Stable Topological Insulator Bi₂Te₃ Created by Ion Beam Irradiation

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1. Introduction

To date, ion beam irradiation on the topological matter has not been nearly imagined what would be happened to its topological properties. It is not well understood how implanted ions into the matter have to do with the topology. Depending on beam energy, ion species, and fluences, the irradiation may result in substantial distinct effects for the matter, thus finding optimum irradiation condition in achieving practical application materials becomes one of the important issues. Since topological matter with stable surface conduction channel is generally hard to find in an as-grown narrow band-gap semiconductor Bi₂Te₃, we employed the beam irradiation technique to realize the practical stable topological matter in this work.

Topological insulators (TIs) consist of charge carriers at the surface, characterized by an intrinsic chirality of spin-momentum with locking suppression of backscattering, making them of interest in spintronics [1-3]. The constituent atoms of TIs are typically heavy elements with strong spin-orbit coupling (SOC), by which a 'band inversion' can be observed at the surface band structure. Relativistic modifications of the band structure closely linked to strong SOC can influence nuclear magnetic shielding, and thus may be detectable by one of the local sensitive methods such as nuclear magnetic resonance (NMR).

Herein, we have irradiated ion beam onto topological insulator Bi₂Te₃, with various ion species, irradiation energy, and fluences. For H⁺ beam irradiated sample, higher density defects created were manifested by analysis of NMR spectra depending on the temperature. After H⁺ beam irradiation, orbital contribution in NMR Knight shift turns out to increase, whereas the freecharge carriers at the Fermi level dominantly contribute to the Knight shift in the unirradiated sample [3]. For Cu⁺ beam-irradiated sample, we found that the ferromagnetic coupling increases, exhibiting higher remanent magnetization and coercive field compared with the unirradiated sample showing unexpected ferromagnetic coupling. ¹²⁵Te NMR spectra and spin-lattice relaxation time (T₁) for Cu⁺ beam-irradiated sample are discussed in detail in view of achieving stable topological insulator.

2. Experiments

Polycrystalline Bi₂Te₃ with a purity of 99.99% from Sigma Aldrich was used as received without further purification, and is of a fairly large (μ m) average grain size. Particle sizes measured are mean values determined from a field emission scanning electron microscope. Powder X-ray diffraction (PXRD) was also used to confirm the crystallinity of the samples using a Philips XPERT MPD x-ray diffractometer with Cu K α (λ = 1.5405 Å) radiation. The H⁺, Cu⁺, and Cr⁺ beam irradiations were performed using ion beam facilities at the Korea Multi-purpose Accelerator Complex (KOMAC). ¹²⁵Te NMR data were acquired with a Bruker Avance II⁺-400 solid-state NMR spectrometer operating at 126.3 MHz. Spectral data were acquired using a spinecho sequence [($\pi/2$)_x- τ -(π)_y-acquire] with the echo delay τ set to 20 μ s. The NMR spectra were obtained at various temperatures of 180K–450K.

3. Experimental Results and Discussion

3.1 Calculated Implantation Profiles for H⁺ beam

Figure 1 shows a distribution of implantation depths and profile for the 200 keV H⁺ beam on Bi₂Te₃, Bi, and Te layers using the SRIM2008 package. The computer simulation of ion stopping gives us a reliable means for simulating the implantation profile. The results indicate that the mean implantation depths are about 1.36, 1.19, and 1.50 μ m for the Bi₂Te₃, Bi, and Te layers, respectively. The shorter penetration depth is thus mainly due to Bi atoms, whereas the longer depth is due to Te atoms.



Fig. 1. Calculated implantation profiles for H^+ in Bi₂Te₃, Bi, and Te from SRIM2008 with an energy of 200 keV used in the experiment.



Fig. 2. a) ¹²⁵Te NMR spectra measured at various temperatures of Bi_2Te_3 before and after H⁺ irradiation. The vertical dashed lines denote the central frequency of the spectra at 180 K. (b) ¹²⁵Te NMR spectra at 180 K together with the fitted red lines by a single Lorentzian function for Bi_2Te_3 before and after irradiation.

The simulation calculates the data without taking account of the crystal structure of the host, and thus excludes implantation channeling, based on the binary collision approximation. Considering our polycrystalline structured sample, it is possible for such channeling to occur, thus resulting in a long tail of the implantation profile deeper into the crystal.



Fig. 3. 125 Te NMR spectra for Cu⁺ beam irradiated Bi₂Te₃ under various fluences, together with the spectrum of unirradiated

sample measured at room temperature. The vertical dashed line denotes the central frequency of the spectrum for the unirradiated sample.

3.2 ¹²⁵Te NMR spectra for H^+ beam-irradiated Bi₂Te₃

Figure 2(a) shows the ¹²⁵Te NMR spectra measured at various temperatures for Bi2Te3 before and after irradiation. All the spectra exhibit a single structureless line, and were well fitted by a single Lorentzian function. The ¹²⁵Te resonance line shapes are clearly asymmetric as evidenced by a slight inconsistency between the symmetric Lorentzian lines and the spectral lines (Fig. 2(b)). This asymmetry appears to be stronger after beam irradiation. arising predominantly from an inhomogeneous distribution of defects with the introduced charge carrier concentrations having different Knight shifts. None of the spectra exhibit shoulder peaks at the negative frequency, which was attributed to TI surface electronic states. On the other hand, the peak in the positive frequency shifts may arise from the bulk electronic states, as displayed in Fig. 2.

3.3 ¹²⁵Te NMR spectra for Cu⁺ beam-irradiated Bi₂Te₃

Figure 3 shows the ¹²⁵Te NMR spectra measured at various temperatures for Bi₂Te₃ before and after Cu⁺ beam irradiation. All the spectra for the irradiated samples exhibit broaden linewidths compared to that of the unirradiated sample, and were well fitted by two

Lorentzian functions. The line broadening in the irradiated samples may be ascribed to the sample inhomogeneity and/or the ferromagnetic coupling created by the introduction of Cu^+ ions. The analysis for the spectra at various temperature will be discussed in detail in the presentation. In addition, the carrier concentration in the Fermi level would be discussed from the T_1 data.

3. Conclusions

In summary, we have investigated the bulk electronic states in the topological insulator Bi_2Te_3 by employing NMR spectroscopy. We have observed the perturbed electronic states which were induced by H^+ and Cu^+ beam irradiation. The change in the Fermi level before and after irradiation was observed by the Knight shifts and spin-lattice relaxation rates.

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