## Single crystal growth and physical properties of layered oxychalcogenide $Sr_2ZnCu_2(S_{1\text{-}x}Se_x)_2O_2$

Takahiro Kato<sup>1,2</sup>\*, Yuki Iwasa<sup>1</sup>, Yuui Yokota<sup>3</sup>, Shigeyuki Ishida<sup>1</sup>, S. Pavan Kumar Naik<sup>2</sup>, Yoichi Higashi<sup>1</sup>, Izumi Hase<sup>1</sup>, Kenta Hongo<sup>4</sup>, Ryo Maezono<sup>4</sup>, Takahiko Horiai<sup>3</sup>, Akira Yoshikawa<sup>3</sup>, Taichiro Nishio<sup>2</sup>, Hiroshi Eisaki<sup>1</sup>, Hiraku Ogino<sup>1</sup>

\*lead presenter: katou.takahiro@aist.go.jp

- 1 National Institute of Advanced Industrial Science and Technology (AIST), Japan
- 2 Tokyo University of Science, Japan
- 3 Tohoku University, Japan
- 4 Japan Advanced Institute of Science and Technology (JAIST), Japan

Layered mixed-anion compounds, which contain multiple anions, have attracted much attention in recent years because of their large flexibility in the structure and composition and various applications such as superconductors, thermoelectric materials, photocatalysts, and so on<sup>[1]</sup>. On the other hand, it is generally difficult to grow single crystals of such compounds owing to low-temperature stable phases and incongruent melting. Oxychalcogenides with CuCh (Ch=S, Se, and Te) layers such as  $Sr_2ZnCu_2Ch_2O_2$  are reported to have the potential to use as p-type transparent conductors as well as thermoelectric applications<sup>[2,3]</sup>. However, owing to the lack of single crystals, their intrinsic physical properties have not been investigated so far. In this presentation, we report the single crystal growth and physical properties of layered oxychalcogenide  $Sr_2ZnCu_2(S_{1-x}Se_x)_2O_2$  ( $0 \le x \le 1$ ).

Utilizing a peculiarity of the rapid grain growth of the compounds, single crystals were synthesized by solid state reaction. The raw materials of SrO, Zn, Cu, S and Se were mixed in stoichiometric molar ratios, sealed in evacuated quartz tubes, and sintered at 1173-1373 K for 48 h. As a result, single crystals of  $Sr_2ZnCu_2(S_{1-x}Se_x)_2O_2$  ( $0 \le x \le 1$ ) were successfully synthesized as shown in Fig 1. Only (001) Bragg peaks were observed in the XRD as shown in Fig.2. The lattice parameters changed in accordance with the Vegard's law, and the value of a band gap also changed with the composition. The details of the grown single crystals of  $Sr_2ZnCu_2(S_{1-x}Se_x)_2O_2$  ( $0 \le x \le 1$ ) and their properties will be discussed in the presentation.

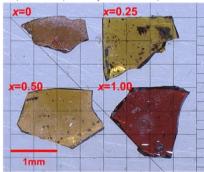


Fig.1 Photographs of single crystal  $Sr_2ZnCu_2(S_{1-x}Se_x)_2O_2$ 

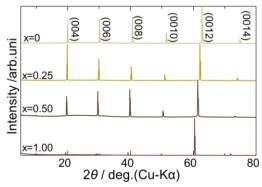


Fig.2 XRD patterns of  $Sr_2ZnCu_2(S_{1-x}Se_x)_2O_2$  single crystals

## Reference

- [1] H. Kageyama, K. Hayashi, K. Maeda, J.P. Attfield, Z. Hiroi, J.M. Rondinelli, K.R. Poeppelmeier, Expanding frontiers in materials chemistry and physics with multiple anions, Nat. Commun. 9 (2018).
- [2] J. Willis, D.O. Scanlon, Latest directions in p-type transparent conductor design, J. Mater. Chem. C. 9 (2021) 11995–12009.
- [3] Y. Yang, Z. Zhou, B. Wei, J. Liu, J. Le Lan, M. Zou, Y. Xu, Y. Zheng, C.W. Nan, Y.H. Lin, Thermoelectric properties of layered oxyselenides with 3d transition metal ions, J. Am. Ceram. Soc. (2022) 35–37.