Effect of tin substitute on electrical properties of tantalum thiophosphates $TaPS_6$

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In recent years, with the increasingly serious energy problem, thermoelectric technology has attracted more and more attention due to their clean Peltier cooling and recovery of waste heat energy. We are continuing the development of novel sulfide thermoelectric materials, according to the environmentally and friendly point of view.

In this study, we focus on the tantalum thiophosphate $TaPS_6$ and the substitution materials, Figure 1 shows the crystal structure of mother material $TaPS_6$. Each Ta atom has eight nearest S neighbors, arranged in the form of a double-sided triangular prism. It has complex crystal structure and free channels with a diameter of about 4.65Å. [1, 2]

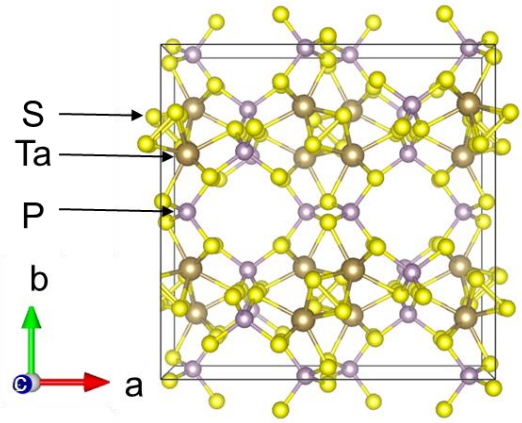

Fig. 1 Crystal structure of $TaPS_6$

According to our preliminary density functional theory (DFT) calculation, undoped $TaPS_6$ is a semiconductor with band gap E_g=830 meV, the calculated $Z_{el}T(=S^2\sigma T/\kappa_{el})$ value will increase to 80-100 by slightly changing of chemical potential.

This study attempts to reduce the chemical potential of $TaPS_6$ by Sn substitution to P-site and investigates the thermoelectric properties of the substitution samples.

The $TaP_{1-x}Sn_xS_6$ (x=0, 0.25, and 0.375) polycrystalline samples were synthesized by melting method. Sealing the starting materials in quartz tube was kept 650℃ for 1 day. After the XRD analysis, the obtained powder samples are pressed in a pellet by hot-press (400℃, 300 MPa).

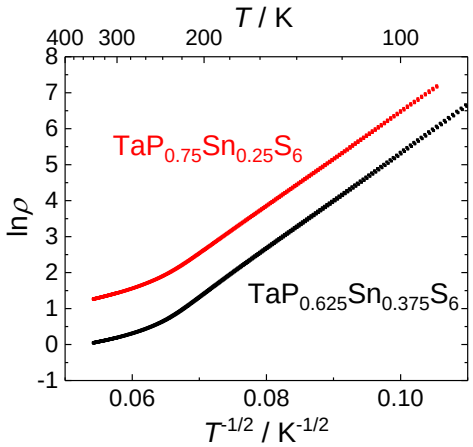

Fig. 2 lnρ-$T^{-1/2}$ curves of $TaP_{1-x}Sn_xS_6$ (x=0.25, 0.375)

We measured the temperature dependence of electrical resistivity ρ. The mother material $TaPS_6$ (x=0) was an insulator, however, the ρ of $TaP_{1-x}Sn_xS_6$ decreases compared to the mother sample (x=0). This result indicates that the Sn substitution makes a hole doping and changes the chemical potential.

The ρ of $TaP_{1-x}Sn_xS_6$ (x = 0.25 and 0.375) decrease with increasing temperature as semiconductor behavior. The data plot of lnρ-$T^{-1/2}$ in the Fig. 2 shows a linear dependence compared to the simple Arrhenius plot. This result suggests that, the carrier conduction mechanism of system is one-dimensional variable-range hopping (VRH).

[1] S. Fiechter and W. F. Kuhs, Acta Cryst, **B36**, 2217-2220 (1980).
[2] K. Momma and F. Izumi, J. Appl. Crystallogr, **41**, 653-658 (2008).