Biological Science

12C/2008G582

Analysis of Cu K-edge XANES spectra in COMMD1 with Multiple scattering Theory

Kei TAKAHASHI[1], Hiroyuki TAKI[2], Takahito MARUO[2], Yoshihiro MIYAGAWA[1],Takehisa KONISHI[1], Takashi FUJIKAWA[1] Naoto YONEZAWA[2], Masaharu NOMURA[3]
[1]Graduate School of Avanced Integration Science, Chiba University,
1-33 Yayoi-cho, Inage, 263-8522 Chiba, Japan
[2]Department of Chemistry Chiba University, 1-33 Yayoi-cho, Inage, 263-8522 Chiba, Japan
[3]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan

Introduction

COMMD1 belongs to COMMD (COpper Metabolism gene MURR1 Domain) family and, in human, the family consists of 10 members. COMMD1 has 190 amino acids residues. In COMMD family, COMMD1, which is related to copper metabolism[1], has been most studied. Although its N-terminal domain structure has been reported[2], its full length structure and the residues which bind the Cu ion are not known. In order to specify the amino acid residues which surround the Cu ion, XANES and EXAFS measurement and the multiple scattering analysis of Cu K-edge XAFS spectra are carried out.

Experimental

COMMD1 were dissolved in Tris buffer (20mM Tris, 100mM NaCl, pH7.5). Cu K-edge X-ray absorption measurements were performed on three samples with the concentration of protein of 1mM and the concentration of Cu of 40μM, 200μM and 400μM. The measurements were performed at BL-12C of Photon Factory equipped with a Si(111) double crystal monochromator. X-ray absorption spectra were recorded in the fluorescence mode using a 19 element solid state detector[3]. The protein solutions were sealed in PET sample cells which have polyimide windows and frozen by liquid nitrogen prior to the measurements. The samples were kept at 100K using a cryocooler during the measurements.

Theory

Cu K-edge XANES spectra are calculated with multiple scattering theory[4]. The X-ray absorption cross section at site *A* is given by.

$$\sigma = -\frac{8}{3}\mathrm{Im}\left[\sum_{m_c,L,L'} i^{l-l'}\exp\{i(\delta_l^A+\delta_{l'}^A)\}\rho_c(l)\rho_c(l')G(L_c10|L)G(L_c10|L')(t^{-1})_{LL'}^{AA}[(1-X)^{-1}]_{LL'}^{AA}\right] \quad (1)$$

$$X_{LL'}^{\alpha\beta} = t_l^{\alpha} G_{LL'}(\mathbf{R_a}-\mathbf{R_b})(1-\delta_{\alpha\beta})$$

$(1\text{-}X)^{-1}$ accounts for the full multiple scattering in the model cluster. T-matrix t_l^{α} at site α reflects the electronic state of atom α. Green function $G_{LL'}$ contains information about the geometrical structure around the X-ray absorbing atom.

Result and Discussion

Fig.1 shows EXAFS spectra and Fig.2 shows calculated and experimental XANES spectra. These data imply that local environment of the Cu ion changes with increasing the concentration of the Cu ion. In theoretical XANES spectra, a structure model which consists of four amino acids which are two Histidine, Serine, and Lysine was considered. Further analysis is now under way to obtain detailed local structural information.

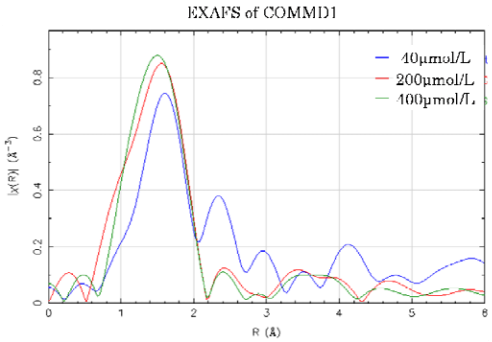

Fig.1: Fourier transformed EXAFS spectra
The numbers are the concentrations of Cu ion

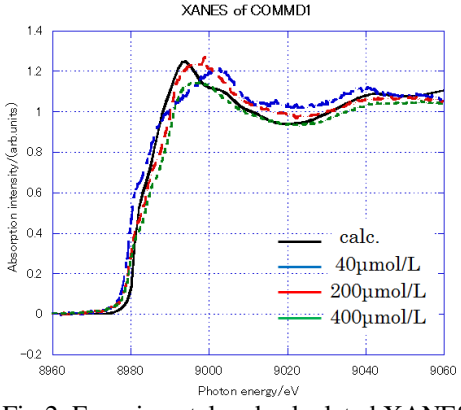

Fig.2: Experimental and calculated XANES spectra

References

[1] S.Narindrasorasak et al., Biochemistry 46,3116(2007)
[2]Monika Sommerhalter et al., J. Mol. Biol. 365.715-721 (2007)
[3]M. Nomura, *J. Synchrotron Rad.*, **5**, 851 (1999)
[4] T. Fujikawa., J. Phys. Soc. Jpn. **62** (1993) 2155

* a5205061ym0113@graduate.chiba-u.jp