Crystalline electric field excitation of $Nd_3Co_4Sn_{13}$

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Topological electronic states in chiral crystal structure attract attentions in condensed matter physics fields [1]. We have studied materials exhibiting phase transitions to chiral symmetry structures to establish spontaneous formation of the topological electronic state. Further, magnetic ordering is attractive because of breaking of time-reversal symmetry in addition to breaking of spatial inversion.

The $R_3Co_4Sn_{13}$ class of materials undergo structural transformations to the chiral structures [2, 3]. The R = Ce compound shows a semimetal behavior, and the R = La one is a superconductor below 2.7 K. It is noteworthy that these properties are expected to be associated with the topological electrons under the chiral crystal structure. In present study, we investigated 4*f*-electron state in $Nd_3Co_4Sn_{13}$, which was reported to show a structural superlattice below 124 K and magnetic ordering at 2.1 K [4, 5].

Inelastic neutron scattering (INS) experiments for the sample of $Nd_3Co_4Sn_{13}$ synthesized using the molten Sn-flux method was performed at the triple-axis spectrometer PONTA (5G). Measurement was conducted with final neutron energy fixed at 14.685 meV.

Figure 1 shows INS spectra at fixed Q = 3 $Å^{-1}$ of $Nd_3Co_4Sn_{13}$. Red and blue marks are data measured at 2.3 and 100 K, respectively. The spectrum at 2.3 K comprises broad response located between 5 and 25 meV, and the 100 K data show an additional peak near 5 meV. The observed intensities are attributed to excitations between the crystalline electric field (CEF) splitting levels of Nd^{3+} $4f^3$ electronic states because the Q dependence of scattering intensity in the fixed energy transfer is consistent with the magnetic form factor. Considering the structural superlattice, we suppose the two inequivalent Nd-ion Wyckoff sites in $Nd_3Co_4Sn_{13}$ as in $R_3Co_4Sn_{13}$ (R = La and Ce). The J = 9/2 multiplets for total angular momentum should split into five Kramers doublets, and four excitations should occur at low temperatures. Thus, we expect eight excitation peaks at most. A least-squares fitting analysis of the 2.3-K data based on eight Gaussian INS peaks together with an incoherent elastic peak and a background slope was conducted. The spectral width was evaluated by the approximate form of E_i dependence of resolution width [6] and the incoherent elastic peak width. The result shown by thick red line comprised of the Gaussian components (thin red lines) reproduces the observed result. It is a further issue to determine the CEF ground-state wave function to discuss a magnetic ordering mechanism.

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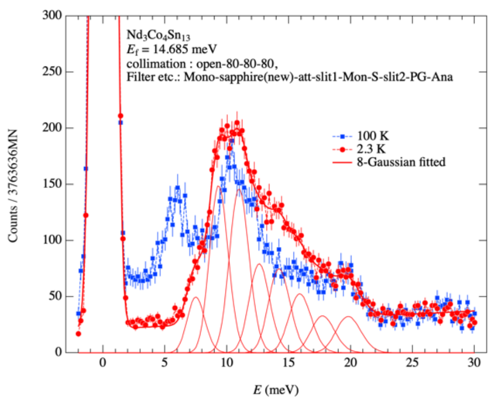

Fig. 1. INS spectra at fixed Q = 3 $Å^{-1}$ of $Nd_3Co_4Sn_{13}$. Red and blue marks are data measured at 2.3 and 100 K, respectively. Thick red line is a fitted result to the 2.3-K data, and thin red lines are Gaussian components.