS_2$ phases is determined by Precession Electron Diffraction and tilting experiments. The interplanar distances calculated from the electron diffraction experiments suggest the growth of PbS or $Pb_{0.9}Sn_{0.1}S$ phase, endotaxially grown in the matrix, having good crystallographic alignment with the matrix. Standard data from JCPDS cards was used for the identification of all phases. High Resolution Transmission Electron Microscopy study was performed for better elucidation of the structural phases. HRTEM images were improved using FFT and IFFT processing. Three theoretical models were designed for the description of the crystal structure and computer image simulations based on the theoretical models were performed using the JEMS software. The combination of electron diffraction and HRTEM images with the simulated images were useful for finding the appropriate structural models.