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審査研究科	数理物質科学研究科
学位論文題目	Magnetic Ion Doping and Secondary Phase Assisted Enhancement in Thermoelectric Properties of Chalcopyrite Type Compounds for Energy Applications （エネルギー応用カルコパイライト型化合物における磁性イオンドーピングと第二相の効果による熱電高性能化）

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論　文　の　要　旨

An investigation on introducing magnetism into nonmagnetic thermoelectric materials was made. Namely, it was demonstrated that by substituting a magnetic ion, Mn, into $CuGaTe_2$, a significant enhancement in the power factor was observed. Using theoretical model interpretations and evaluating magnetic properties, it was showed that the power factor surpasses the normal carrier tuning effect. It was indicated that this is because the magnetic ion couples with the electrical carriers and increase their effective mass to a beneficial level. Therefore, these results have demonstrated that magnetic ion doping is an effective technique to improve thermoelectric properties.

Thermoelectric and magnetic properties of $CuIn_{1-x}Mn_xTe_2$, which is another chalcopyrite system, were also investigated. Results showed that the Mn ions doped in $CuInTe_2$ are in the Mn^{3+} state. From the Curie-Weiss fitting, a strong antiferromagnetic interaction between Mn and carriers was inferred, which suggests the magnetic interaction is a probable origin for the enhanced power factor. Thermoelectric and magnetic properties of $CuIn_{1-x}Mn_xTe_2$ provides further evidence of carrier magnetic moments correlations presented Results reinforced the idea of magnetic enhancement in chalcopyrite type compounds and also revealed further that magnetic moment and charge carrier interactions plays an essential role in enhancement of

thermoelectric properties.

Finally, Fe substitution and its effects on thermal transport and structural properties in chalcopyrite-type $CuGaTe_2$ were also investigated. In this case, Fe was found not to dope into the compound atomic sites, but rather was shown to form secondary phases. Thermal conductivity was mainly reduced due to the secondary phase. Thereby, Figure of merit (ZT) was enhanced and maximum value of 0.92 is obtained at 770 K for composition $CuGa_{0.98}Fe_{0.02}Te_2$. This is around 60 % improvement as compared to pristine $CuGaTe_2$. As a result, the role of secondary phases and microstructural analysis towards improvement in thermoelectric properties of chalcopyrite $CuGaTe_2$ was demonstrated.

審　　査　　の　　要　　旨

〔批評〕

A new idea of magnetic enhancement in thermoelectric power factor was apparently presented by the applicant's work. The applicant doped Mn into $CuGaTe_2$ and discovered that the power factor could be enhanced significantly beyond carrier optimization effects. The magnetic ion Mn was indicated to couple with the electrical carriers and as a result enhance the carriers effective mass, and overall lead to an enhancement in the power factor for certain doping levels. A similar magnetic enhancement effect was also shown by the applicant for Mn doped $CuInTe_2$. This is an interesting effect and well researched and indicated. Furthermore, a different effect was found for composite materials, when Fe doping into $CuGaTe_2$ was found to have little solubility, and resulted in the formation of secondary phase which selectively scattered phonons effectively, leading to an especial decrease in the thermal conductivity. Overall this effect led to substantial enhancement of ZT.

The applicant has achieved interesting results into control over electrical, thermoelectrical, and thermal properties, to achieve enhancement in thermoelectric performance. The magnetic ion doping enhancement appears to be especially interesting and opens opportunities for magnetic enhancement in other thermoelectric materials also, and appears to be of wide impact. It is judged that the work by the applicant merits awarding of PhD of Engineering.

〔最終試験結果〕

The final examination committee conducted a meeting as a final examination on February 19, 2019. The applicant provided an overview of dissertation, addressed questions and comments raised during Q&A session. All of the committee members reached a final decision that the applicant has passed the final examination.

〔結論〕

Based on the results of the above-mentioned dissertation defense and final examination, the final examination committee approved that the applicant is qualified to be awarded Doctor of Philosophy in Engineering.