Layered TiS$_2$ single crystals have been reported to possess a large power factor (37.1 $\mu$W/K$^2$) but show a relatively low ZT value (0.16 at 300K) because of a high thermal conductivity (6.8 W/mK). In this study, we intercalate organic molecules (Lewis base) into the van der Waals gap of the layered TiS$_2$ single crystal to form an inorganic/organic hybrid superlattice structure. The thermal conductivity would hopefully be reduced, while the electronic properties would almost be maintained, resulting in an improvement in thermoelectric performance. Various molecules have been intercalated in order to optimize the thermoelectric properties of the hybrid material.

TiS$_2$ single crystal is grown by the vapor transport method. An electrolysis method was then used to intercalate organic molecules into the van der Waals gap of a TiS$_2$ single crystal. The cathode and anode were set as TiS$_2$ single crystal and Pt respectively. The electrolyte is composed of amine hydrochloride solution. The electrolysis reaction was conducted at a voltage around 2.0V for different duration. The electronic properties were measured by the van der Pauw method using a home-made apparatus. The thermal conductivity was measured by the Parallel Thermal Conductance method.

A variety of organic molecules have been successfully intercalated into the van der Waals gaps of TiS$_2$ single crystal, leading to different expansions of the interlayer distance. It was found that the intercalated organic molecules could donate electrons into the TiS$_2$ layers, resulting in an increase in electrical conductivity and a decrease in Seebeck coefficient. The thermal conductivity of this superlattice was found to be sensitive to the manner of arrangement of organic molecules inside the van der Waals gap and consequent interlayer distance. In the case of intercalation of large molecules, such as hexylamine or tri-n-octylamine, the thermal conductivity was significantly reduced and the ZT value was improved compared with the pristine TiS$_2$ single crystal. All the TiS$_2$-based hybrid materials have shown high softness and bending tolerance, which can be considered as a promising mechanically flexible thermoelectric material. Furthermore, robust organic material, such as glycerol was co-intercalated together with the Lewis base and the thermal stability of the hybrid material was found to be improved significantly.

Fig. 1. SEM image of (a) TiS$_2$ nanosheet and (b) cross section of organic/inorganic superlattice of TiS$_2$(Hexlamine)$_x$(Glycerine)$_y$. 