Transport properties deviation of polycrystalline Bi₂O₂Se: Causes and solutions

<u>Jan Zich</u>^{1,2}, Antonín Sojka¹, Jiří Navrátil^{1,2}, Karel Knížek², and Čestmír Drašar¹

¹University of Pardubice, Studentská 95, Pardubice 532 10, Czechia ²Institute of Physics of ASCR, Cukrovarnická 10, 162 00 Praha, Czech Republic

Bismuth oxyselenide (Bi_2O_2Se) is a promising thermoelectric (TE) material known for its high carrier mobility, non-toxic composition, and cost-effectiveness. However, its low intrinsic electrical conductivity necessitates doping to enhance performance. A major challenge is the significant variation in transport properties of bulk polycrystalline samples, even when synthesized using similar methods. This study examines the causes of these deviations and suggests solutions.

Through analysis of literature and synthesis of samples using different compounds and methods, we identified that impurities and foreign phases significantly impact the transport properties of undoped Bi_2O_2Se . Techniques such as powder X-ray diffraction (PXRD), scanning electron microscopy/energy dispersive X-ray spectroscopy (SEM/EDS), Raman spectroscopy, and ATR IR spectroscopy were used to detect these impurities.

To combat this issues, we propose a reproducible low-temperature solid-state synthesis process to produce high-purity $\mathrm{Bi_2O_2Se}$. This method minimizes presence of high temperature associated secondary phases and ensures a consistent crystal structure, leading to improved and reliable transport properties. By refining synthesis techniques and controlling impurity levels, we aim to establish a standard for achieving consistent performance in $\mathrm{Bi_2O_2Se}$.

The authors thank the Czech Science Foundation for financial support (Project No. 22-05919S) and Ministry of Education, Youth and Sports of Czech Republic (grant LM2023037).

- [1] Zhang Z-l, Wang T, Nisar M, et al. Enhanced thermoelectric properties of n-type Bi2O2Se by KCl doping. Journal of Advanced Ceramics, 12(9): 1767-1776 (2023)
- [2] Si Young Bae, Hyun-Sik Kim, Se Woong Lee, Okmin Park, Hyunjin Park, Sang-il Kim, Enhanced thermoelectric properties of I-doped polycrystalline Bi2O2Se oxyselenide, Journal of Materials Research and Technology, Volume 19 (2022)
- [3] Yuping Li, Haojie Huo, Hai Huang, Kai Guo, Xinxin Yang, Juanjuan Xing, Optimization of electrical and thermal transport properties of layered Bi2O2Se via Nb doping, Journal of Materials Science, vol. 56 (2021)
- [4] P. Ruleova, C. Drasar, P. Lostak, C.-P. Li, S. Ballikaya, C. Uher, Thermoelectric properties of Bi2O2Se, Materials Chemistry and Physics, Volume 119, Issues 1–2 (2010)