AMTC Letters
Vol. 2 (2010)

Observation of the Anisotropy of Inelastic Scattering Cross-Section of the Boron *K*-shell Excitation of MgB_2

K. Momonoi[1], K. Saitoh[2] and N. Tanaka[2]

[1]Department of Crystalline Materials Science, Nagoya University, Nagoya, 464-8603, Japan
[2]EcoTopia Science Institute, Nagoya University, Nagoya, 464-8603, Japan

When a fast electron penetrating a solid experiences an inelastic scattering accompanied by an inner-shell excitation, the momentum transfer (**q**) dependence of the inelastic scattering cross section, differential in angle, becomes anisotropy if initial state $|i\rangle$ and final state $|f\rangle$ is of anisotropy. Botton observed the two-dimensional angular distribution of inelastic scattered electrons using a post-column energy-filtering system for transmission electron microscopy [1]. This technique was applied to a single carbon nanotube and the partial EELS spectra were obtained by the analysis of this experiment [2].

The present paper is aimed to obtain a **q**-dependence of inelastic scattering cross section and the partial EELS spectra accompanied by the boron *K*-shell excitation $|1s\rangle \rightarrow |2p\rangle$ of MgB_2. It is known that boron $2p$ orbitals splits into $2p_{xy}$ and $2p_z$ orbitals because of the hexagonal symmetry of the MgB_2 structure. Inelastic scattering angular distributions were taken by using JEM-2010FEF operated at 120kV equipped with Gatan Imaging Filter. The incident direction was perpendicular to the *c*-axis. A series of inelastic scattering angular distributions was obtained at successive energy losses from 160 eV to 230 eV. Figs.1(a), 1(b), 1(c) and 1(d) show inelastic scattering distributions at energy losses of 180 eV (pre-edge of boron K-shell excitation), 190 eV, 198 eV and 204 eV respectively. Fig.1(a) shows an isotropic distribution which has the peak at the origin (q_{xy}, q_z) = (0, 0). On the other hands, Fig.1(b) shows an anisotropic distribution which is extended to the q_z direction indicating the contribution of $|1s\rangle \rightarrow |2p_z\rangle$ excitation. Fig.1(c) again shows an isotropic distribution. Fig.1(d) shows an anisotropic distribution, which is extended to the q_{xy} direction, indicating the contribution of $|1s\rangle \rightarrow |2p_{xy}\rangle$ excitation.

It is considered that each scattering patterns is an incoherent superposition of the inelastic cross sections accompanied by the $|1s\rangle \rightarrow |2p_{xy}\rangle$ and $|1s\rangle \rightarrow |2p_z\rangle$ excitations. By the quantitative comparison of the experimental and simulated scattering patterns, the weight coefficients of the two components p_{xy} and p_z was obtained as the function of energy loss, that is to say the partial EELS spectra. Fig.2 shows the partial EELS spectra of the p_{xy} and p_z components. The partial EELS spectra show a good agreement to the partial density of states which is obtained by the first principle calculation [3].

References
[1] G. A. Botton, *J. Electron Spectrosc. Rel. Phenom.* **143** (2005) 129.
[2] K. Saitoh, K. Nagasaka and N. Tanaka, *J. Electron Microsc.* **55** (2007)
[3] R. F. Klie , Y. Zhu, *Phys. Rev. B* **73**, 014513 (2006).

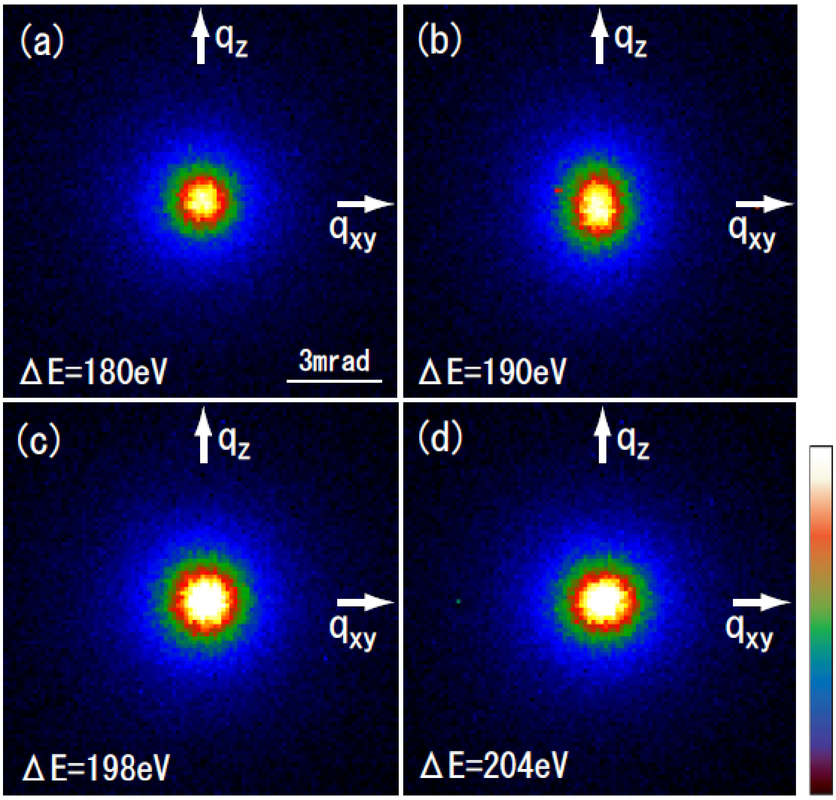

Fig.1. Series of inelastic scattering distributions of MgB_2 at energy losses of 180 eV (a), 190 eV (b), 198 eV (c) and 204 eV (d). Anisotropic scattering distributions in (b) and (d) indicate the excitations of $|1s\rangle \rightarrow |2p_z\rangle$ excitation and $|1s\rangle \rightarrow |2p_{xy}\rangle$, respectively.

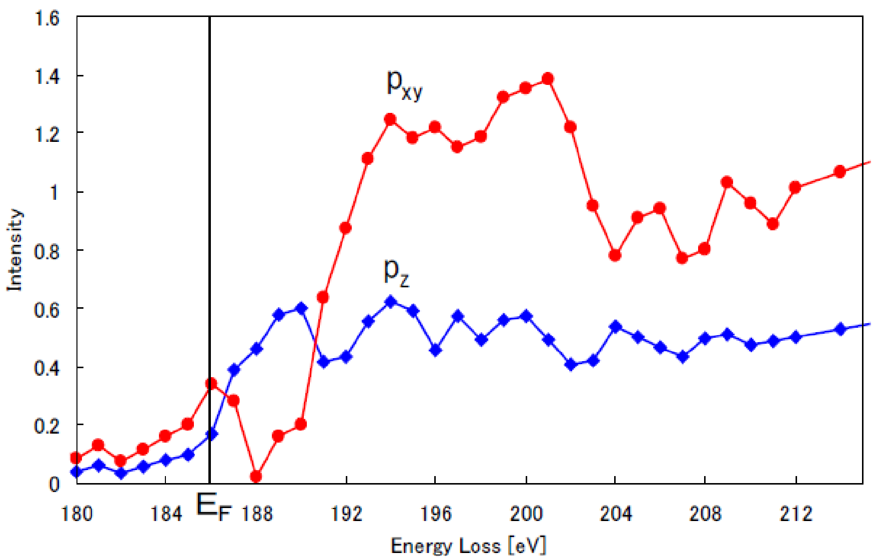

Fig.2. Partial EELS spectra of the boron p_{xy} and p_z components. The red and blue lines show p_{xy} and p_z components, respectively. E_F indicates the Fermi energy at 186 eV.