IOCC 2024 Conference

The 4th International Online Conference on Crystals

18–20 September 2024 | Online

The influence of the substitution in cation and anion sublattice on the HT-Pb_2GeS_4 structure

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INTRODUCTION & AIM

The HT-Pb_2GeS_4 (SG *I*-43*d*) is prospective material for investigation. The structure of HT-Pb_2GeS_4 crystallizes in cubic symmetry. The position 24*d*, 16*c* and 48*e* can be modified by substitution of atoms Pb and S. We investigated the crystalline structure of four compositions: $Pb_{1.9}Sn_{0.1}GeS_{3.52}Se_{0.48}$, $Pb_{1.86}Sn_{0.14}GeS_{3.32}Se_{0.68}$, $Pb_{1.82}Sn_{0.18}GeS_{3.16}Se_{0.84}$ and $Pb_{1.58}Sn_{0.42}GeS_{3.64}Se_{0.36}$ changing the cation and anion sublattice simultaneously.

METHOD

Samples with the nominal compositions of $Pb_{2-x}Sn_xGeS_{4-y}Se_y$ (x = 0.1, 0.14, 0.18, and 0.42; y = 0.36, 0.48, 0.68, and 0.84) were prepared by melting high-purity Pb (shot, 99.99 %), Sn (shot, 99.99 %), Ge (shot, 99.999 %), S (shot, 99.99 %), and Se (shot, 99.99 %) in quartz containers evacuated to a residual pressure of 10–2 Pa. The total mass of every sample was 1 g. The ampules with the stoichiometric mixtures of elements were heated up to 1423 K at a rate of 12 K/h; kept at this temperature for 4 h; cooled down to 773 K at a rate of 12 K/h; annealed at this temperature for 500 h; and quenched in cold water without breaking the containers.

Powder X-ray Diffraction, thermal analysis and Scanning Electron Microscopy (SEM). Phase identification was performed with a DRON-4-13 X-ray diffractometer using Cu *K*α radiation (λ = 1.5418 Å, $\Delta 2\Theta$ = 0.005 °, 2Θ range 10 – 100 °) with Bragg-Brentano geometry. Rietveld refinement of the crystal structure was carried out using the WinCSD program package [1].

RESULTS & DISCUSSION

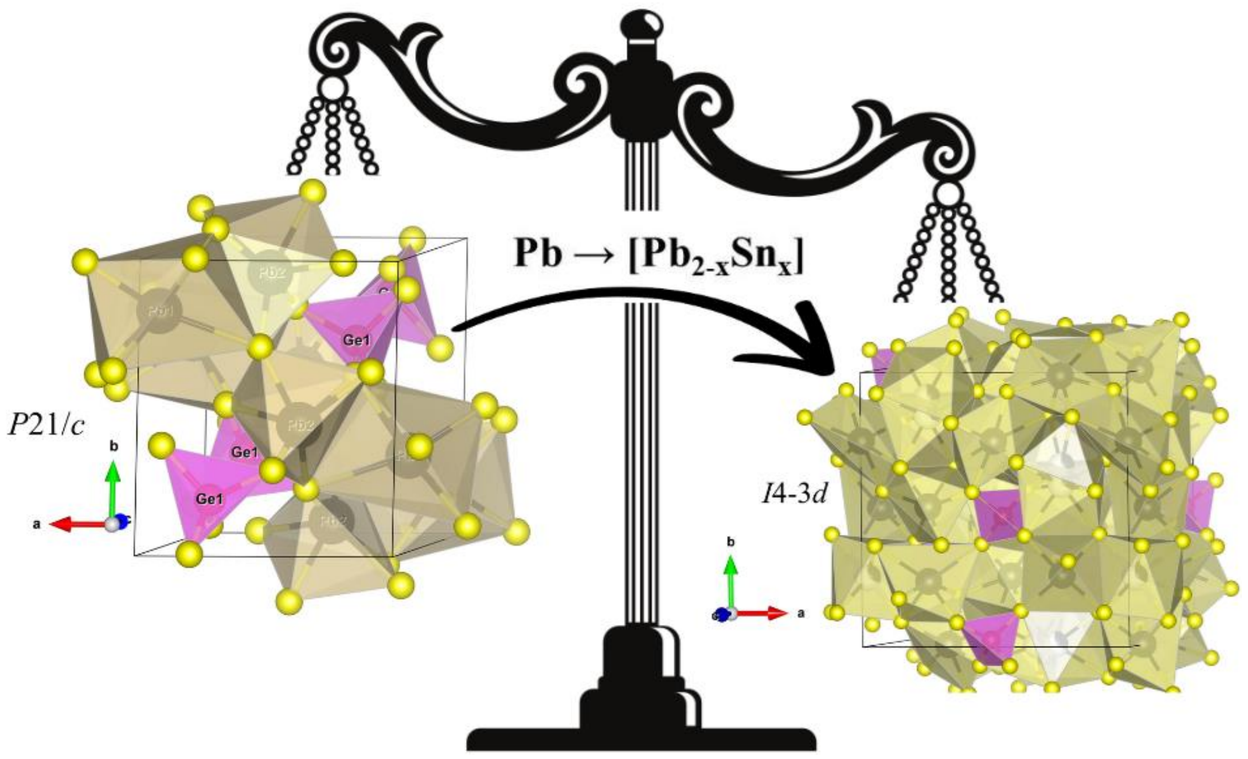

Fig.1. Phase transition of $Pb_{2-x}Sn_xGeS_{4-y}Se_y$ (x = 0.1, 0.14, 0.18, and 0.42; y = 0.36, 0.48, 0.68, and 0.84) samples

The substitution in cation and anion sublattice on the Pb_2GeS_4 crystal structure leads to the increasing of the volume of the lattice from 2794.9 Å to 2852.2 Å due to the change of y. The lattice parameter a is changing from 14.086 Å to 14.1816 Å. The distortion of the cation sublattice is observed.
Hence, such peculiarities of the crystal structure may improve some thermoelectric and optical properties.

CONCLUSION

Materials with phase transition based on $Pb_{2-x}Sn_xGeS_{4-y}Se_y$ (x = 0.1, 0.14, 0.18, and 0.42; y = 0.36, 0.48, 0.68, and 0.84) samples are perspective due to n→p electronic transition.

FUTURE WORK / REFERENCES

1. Akselrud, L.; Grin, Y. WinCSD: Software Package for Crystallographic Calculations (Version 4). J. Appl. Crystallogr. 2014, 47 (2), 803– 805, DOI: 10.1107/S1600576714001058 46.