

---

**Yun Choi**<sup>1</sup>

Keunui Kim<sup>1</sup>, Jungcheol Kim<sup>1</sup>, Soo Yeon Lim<sup>1</sup>, Jung Hwa Kim<sup>2</sup>, Zonghoon Lee<sup>2</sup>,  
Hyeonsik Cheong<sup>1,\*</sup>

<sup>1</sup>Department of Physics, Sogang University, Seoul, 04107, Korea

<sup>2</sup>School of Materials Science and Engineering, Ulsan National Institute of Science and Technology, Ulsan  
44919, Korea

yunchoi@sogang.ac.kr

---

## Crystallographic axis of ReX<sub>2</sub> (X= S, Se) identified by polarized Raman spectroscopy

In-plane anisotropy of rhenium dichalcogenides (ReX<sub>2</sub>, X= S, Se), members of the group-VII transition metal dichalcogenides (TMDs), give additional degrees of freedom in manipulating device properties using anisotropic electronic and optoelectronic properties. The covalent bonding of the transition metal atoms (Re-Re) causes the anisotropic 1T' (distorted trigonal) structure and all axes are not normal to other axes of the crystal. Therefore, up- and- down faces of monolayer ReX<sub>2</sub> are not equivalent. Hence, there are two types of fabricated samples; one is 'c-up' type and the other one is 'c̄-up'. Furthermore, physical properties are originated by structural unisotropy and related to the crystallographic orientation (in plane) [1][2]. Therefore, identification of crystal axis is important in fabricating devices.

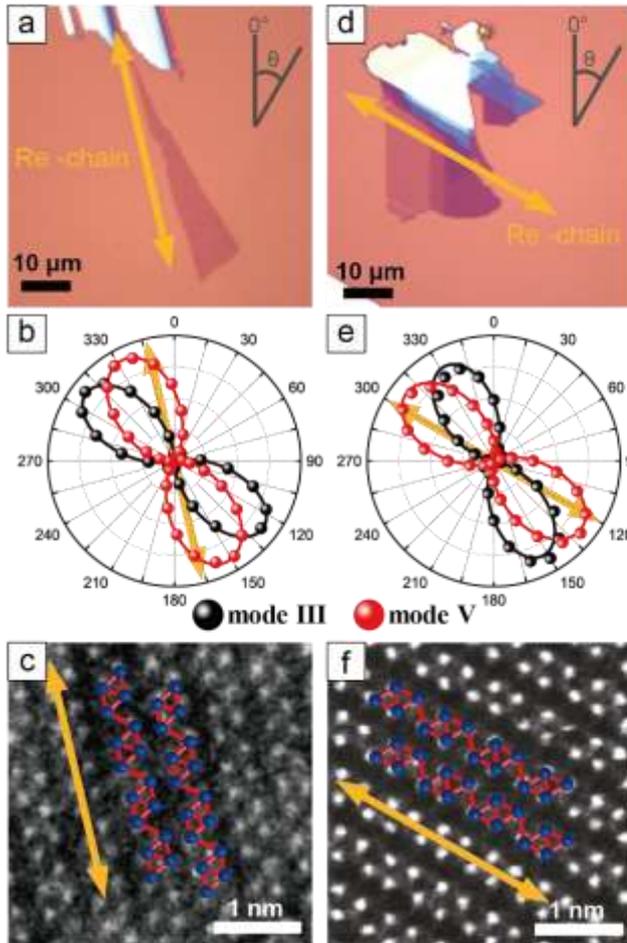
In this study, we performed linearly polarized Raman measurements on 1- to 3-layer ReX<sub>2</sub> on both up- and down-sides. The thickness was determined by interlayer vibration modes in the low frequency region (< 40 cm<sup>-1</sup>) [3]. We investigated the polarization dependences of the 18 Raman modes with the excitation energies (2.81, 2.41, 2.33 and 1.96 eV). The polarization dependences of the Raman modes vary with the excitation wavelength. From the relation of the polarization dependence of two Raman modes (mode III and V for ReS<sub>2</sub>: 152, 212 cm<sup>-1</sup> and mode IV and V for ReSe<sub>2</sub>: 125 cm<sup>-1</sup> and 160 cm<sup>-1</sup>), we classified the sides of the samples corresponding to the two vertical orientations (c-axis) by comparing the relations of two Raman modes from the samples. To investigate the polarization dependences of the Raman signals from both sides of the same sample, we fabricated ReX<sub>2</sub> sample on transparent quartz substrate and measured both sides by flipping. We also identified the Re-chain direction, b-axis, using the polarization direction of the Raman modes at 212 cm<sup>-1</sup> (ReS<sub>2</sub>) and 160cm<sup>-1</sup> (ReSe<sub>2</sub>) by comparing with scanning transmission electron microscopy (STEM) measurements. The crystallographic orientation of ReS<sub>2</sub> including can be determined using excitation energies of 2.41, 2.33 and 1.96 eV, but the same information on ReSe<sub>2</sub> can be determined by using the 1.96 eV excitation energy only.

### References

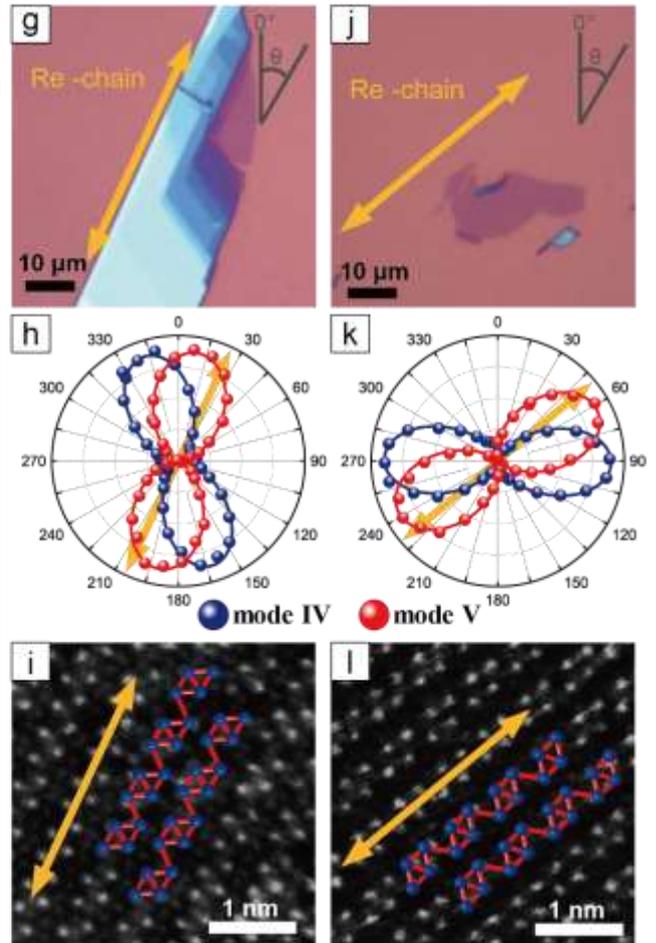
- [1] Y. Lin *et al.*, ACS Nano, 9 (2015) 363
- [2] S. Sim *et al.*, Nature communication, 9 (2018) 351
- [3] E. Lorchat *et al.*, ACS nano, 10 (2016) 27525

### Figures

### ReS<sub>2</sub> (1L, 2.33 eV)



### ReSe<sub>2</sub> (1L, 1.96 eV)



**Figure 1:** (a, d, g, j) Optical images of 1L ReX<sub>2</sub> samples. (b, e, h, k) polarization dependences of the intensities of Raman modes III and V at 152 and 213 cm<sup>-1</sup> for ReS<sub>2</sub> (c, f, i, l) HR-STEM images of samples. The Re-chain directions are indicated by the arrows. The orientations are (c, i) 'c-up' and (f, l) 'c<sup>-</sup>-up'.