Inelastic Neutron Scattering Study of Crystal Electric Field Excitations in the Antiferromagnetic Topological Insulator NdBi

Y. Fukushima[A], H. S. Suzuki[A], H. Saito[A], T. Nakajima[A], T. Kondo[A]

[A]ISSP, The Univ. of Tokyo

Recently, the rare-earth monobismuthide NdBi has attracted significant attention as a promising candidate for an antiferromagnetic topological insulator (AFM-TI)[1]. NdBi has a NaCl crystal structure and shows type-A antiferromagnetic order, where ferromagnetic (001) planes are stacked antiferromagnetically along the c-axis. At the topmost surface layer, this ferromagnetic order breaks time-reversal symmetry, opening a gap at the Dirac cone. Within this energy gap, a one-dimensional, spin-polarized electronic state is expected to emerge, providing a dissipationless conduction channel highly desired for next-generation spintronics.

Beyond its exotic topological properties, NdBi is particularly attractive due to its unusually high magnetic transition temperature (T_N = 24 K). This transition temperature is nearly eight times higher than expected from standard de Gennes scaling in other rare-earth monobismuthides (~3 K). However, the microscopic origin of this anomalously strong coupling remains elusive. A sister compound CeBi also exhibits a high transition temperature. In CeBi, it is well-established that a strong interaction between the Ce 4f and Bi 6p orbitals (p-f mixing) drives this behavior. Because the Bi 6p valence band forms two Fermi pockets possessing Γ_8 symmetry, it couples strongly with the rare-earth 4f electrons that share the same Γ_8 symmetry within the crystal electric field (CEF) split levels. Consequently, this intense p-f interaction stabilizes the Γ_8 state as the ground state, reversing the standard CEF ground state for an NaCl-type crystal structure where the Γ_7 state should typically be the most stable. To determine whether a similar p-f interaction scenario is responsible for the enhanced transition temperature in NdBi, it is crucial to experimentally identify its CEF level scheme and establish the true ground state symmetry.

Inelastic neutron scattering (INS) experiments were performed to observe the CEF excitations of NdBi. The measurements were conducted at the PONTA-5G beamline. Single-crystal samples of NdBi were loaded into an aluminum cell and cooled down to 2.3 K using a closed-cycle helium refrigerator.

Figure 1 shows the inelastic neutron scattering spectra of NdBi measured at paramagnetic phase of 42 K. Excitation peaks corresponding to transitions between the CEF split levels of the Nd^{3+} ions were successfully observed in addition to a dispersive phonon mode. Our quantitative analysis revealed that the Γ_8 is the ground state. This result supports the p-f interaction scenario for the anomalously high transition temperature in NdBi.

To gain a more comprehensive understanding of this mechanism, analysis of the INS data within the AFM phase is currently underway. Resolving the exchange-splitting of the CEF levels in the magnetically ordered state will provide further critical insights into the microscopic anisotropy and strength of the p-f interaction.

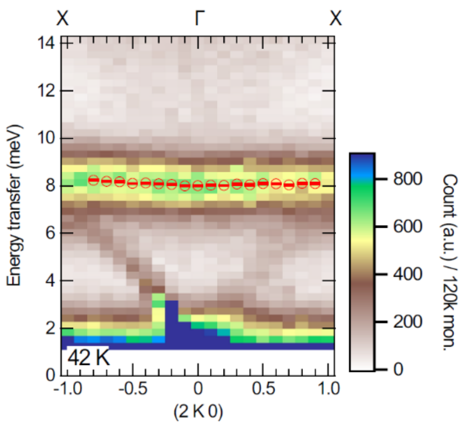

Figure 1 Inelastic neutron scattering spectra of NdBi measured at 42 K.

[1] A. Honma *et al.* Nat. Commun. **14**, 7396 (2023).