

Topic for a Master's Thesis (English)

" Exploring the extraordinary Ge-Ge bond in GeTe-SeTe system"

INTRODUCTION...Member of the $GeTe - Sb_2Te_3$ family are the most common phase change materials(PCMs) for date storage. To break the limitation of the traditional PCMs, chalcogenide superlattices and chemically synthesized nanocrystals are being examined ^[1]. Besides the pseudo-binary line from GeTe towards Sb2Te3, an interesting compound $GeSe_{0.75}Te_{0.25}$ has seen in the pseudo-binary and sparsely studied GeTe–GeSe system^[2]. This single crystal is a layered 2D material held together by the van der waals type weak chalcogenide–chalcogenide interactions but also display unexpected Ge–Ge contacts, as confirmed by electron microscopy analysis. Furthermore, most of these 2D structures in the GeTe/Sb2Te3 system are



Fig.1. a) The layered structure of Ge4Se3Te with Ge sites in gray and mixed chalcogenide sites A1 and A2 (black/red) with an approximate 3:1 ratio of Se and Te. b) Germanium coordination. c) Top view of the crystal structure along the c axis.

dominated by strong metal–chalcogenide interactions while only very few compounds exhibit (weaker) metal–metal bonds ^[3]. The unexpected and significantly stronger Ge–Ge contacts reshuffle electrons from antibonding Ge–Te into bonding Ge–Ge contacts, thereby lowering the energy. The analysis of the density of energy (DOE) function clarifies the importance of both offsite and on-site energetic contributions for phase stability.

THESIS DETAILS...In this master thesis, we will focus on studying the electronic transport properties of $GeSe_{0.75}Te_{0.25}$ single crystal in the out of plane direction to explore the special Ge-Ge bond. A four contacts geometry device should be accomplished first. The fabrication flow is shown as the following. In this process, you can have chance to obtain the Nano-device fabrication skills and two-dimensional materials fabrication techniques. To the end, Hall measurement and magnetoresistance measurement will be performed on the sample to detect the effect of the Ge-Ge contact on its electrical properties.



Fig.2 structure of the out of plane device

[1] P. M. Konze, V. L. Deringer, R. Dronskowski, Chem. Mater. 2016, 28, 6682–6688.

[2] Küpers,Wuttig, M. (2017). Unexpected Ge-Ge Contacts in the Two-Dimensional Ge4Se3Te Phase and Analysis of Their Chemical Cause with the Density of Energy (DOE) Function. Angewandte Chemie International Edition, 56(34), 10204-10208.

[3] T. Matsunaga, N.Yamada, Y. Kubota, Acta Crystallogr. Sect. B 2004, 60, 685–691.