報告番号	※ 甲 第 10395 号

主 論 文 の 要 旨

論文題目 Study on $(Bi_{1-y}B_yS)_n$ $(Ti_{1-x}A_xS_2)_2$ Misfit Layer Sulfide as a Novel Thermoelectric Material
（ミスフィット層状硫化物 $(Bi_{1-y}B_yS)_n$ $(Ti_{1-x}A_xS_2)_2$ の熱電半導体物性に関する研究）

氏　　名 YULIA EKA PUTRI

論 文 内 容 の 要 旨

Thermoelectric materials can help the worldwide demand for energy by converting waste heat into electricity. A single crystal of titanium disulfide (TiS_2) is a potential thermoelectric material because of its high power factor, which is comparable with that of Bi_2Te_3 alloy at room temperature. However, despite its large power factor, the thermoelectric performance of TiS_2 is limited by its relatively large thermal conductivity, so its ZT is not optimum. Reducing the thermal conductivity of TiS_2 by intercalating a bismuth sulfide (BiS) layer into the van der Waals gap to form $(BiS)_{1.2}$ $(TiS_2)_2$ successfully reduced its lattice thermal conductivity without reducing its high power factor. However, electron transfer occurs from the BiS layers to the TiS_2 layers in $(BiS)_{1.2}(TiS_2)_2$, which greatly increases its carrier concentration and electrical conductivity. As a result, the Seebeck coefficient of $(BiS)_{1.2}(TiS_2)_2$ decreases and its power factor is sub-optimum. The study on $(Bi_{1-y}B_yS)_n$ $(Ti_{1-x}A_xS_2)_2$ misfit layer sulfide as a novel thermoelectric material reveals that the thermoelectric performance of this compound can be improved by dope of low valency dopants, as so called the modulation or selective doping. We have tried to dope several dopants from alkaline earth elements and transition metal elements into the different layer; host layer TiS_2 or phonon barrier layer BiS. In this work we have successfully improved the thermoelectric properties of $(BiS)_{1.2}(TiS_2)_2$ misfit layer sulfide through the optimization of carrier concentration by chromium doping. The chromium ions substituted for the titanium sites reduced the carrier concentration and increased the Seebeck coefficient. Unlike other acceptor dopants, chromium increased the effective mass, which further enhanced the Seebeck coefficient. It is assumed that additional resonant states may be formed near the Fermi level which can account for the increase in effective mass and further investigation is required in the near future. The electronic thermal conductivity was significantly reduced due to the decrease in electrical conductivity. Consequently, the overall ZT value measurably improved.