

## X-RAY POWDER DIFFRACTION CHARACTERIZATION OF THE SEMICONDUCTING COMPOUNDS $\text{Ag}_2\text{FeSnS}_4$ AND $\text{Ag}_2\text{FeSn}_3\text{S}_8$

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The crystal structures of the semiconducting compounds  $\text{Ag}_2\text{FeSnS}_4$  and  $\text{Ag}_2\text{FeSn}_3\text{S}_8$  were established simultaneously from the same X-ray powder diffraction pattern.

$\text{Ag}_2\text{FeSnS}_4$  belongs to the  $\text{I}_2\text{IIIVVI}_4$  semiconducting system. It can be considered as a member of one of the two possible families of four-fold normal derivatives ( $\text{A}_2\text{BCD}_4$ ) of the II VI binaries in which the II cation has been substituted by three types of cations. The other family is  $\text{I II}_2\text{III VI}_4$ .  $\text{Ag}_2\text{FeSn}_3\text{S}_8$  can be described as an eight-fold defect derivative of the II VI binaries which belong to the  $\text{I}_2\text{IIIV}_3\text{VI}_8$  semiconducting family.

In a synthesis attempted to prepare  $\text{Ag}_2\text{FeSnS}_4$  by direct fusion of the constituent elements in vacuum-sealed quartz ampoules, both  $\text{Ag}_2\text{FeSnS}_4$  and  $\text{Ag}_2\text{FeSn}_3\text{S}_8$  were obtained. The X-ray powder diffraction data of the product were collected at room temperature with a Siemens D5005 diffractometer using a diffracted beam graphite monochromator ( $\text{CuK}\alpha$  radiation:  $\lambda = 1.54059\text{\AA}$ ). The specimen was scanned in the  $2\theta$  range of  $10^\circ$ - $100^\circ$ , the scan step was  $0.02^\circ$ , and the time of counting in every step was 40s.

The unit cell parameters for both materials were refined using the program NBS\*AIDS83. The compound  $\text{Ag}_2\text{FeSnS}_4$  crystallizes in the tetragonal space group  $\text{I}\bar{4}2\text{m}$  ( $\text{D}_{4h}^{2d}$ ,  $N^\circ$  121),  $Z=4$ , with unit cell parameters:  $a=5.7706(2)\text{\AA}$ ,  $c=10.9685(4)\text{\AA}$ . The second phase  $\text{Ag}_2\text{FeSn}_3\text{S}_8$  crystallizes in the tetragonal space group  $\text{I}4_1/a$  ( $\text{D}_{4h}^6$ ,  $N^\circ$  88),  $Z=4$ , with unit cell parameters:  $a=7.4833(2)\text{\AA}$ ,  $c=10.5674(4)\text{\AA}$ .

Rietveld refinement of the structure of each compound was carried out in the same pattern. The atomic coordinates of the isostructural compounds  $\text{Cu}_2\text{FeSnSe}_4$  and  $\text{Cu}_2\text{FeSn}_3\text{S}_8$  were used as starting model.

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