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X-ray diffraction experiments in quadrupolar Kondo candidate $PrTi_2Al_{20}$ and PrV_2Al_{20}

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Crystal structure analyses in $PrTr_2Al_{20}$ (Tr = Ti and V) has been carried out. We found that Pr-Al cage for PrV_2Al_{20} is anisotropically deformed from sphere, which modify the crystalline-electric-field levels of Pr^{3+}. The information would provide a clue to understand the anomalous properties in $PrTr_2Al_{20}$.

1 Introduction

Non-magnetic $PrTr_2X_{20}$ (Tr = transition metal, X = Al and Zn) compounds have been extensively studied as candidates for the two channel (quadrupolar) Kondo effect. In PrV_2Al_{20}, magnetic susceptibility and electric resistivity show anomalous $T^{1/2}$ behavior at low temperatures, which is in good accordance with the theoretical prediction for the two channel Anderson lattice model [1]. In stark contrast, $PrTi_2Al_{20}$ shows T^2 behavior below ~ 20 K. They show quite different ordering behavior. $PrTi_2Al_{20}$ shows ferro-quadrupolar order at T ~ 2 K [2]. In contrast, PrV_2Al_{20} shows successive non-magnetic anomalies at much lower temperatures around 0.6 K, of which the origin is suggested to be antiferro-quadrupolar type [3]. The crystal-electric-field (CEF) levels of Pr^{3+} in $PrTi_2Al_{20}$ were determined as Γ_3 (quadrupolar- and octapolar-active ground state) - Γ_4 (5.61) - Γ_5 (9.30) - Γ_1 (13.5 meV), whereas it was not explored in PrV_2Al_{20} [2]. The detailed knowledge on the crystal structures would provide a clue to understand the difference of the anomalous transport behavior. Thus, we reinvestigated crystal structure analysis of the $PrTr_2Al_{20}$.

2 Experiment

X-ray diffraction experiments were performed using single crystals with diameters of about 30 μm on the BL-8A. The photon energy of the incident X-rays was tuned at 18 keV. X-ray beams were shaped into a square of 200 x 200 μm^2 by a collimator. The intensity data were converted to the |F|-tables by using Rapid- Auto program, Rigaku. We used CrystalStructure program of Rigaku for analyzing the crystal structure from the |F|-table.

3 Results and Discussion

The crystal structure analyses for single crystals of $PrTi_2Al_{20}$ and PrV_2Al_{20} were performed. The comparisons between observed and calculated structure factors are shown in Fig. 1(a). The crystal structure consists of two Al-cages with individually capturing Pr and Tr atoms as shown in Fig. 1(b). The CEF x and W parameters were known as x s= 0.25(1) and W = -1.53(3) K for $PrTi_2Al_{20}$ [2]. Using the point charge calculation based on the refined structural parameters of Tr = Ti, we estimated the Al-charges that are consistent with the x and W parameters. The estimated Al-charges are +0.9 for Al(1) and +0.88 for Al(3). Next, we assumed that Al-charges estimated at Tr = Ti are also applied to Tr = V, and obtained x ~ 0.41 and W ~ -2.1 K using the point charge model based on the refined structural parameters for Tr = V. By these parameters, the CEF excited levels can be estimated as Γ_4 ~ 5.6, Γ_5 ~ 11.1, and Γ_1 ~ 13.5 meV for PrV_2Al_{20}. Detailed information is found in [4].

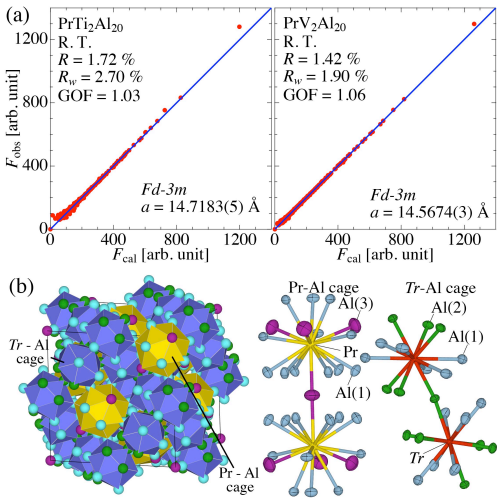

Fig. 1: (a) Observed (F_{obs}) and calculated (F_{cal}) structure factors for $PrTr_2Al_{20}$ (Tr = Ti and V). (b) Schematic of crystal structure of $PrTr_2Al_{20}$.

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