Improvement of thermoelectric conversion properties by controlling local crystal structure in half-Heusler NiZrSn compounds

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Half-Heusler NiZrSn compounds have excellent thermoelectric properties [1], mechanical strength [2], and oxidation resistance [3], and are being commercialized for the development of thermoelectric power generation devices that operate in high temperature environments. The excellent thermoelectric conversion properties of half-Heusler NiZrSn compounds are attributed to their semiconducting electronic structure with a narrow band gap near the Fermi level and low thermal conductivity. The half-Heusler structure with high crystal symmetry inherently results in high thermal conductivity, but this is inconsistent with actual experimental results. Therefore, in order to elucidate the origin of the high thermoelectric conversion properties in half-Heusler NiZrSn compound, we have investigated the detailed crystal structure of half-Heusler NiZrSn compound by synchrotron powder diffraction [4] and X-ray absorption fine structure measurements [5]. As shown in Fig. 1, interstitial atomic defects exist in the vacancy sites and the surrounding atoms are distorted. This has been found to contribute to a significant decrease in thermal conductivity and a pseudogap-like semimetallic electronic structure can be formed and the thermoelectric properties can be controlled by Fermi-level control. In this presentation, we will show that high thermal conversion properties can be realized by utilizing the defect structure at the vacancy site, together with the latest research results.

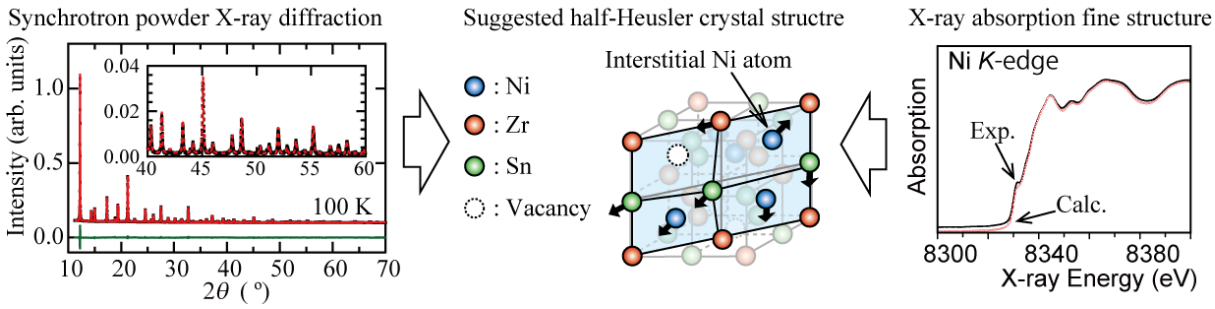

Figure 1 Local structure of the half-Heusler structure proposed by X-ray diffraction and XAFS measurements in the half-Heusler NiZrSn compound. The constituent atoms around the Ni atoms invaded into the vacancy site are distorted.

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