# Development of Convenient Experimental and Analytical Methods for Diffraction Anomalous Fine Structure

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Diffraction anomalous fine structure (DAFS) is a spectroscopic analysis established by coupling XRD and XAFS [1]. DAFS has some remarkable aspects such as a site-selectivity and a spatial-selectivity, with which XAFS-like spectra can be obtained at a certain site and a certain phase by selecting diffraction peaks. Though it is a power-full tool for the materials science, DAFS previously took a relatively long measurement time. (e.g. 0.5 day for 1 spectrum), because of optical alignment at every incident energy. In addition, the data analysis of the DAFS spectrum is complicated due to the phase problem to extract resonant terms from the spectrum. In the present study, we have developed the measurement techniques of DAFS at BL28XU in SPring-8 by using a channel cut monochromator with a small gap, a one-dimensional detector and a polycrystalline sample. Furthermore, we also have developed a direct solution method of DAFS without any iteration process.

Figure 1 shows a DAFS spectrum from 111 diffraction of metallic Ni polycrystalline foil (left) and a resultant imaginary part of the resonant term, $f''_{\mathrm{Ni}}$, and $\mu tE$ of XAFS measured simultaneously (right). The total DAFS spectrum of 430 eV energy width around Ni K-edge was acquired for 326 s, which is extremely fast compared with the conventional measurement (e.g. 0.5 day). The measured spectrum was analyzed by the method mentioned above. $\mu tE$ should be equivalent to $f''_{\mathrm{Ni}}$ since Ni atoms occupy only one site in a Ni fcc metal unit cell. The shape of $f''_{\mathrm{Ni}}$ at the absorption edge and the energy of the oscillation above the edge show a good agreement with that of $\mu tE$ except for some difference of the two spectra above the edge due to the truncation error in the Kramers-Kronig relation. These results verified the measurement technique and analysis method in this study.

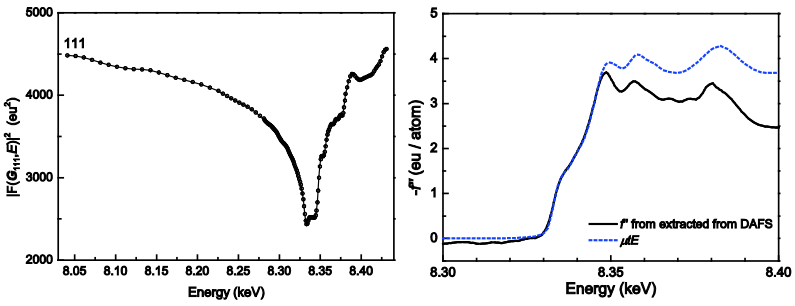


**Fig. 1.** DAFS spectrum from 111 diffraction of Ni metal foil (left), $f''$ and $\mu tE$ (XAFS) near the Ni K-edge (right).

[1] H. Stragier, J. Cross, J. Rehr, L. Sorensen, C. E. Bouldin, and J. C. Woicik, Phys. Rev. Lett. **69**, 3064 (1992).