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Characterization of PbTe-based thermoelectric materials by scanning/ transmission electron microscopy (S/TEM)

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Thermoelectric conversion of waste heat to electrical power represents one approach toward improving our current energy consumption and utilization. If bulk materials with low-cost processing and high figure of merit (ZT) can be developed, their application to widespread markets may be realized [1]. Many techniques have been developed to increase ZT such as solid solution alloying, nanostructuring [2,3], which may enhance thermal scattering without significant loss of electrical conductivity. Accordingly, a precise characterization and analysis of microstructure and chemical composition as they relate to thermo-electrical transport are vitally important for the fundamental understanding of thermoelectric materials. Here, we present PbTe-PbS as a model system which is an intrinsically immiscible system with multitude of precipitates and interfaces. The nature and character of the precipitates and interfaces are examined with analytical S/TEM [5].

Fig.1 shows the spinodal decomposition of PbTe-PbS30%., details are featured in (a-e). Fig.1(a) shows a low magnification STEM image together with three elements composition mapping crossing one boundary, clearly indicating two phases PbS (light white part) and PbTe (grey part). (b) Intermediate magnification bright field image shows pretty homogeneous contrast in PbTe region and nano-scale precipitates in the PbS region. (c) and (d) HRTEM images of PbS area show two typical of inclusions, small size PbTe and straight line-like defect with Te vacancy. (e) Lattice image shows one kind of modulation structures at the boundary between PbTe and PbS, mainly due to the overlap these two phases, further strain analysis reveal a series of misfit dislocations at the boundary because of large lattice mismatch between PbTe and PbS.

Fig.2 shows another type of spinodal decomposition in sample $Pb_{0.8}Sn_{0.2}Te$-PbS30%, the observed two phases are PbTe and $PbSnS_2$ rather than PbTe and PbS. (a) Low magnification STEM image, comparing to Fig.1a, we can find the difference of phase contrast of these two phase much higher than that in Fig.1a. Further experiments, such as electron diffraction patterns (b) and (c) which show super lattice along one direction and split spots, reveal the two phases are PbTe and $PbSnS_2$. $PbSnS_2$ is orthorhombic structure with space group Pnma and lattice parameters of a=1.1412 nm, b=0.408 nm, and c=0.428 nm. (d) and (e), different region HRTEM images, show the two directions of $PbSnS_2$ phase, 100 and 011, respectively. (f) High magnification lattice image of $PbSnS_2$ phase together with its model (insert) show the layered structures. (g) HRTEM image shows the different direction orientation sequence 001, 110, and 001 in $PbSnS_2$ phase.

The presentation will cover S/TEM microscopy and microanalysis strategy to unravel microstructural influence on thermoelectric properties and associated phenomena.

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[4]This work is supported by the Office of Naval Research MURI program.

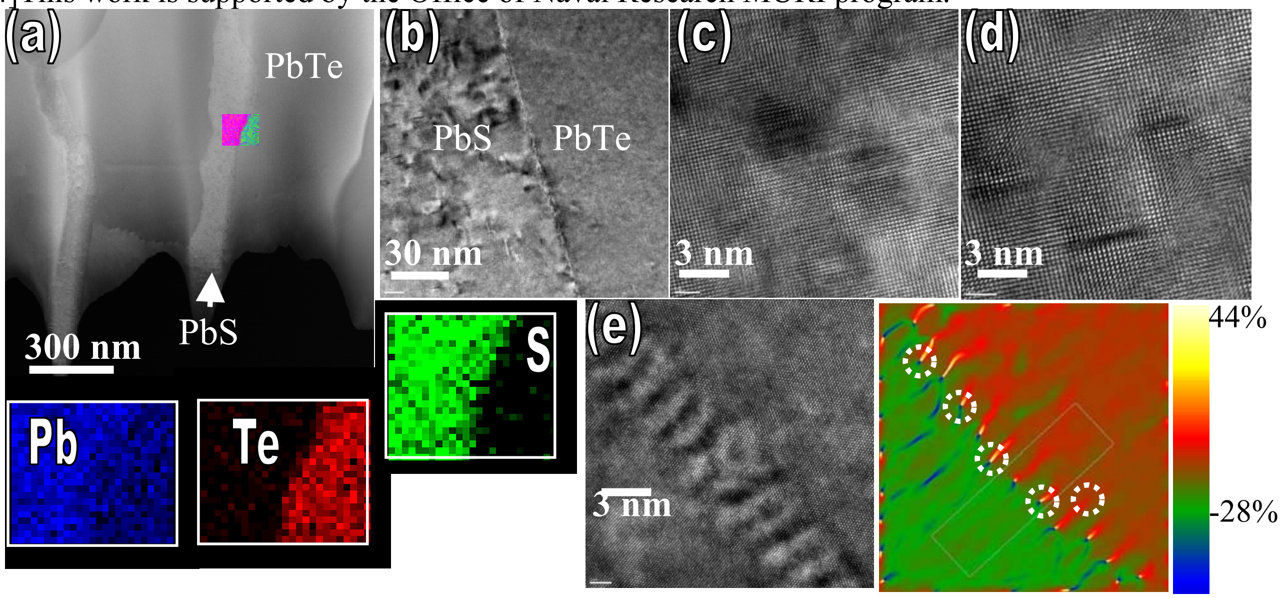

Fig.1 Spinodal decomposition of PbTe-PbS30%. (a) Low magnification Z-contrast image with selected area crossing the boundary together with distributions of three types elements (b) intermediate magnification bright field image with inhomogeneous contrast in the PbS region. High magnification lattice images (c) and(d) show two typical inclusions(or defects) (e) HRTEM image show one kind of modulation structures at the boundary, further strain analysis reveal a series of misfit dislocations at the boundary.

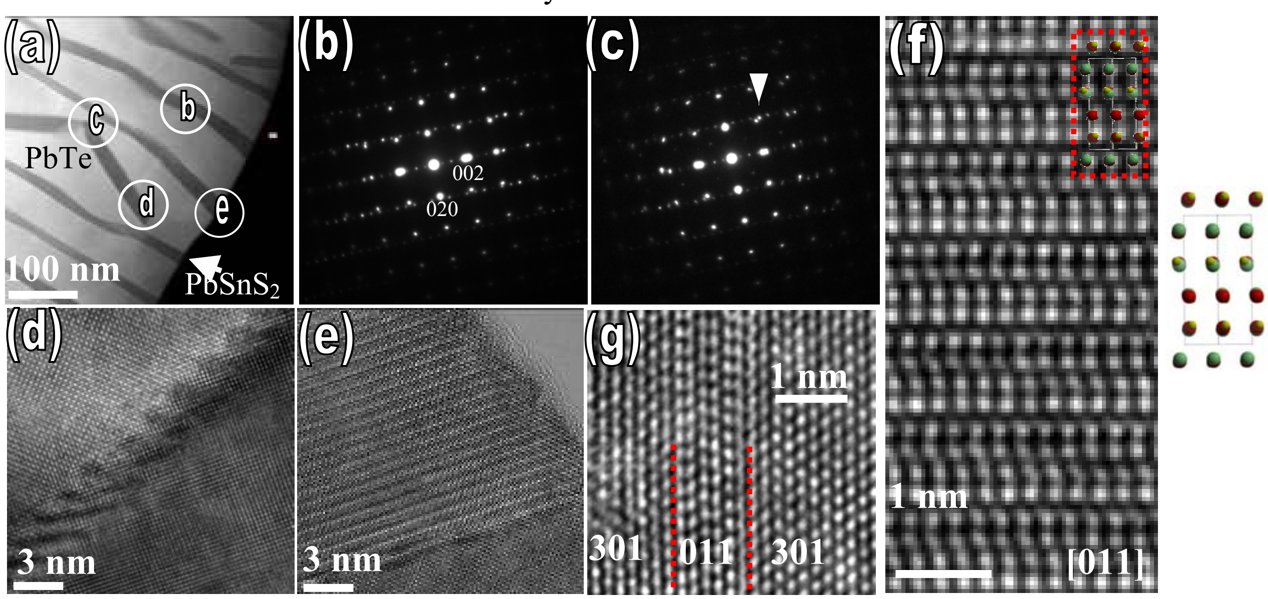

Fig.2 Spinodal decomposition of $Pb_{0.8}Sn_{0.2}Te$-PbS 30%: (a) Low magnification STEM image. The electron diffraction patterns in (b) and (c), which are from different regions as shown in (a), can be indexed PbTe and new phase $PbSnS_2$. The different region HRTEM images (d) and (e) further confirm the dark area is $PbSnS_2$. (f) high magnification lattice image of $PbSnS_2$ and the model (insert), (g) HRTEM image shows the different direction orientation sequences.

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