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Vibrational mode analysis of SnS thin films by density functional perturbation theory

Tin sulfide (SnS) is attracting much attention as thermoelectric and solar power generation materials, which consist of abundant resources. It has a high thermal conductivity owing to low crystal density.[1] Monolayer growth and control of layer number are demanded for the future application toward transparent and flexible thermoelectric devices. In order to identify the number of layers using Raman spectroscopy, it is necessary to analyze the layer number dependence of phonon vibration mode. In this paper, we investigate the phonon vibration modes of SnS thin films using first-principles calculations based on density functional perturbation theory.

Figure 1(a) shows the crystal structure of bulk SnS. It has an orthorhombic structure and double layers in unit cell. The interaction between layers is van der Waals forces. Figure 1(b) is the corresponding 1st Brillouin Zone of bulk SnS. Bulk SnS is an indirect transition semiconductor with a band gap of 1.16eV. The phonon vibration modes at Γ-point are calculated for several different number of layers as shown in Fig. 2. The red solid lines represent the frequency of Raman active modes, and the blue dotted lines indicate Raman inactive modes. In the range of 150 to 200 cm^{-1} , the out-of-plane modes for bilayer shift lower frequency compared with those of bulk, because of the reduction of interlayer interaction. For same reason, in the range of 200 to 250 cm^{-1} , the out-of-plane modes for monolayer, which are Raman active, shift lower frequency than those of bilayer. In addition, the out-of-plane mode for monolayer disappears. Thus, it is found that SnS thin films show the strong layer-number dependence in the phonon vibration modes near the region of 200 cm^{-1} .

References

[1] Q. Tan, *et. al.*, J. Electron. Mater., (2014) 373 [508]

Figures

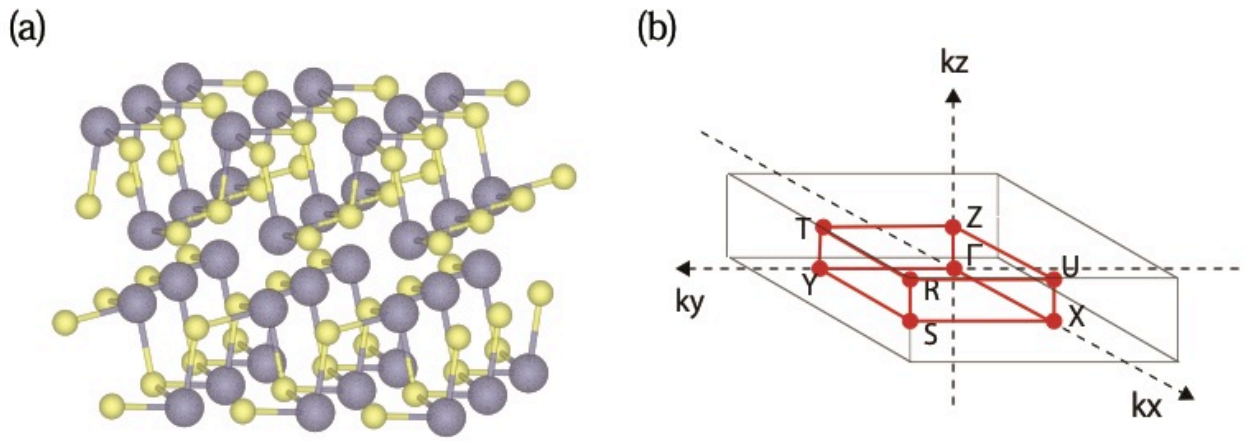

Figure 1: (a) Bulk crystal structure of SnS. It has a structure in which S and Sn are alternately bonded. (b) The corresponding first Brillouin zone.

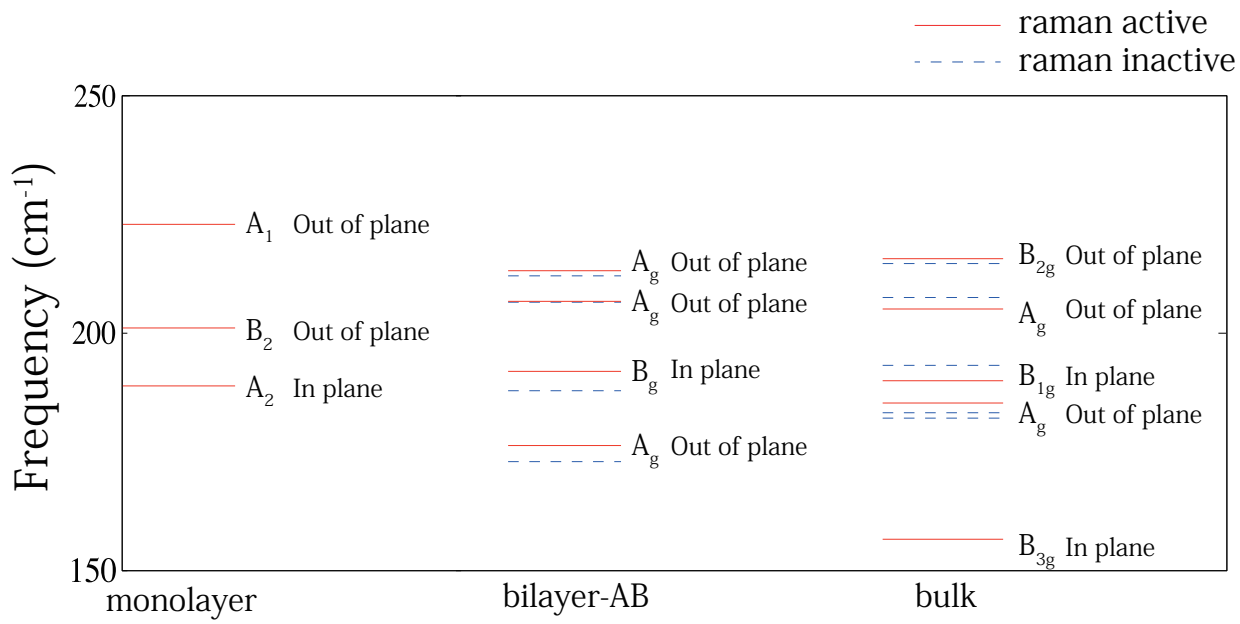

Figure 2: Raman active vibration modes at 150 to 250 cm^{-1}. The appearance of changes in the Raman active vibration modes corresponds to the number of layers. A_1 etc. in the figure show irreducible representations of the vibration mode.