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Electronic Structure of Ca 3d Levels of Superconducting CaC_6 using Soft X-rays Absorption and Emission Spectroscopy

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1 Introduction

CaC_6 is known as a superconductor with the highest superconducting transition temperature, T_c, of 11.5 K among graphite intercalation compounds (GICs) [1]. The mechanism of superconductivity of alkali-metal GIC might be due to a large charge transfer from alkali metal to carbon layers. However, in CaC_6, theoretical calculations suggest that Ca 3d electrons forms an interlayer (IL) band and will play an important role on the superconductivity, which is consistent with Ca isotope effect and photoelectron experiments [2-5]. XAS and XES near Ca-L edge give unoccupied and occupied partial electron density of states of Ca 3d levels, respectively. The purpose of the present study is to elucidate the electronic structures of Ca 3d in CaC_6 using XAS and XES methods.

2 Experiment

Sample was synthesized by a conventional liquid-solid reaction between molten Li-Ca alloy and the graphite. As the graphite, HOPG plates and/or Grafoil sheets were used. X-ray diffraction patterns show that the samples are almost single phase of first stage CaC_6 with a small amount of intermediate products, Li-GIC. In these patterns, only (00l) peaks are observed, which suggests that the normal axis of the sample plate is highly oriented to the *c*-axis, however they are not the single crystals. It is noted that there is no trace of Ca compounds without CaC_6 in XRD pattern. A magnetization measurement shows the Meissner effect below 11.5 K.

XAS and XES experiments were performed at BL-19B and 2C in KEK-PF.

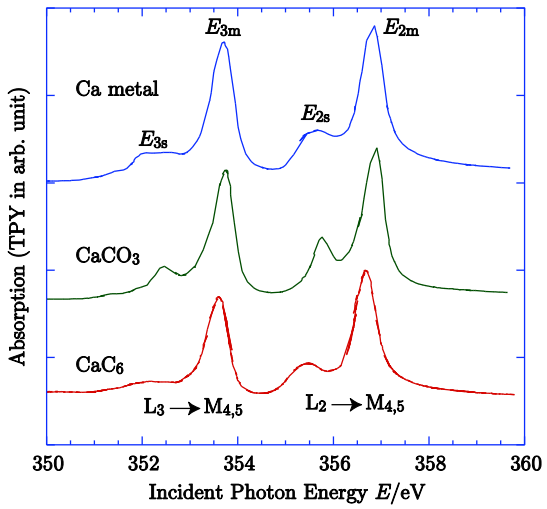

Fig.1: Ca-L XAS spectra of Ca metal, $CaCO_3$ and CaC_6.

3 Results and Discussion

Figure 1 shows Ca-L XAS spectrum of CaC_6. It shows the clear two peaks correspond to the L_2 and L_3 edges. A small satellite peak is observed on the low energy side. In comparison with the spectra of Ca metal and CaCO3, observed satellite peak suggests that Ca in CaC_6 is metallic rather than ionic. Figure 2 shows XES spectra with the excitation energies of E_{3m} in XAS spectra. It shows an elastic peak and some inelastic peaks. These inelastic spectra consist of fluorescence and Raman peaks. The fluorescence spectra indicate that considerable amount of Ca 3d electrons are in occupied states with the hybridization with Ca 4s and C 2p, consistently with the XAS results. The present result supports the important role of Ca 3d in the superconductivity of the compound, as previous theoretical and experimental studies.

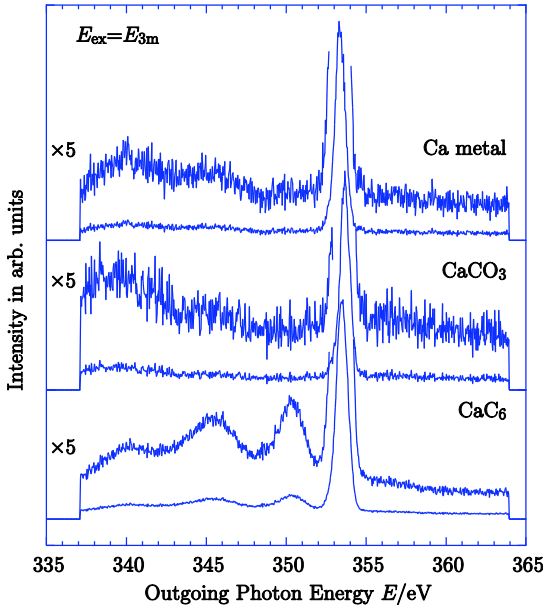

Fig.2: Ca-L XES spectra of Ca metal, $CaCO_3$ and CaC_6.

References

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