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Crystal structure and physical properties of U-based skutterudites

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Among the filled-skutterudite structure compounds, only UFe_4P_{12} is known as the uranium-based skutterudite. As reported for the rare-earths skutterudites, the structural stability decreases with increasing the atomic number because the ionic radius of heavy rare-earth is too small to be filled in the cage formed by pnictogens. Because of the small ionic radius of uranium, it is believed that the skutterudite structure with uranium is not very stable.

In the previous x-ray diffraction study, the existence of defects at the uranium site was reported (occupancy number 0.95) which might be attributed to the structural instability mentioned above. It should be noted, however, the occupancy number looks small when the thermal vibration such as the rattling motion reported for other skutterudites is large.

In the present study we have carried out the x-ray diffraction experiments using the single crystal to determine both the occupancy number and the isotropic atomic displacement factors $B_{\rm iso}$. The single crystal of UFe_4P_{12} was grown by the Sn-flux method. It is characterized as an insulating ferromagnet with $T_{\rm C} = 3$ K by measuring magnetization, specific heat and resistivity[1]. The ^{31}P-NMR can be explained by the transferred field from uranium ions without defects on the uranium site[2].

Cubic structure (space group $Im\bar{3}$) with the lattice parameter $a = 7.768$ $\mathring{A}$ was confirmed as reported previously. The isotropic atomic displacement factor $B_{\rm iso}$ was determined to be 0.49 at room temperature, which is similar to the other uranium compounds such as UBe_{13} indicating the absence of the rattling motion. The site occupancy for the uranium sites is 1 within an experimental error. This result is consistent with the insulating behavior without conduction carriers from impurities as well as the NMR observation.

[1] T.D. Matsud *et al*, JPSJ 73 (2004) 2533.

[2] Y. Tokunaga, 6b4, this workshop.