New lead- and tellurium-free thermoelectric materials: $AgSn_m(Sb_xBi_{1-x})Se_{m+2}$

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The global demand for energy production has intensified the interest in improving the efficiency of energy generation systems. In this context, thermoelectric materials have been used to take advantage of the conversion of residual heat into electricity [1]. High efficiencies have been obtained using lead-based nano-structured thermoelectric materials, such as (PbTe) m-$AgSbTe_2$ systems [2]. Due to the presence of lead, a known toxic element, and tellurium, a rare element in the earth's crust, alternatives must be sought. Chemical modifications and doping of SnSe have generated interest due to its low intrinsic thermal conductivity [3]. Of such modifications, $AgSn_mSbSe_2Te_m$ phases with m = 2 and 10 have shown values of ZT = 0.1 at RT [4]. On the other hand, to enhance the Seebeck coefficient in $AgSbTe_2$ compounds, Bi doping has been used, which increased the ZT value by 10% [5].

Herein, we report the synthesis, characterization, and electrical properties of $AgSn_m(Sb_{1-x}Bi_x)Se_{m+2}$ compounds, with m = 1, 2. These phases were synthesized by the ceramic method at high temperatures (Figure 1A). Rietveld refinement results indicated that the selenides consisted of phases related to NaCl-type crystal structure. The powder X-ray diffraction (XRD) patterns were refined in the *Pm-3m* and *P4/mmm* space group. The backscattered image and EDS analysis of the samples revealed that the chemical compositions were uniform throughout the scanned region. The microstructural features of the samples were analysed using HRTEM. Figure 1B shows the ED patterns for the selected areas. The results suggest the presence of regions with different symmetries at the nanoscale.

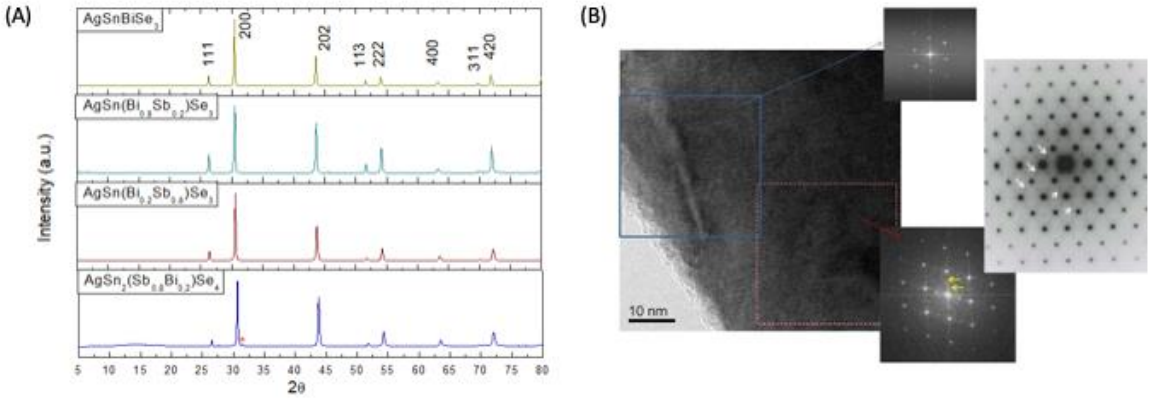

Figure 1. (A) X-ray diffraction patterns (XRD) for $AgSn_m(Sb_{1-x}Bi_x)Se_{m+2}$ (B) HRTEM images showing electron diffraction patterns (ED) and fast fourier transforms (FFTs). The arrows indicate the dots of the reciprocal lattice, which violate the systematic absence of the *Fm-3m* space group.

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Keywords: Rietveld analysis; lead-free Thermoelectric; HRTEM; Selenides

Authors are grateful for FONDECYT Project N° 1190856

Acta Cryst. (2021), A**77**, C1157