X-ray Diffraction Studies of URu_2Si_2 and UPd_2Si_2

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URu_2Si_2 (the tetragonal $ThCr_2Si_2$ type crystal structure; space group *I*4/*mmm*) has attracted much interest because of its peculiar phase transition at 17.5 K ($\equiv T_o$) [1-3]. A sharp peak anomaly of 5f-electronic specific heat at T_o, which involves an entropy reduction of ~ 0.3*R*ln2, indicates a freezing of some degree of freedom of 5f electrons below this temperature. However, despite more than 25 years of intense research trying to identify the order parameter, the intrinsic nature of the phase transition has not been elucidated. The phase transition of URu_2Si_2 has thus been called the "hidden order (HO)", and much effort has now been focused on direct detection of the broken symmetry by using various microscopic techniques [4].

The isostructural compound UPd_2Si_2 shows two successive antiferromagnetic phase transitions at 108 K ($\equiv T_{Nl}$) and 135 K ($\equiv T_{Nh}$). The magnetic structure in the higher temperature range between T_{Nl} and T_{Nh} is a novel longitudinal, sinewave incommensurate structure with a wave vector of $\boldsymbol{q} \sim 0.73\ \boldsymbol{c}^*$ and magnetic moments aligned along the *c* axis [5]. Below T_{Nl}, the system undergoes a first-order phase transition, and a simple type-I structure ($\boldsymbol{q} = \boldsymbol{c}^*$) becomes stable. The magnetic phase diagram constructed in the field range up to 80 T of this material is fairly well described in terms of a phenomenological, frustrating local spin model called the axial-next-nearest-neighbor-Ising (ANNNI) model [6].

The $ThCr_2Si_2$ structure includes a free position parameter, *z*, of the Si 4(e) site. Since the Si ions are located at the nearest-neighbor position of the U ions, the precise determination of the *z* parameter would provide useful information for evaluation of hybridization effects of 5f orbits with Si s, p states, calculations of a band structure, analyses for ^{29}Si-NMR spectra, and so on. These pieces of knowledge might offer a clue to solving the issue of HO in URu_2Si_2 and a microscopic-level understanding of the magnetic interactions in UPd_2Si_2. We will report our latest studies of structural analyses of these materials based on the X-ray diffraction measurements performed in the temperature range 7 K ≤ *T* ≤ 300 K at BL-8A and 8B in the Photon Factory KEK.

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