Crystalline Electric Field Excitations in Pr3Pd20Ge6

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Pr3Pd20Ge6 crystallizes in the cubic Cr23C6-type structure (Fm3m) with two inequivalent Pr sites of 4a (Oh) and 8c (Td). The previous experiments of inelastic neutron scattering (INS) [1] and high-field magnetization [2] suggested that the crystalline-electric-field (CEF) lowest level of the Pr 4f electrons is the quadrupole doublet Gamma3 for both the 4a and 8c sites. On the other hand, the elastic constant c44 was found to show a 1/T behavior at low temperatures [3], which cannot be account for sorely by the Gamma3 ground state. We also found that the magnetic susceptibility of this compound shows no tendency of saturation down to 0.1 K, indicating that the 4f electrons should have a magnetic ground state in at least one of the Pr sites [4]. From the detailed CEF analyses on the M(B, T) and C(B, T) results, we proposed that the magnetic Gamma5 triplet sits at the lowest level in the 4a site while the G3 doublet is in the 8c site [4]. This ”two-site” CEF scheme semi-quantitatively well reproduces the B and T variations of magnetization and specific heat, particularly the step-like fine structures observed in the low-temperature M(B) curves and a field-induced first order phase transition. The energy separations between the lowlying two levels are estimated as Gamma5(0)-Gamma3(~0.5 meV) and Gamma3(0)-Gamma5(~0.3 meV) for 4a and 8c sites, respectively. These excitations, however, are difficult to be distinguished from each other by the energy resolution in the previous INS measurements. In the present project, we reperformed the INS experiments for a powdered Pr3Pd20Ge6 sample on the triple axis spectrometers PONTA at 5G beam hole and HER at C1-1 of the JRR-3M reactor in JAEA, extending the energy window up to 15 meV and improving the energy resolution down to ~ 0.1 meV, respectively. We have observed significant fine structures in the INS spectra. Their intensities and temperature dependencies are quantitatively well reproduced by the numerical calculations based on the two-site CEF model. The CEF parameters determined here, however, are slightly larger than those obtained from the magnetization data, but they give more reasonable fits for C(T). The reanalyses on the M(B, T) curves are now in progress.

[1] L. Keller et al., Physica B 259-261 (1999) 336.
[2] M. Nakayama et al., Physica B 281&282 (2000) 152.
[3] T. Horino et al., Physica B 281&282 (2000) 576.
[4] H. Amitsuka et al., J. Phys. Soc. Jpn. 71 (2002) suppl. 124.

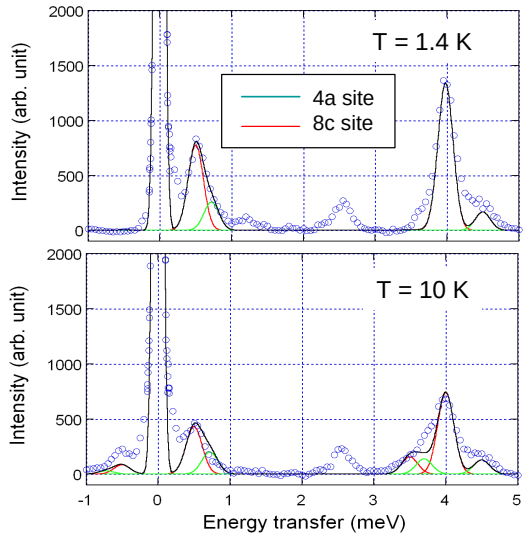

Fig. 1. Part of the inelastic neutrn scattering spectra of Pr3Pd20Ge6 obtained by using C1-1(HER). The lines are numerical calculations based on the two-site CEF model. The peaks observed at about 1.2 meV and 2.5 meV are spurious.