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Construction of Soft X-ray XAFS Database at SR center of Ritsumeikan University

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X-ray absorption fine structure (XAFS) is a very useful tool for study of chemical state of materials. However, reference spectra of standard samples are necessary to analyze XAFS spectra of unknown materials. The researcher has measured some suitable standard samples and cited the reference spectra reported in journals. It is more desirable for them to be able to utilize databases of XAFS spectra which are open access on internet in order quantitatively to compare unknown spectra with standards. Several XAFS spectra databases have been developed on internet [1, 2] and their energy is mainly in hard X-ray region. XAFS databases in soft X-ray region are fewer than those in hard X-ray region, especially in Japan, not present. We then tried to construct a database of soft X-ray XAFS spectra in the SR center.

We referred to the hard X-ray XAFS database “BENTEN” at SPring-8 [3] to decide files included in a dataset. The dataset is composed of raw data (not normalized), normalized data, figures and metadata files. these files are text based, except figures, so as to be easily able to read with data processing soft. The raw data file is written in comma separated values (csv) format and includes all the data collected in used measurement modes. Soft X-ray XAFS beamlines in the SR center have plural measurement modes: total electron yield (TEY), partial electron yield (PEY), partial fluorescence yield (PFY), inverse partial fluorescence yield (IPFY), and total fluorescence yield (TFY). The normalized data files, which are simple column data composed of energy and normalized intensity, are prepared for each measurement mode in order for anyone to use without data processing. The figure file shows the spectrum of the normalized data and the energy region is XANES part of the normalized data. The metadata is composed of key-value pairs and the file is written in yaml format in order for anyone to be able to understand.

We referred the dataset of SPring-8 in NIMS MDR XAFS database [4] for structure of metadata. Large categories of metadata of the SR center are as follows: data_info, sample,

measurement, instrument, file, similar to those of SPring-8 in MDR. Two categories of facility and local of them are not present in the metadata of the SR center. The category of facility is related to information of the ring, and several keys are included in the measurement category of our metadata. The local category corresponds to the file category of our metadata. The values in metadata were extracted from a header of the raw data file and measurement conditions input in an Excel file.

The terms in each category were also changed and some examples are shown below. The terms of energy calibration were added to the measurement category (Table 1) to define the relationship between the energy of incident X-ray and the spectrum. In the databases of

Table 1. Measurement category of metadata.

category	key	description
measurement:		measurement conditions
	absorption_edge:	absorption edge
	energy_calibration:	energy calibration (array)
	- standard sample:	standard sample
	calibration_position:	calibration position
	energy:	calibration energy
	energy_unit:	calibration energy unit
	incident_angle:	incident angle
	incident_angle_unit:	incident angle unit
	tune_angle:	angle of monochromater tuning
	tune_angle_unit:	angle unit
	tune_energy:	energy of monochromater tuning
	tune_energy_unit:	energy unit
	data_points:	data points
	section:	section (array)
	section_number:	section block number
	section_blocks:	section blocks (array)
	- start_energy:	start energy
	start_energy_unit:	start energy unit
	end_energy:	end energy
	end_energy_unit:	end energy unit
	sampling_number:	sampling number
	delta_energy:	delta energy
	delta_energy_unit:	delta energy unit
	waiting_time:	waiting time
	waiting_time_unit:	waiting time unit
	dwelling_time:	dwelling time
	dwelling_time_unit:	dwelling time unit
	start_ring_current:	start ring current of measurement
	end_ring_current:	end ring current of measurement
	ring_current_unit:	ring current unit
	start_time:	start datetime of measurement
	end_time:	end datetime of measurement

hard X-ray XAFS, the measurement category is based on transmission mode using ion chambers, and terms of I0 (incident X-ray) and I1 (transmitted X-ray) are described in the instrument category. In case of soft X-ray XAFS, however, plural measurement modes are used as mentioned above. We, therefore, changed from I1 to the used modes such as TEY and PFY, and added to several terms related to current detection for electron yield and detector for fluorescence yield (Table 2).

Table 2. Instrument category of metadata.

category	key	description
instrument:		instrument information
	I0:	I0
	detector:	detector (array)
	- type:	type
	manufacturer:	manufacturer
	model_number:	model number
	coating_element:	coating element
	aperture_ratio:	aperture ratio
	aperture_ratio_unit:	aperture ratio unit
	applied_voltage:	applied voltage
	applied_voltage_unit:	applied voltage unit
	Ammeter:	Ammeter (array)
	- range:	range
	range_unit:	range unit
	manufacturer:	manufacturer
	model_number:	model number
	additional_data:	additional data
	TEY:	TEY
	Ammeter:	Ammeter (array)
	- range:	range
	range_unit:	range unit
	manufacturer:	manufacturer
	model_number:	model number
	additional_data:	additional data
	PFY:	PFY
	detector:	detector (array)
	- type:	type
	manufacturer:	manufacturer
	model_number:	model number
	amp_gain:	amp gain
	amp_gain_unit:	amp gain unit
	peaking_time:	peaking time
	peaking_time_unit:	peaking time unit
	deadtime:	deadtime
	deadtime_unit:	deadtime unit
	deadtime_setting_energy:	deadtime setting energy
	deadtime_setting_energy_unit:	deadtime setting energy unit
	element_number:	element number
	ROI:	ROI (array)
	- ROI_energy_lower:	ROI energy lower
	ROI_energy_upper:	ROI energy upper
	ROI_energy_unit:	ROI energy unit
	additional_data:	additional data
	PEY:	PEY
	detector:	detector (array)
	- type:	type
	manufacturer:	manufacturer
	⋮	⋮

In the present state, the database is developed at the web site of the SR center (Fig. 1) [5]. 98 datasets are registered. In addition, 75 datasets of them are registered on NIMS MDR XAFS Database [4]. We are planning to add datasets.

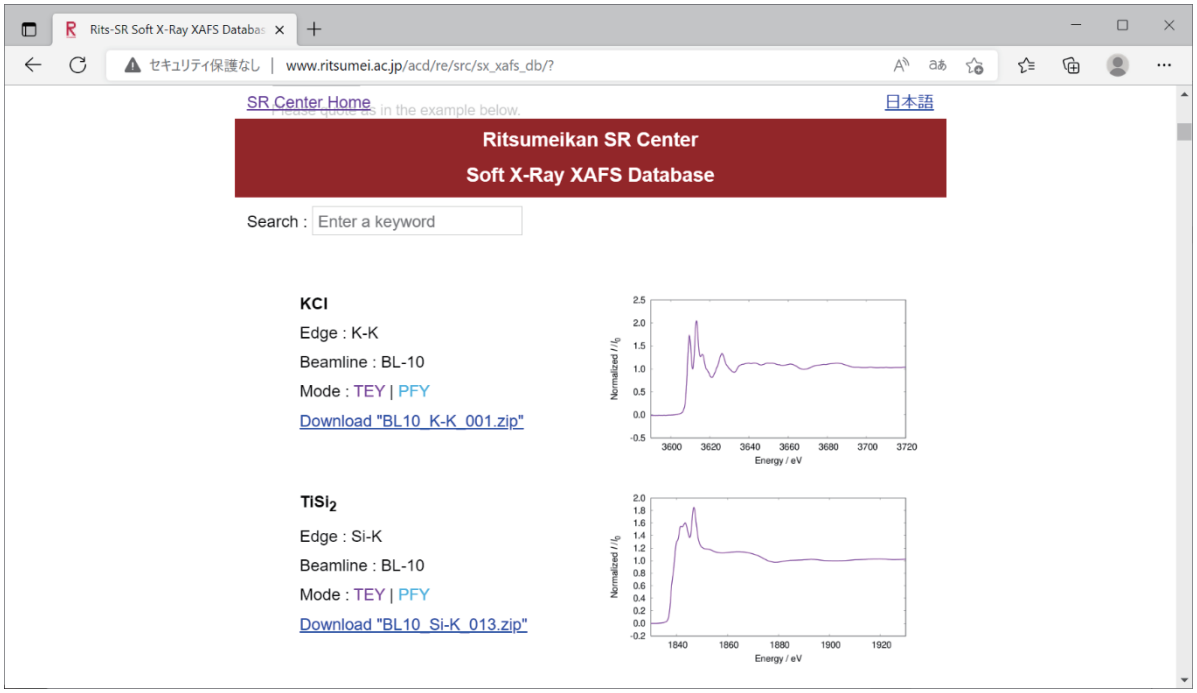

Fig. 1. Database site of the SR center.

References

[1] https://www.jxafs.org/xafs-database/

[2] Kiyotaka Asakura, Hitoshi Abe, Masao Kimura, *J. Synchrotron Rad.*, **2018**, *25*, 967.

[3] https://support.spring8.or.jp/xafs/standardDB_02/standardDB.html

[4] https://doi.org/10.48505/nims.1447

[5] http://www.ritsumei.ac.jp/acd/re/src/sx_xafs_db/