Application of Electronic Laboratory Notebook for Analysis Records in Materials Research

Mineharu Suzuki,[1,]* Yoshitomo Harada,[1] Yutaka Ueshima,[2] Shigeyuki Matsunami,[1] Keisuke Goto,[3] and Hideki Yoshikawa[1]

[1]*Data Platform Center, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0047 Japan*
[2]*QUATRE-i SCIENCE Co. Ltd., 2-1-3 Yamate-Minami, Kyotanabe, Kyoto 610-0354, Japan*
[3]*Emeritus Professor, Nagoya Institute of Technology, Gokiso, Showa, Nagoya, Aichi, 466-8555 Japan*
*corresponding author's e-mail: SUZUKI.mineharu@nims.go.jp

Instead of conventional paper-based laboratory notebook, electronic recording system of experimental conditions is adopted in actual measurements. "Electronic" leads to easiness of retrospective search on computer and sharing of information with collaborators via communications network. The more advantage is that an electronic laboratory notebook (ELN) data can be linked with characterization measurement data. In order to apply an ELN in a research and development sector, various kinds of notebook templates are required with a flexibility and a data recording device should be handy and user-friendly. In our developing ELN system, everyone can make an original ELN template according to the preference and can input data onto the template working on a web software of a tablet or PC. ELN data with essential metadata are stored in an ELN server and they are utilized as digital data file.

1. Introductory

We have generally recorded many kinds of information on experimental procedures onto a laboratory notebook (LN). Everyone knows that LN is very important to perform reproducing/repeating experiments, or to be an evidence data for a manuscript publication or a patent claim.

We are conventionally using a paper-based LN (PLN) because it is very flexible to record everything. It is possible to put a picture or output data sheet on a PLN page. The biggest drawback is the fact that only the person who wrote the PLN can exactly understand the recorded information. One might know that even the person who wrote them cannot read her/his handwritten characters. PLN has also a difficult issue in searching the page of interest. Developing recent digital technologies assist us to perform experiments using computer and network communications. We can see a commercial electronic laboratory notebook (ELN) for pharmaceuticals, chemicals as well as biologicals because of an easy definition to uniform procedures, called as protocol. There are chemical reaction formula, calculation of product yields, citation of toxic materials database, and descriptions of genome. On the other hand, it may be difficult to find out general processes in material sciences and characterization techniques. It is most apparent not least in the sector of research and development, leading to individual notebook template for each scientist or each instrument.

Thus, we have adopted the new type of ELN with a flexibility according to demands by human and instrument. ELN data recorded with a tablet device or PC can be linked with digital measurement data.

2. Features of ELN

The followings are several subjects among features of our ELN system.

1) An application software is not required because of running on a web-browser.

2) Minimum metadata are added automatically by key-value description with persistent identifiers (PIDs) for operators, accessible collaborators, instrument, experimental process, etc. These PIDs are capable to integrate ELN data with other related material data.

3) A photographs, picture, and processing manual can be imported onto an ELN data.

4) One can search and compare ELN data.

5) Related files can be attached with ELN data.

6) Collaborators can share one ELN data.

7) ELN data can be linked with digital measurement data in data collection system.

8) We can easily extract specified item values from multiple ELN data and convert to tabular type data set.

3. Correspondence of PLN and ELN

Figure 1 shows an example of PLN for the absolute AES instrument [1], corresponding to the experimental conditions to take an Auger spectrum shown in Fig. 2. By Fig.1, we know the measurement date and time, the specimen currents and mesh-collector currents before/after the measurement, the Faraday cup and specimen positions given by micrometer gauges, and measurement kinetic energy ranges/energy step sizes. The conditions of primary electron beam such as lens parameters are not recorded in Fig. 1. The elastic peak conditions to determine the specimen position relative to the cylindrical mirror analyzer are not occasionally recorded on PLN. Information not-described on PLN is stored in other media or in the brain memory of person. A linkage/relationship between the actual data shown as Fig. 2 and the PLN may be neither clear except for a specified person. Such situations are not preferable from the viewpoint of traceability.

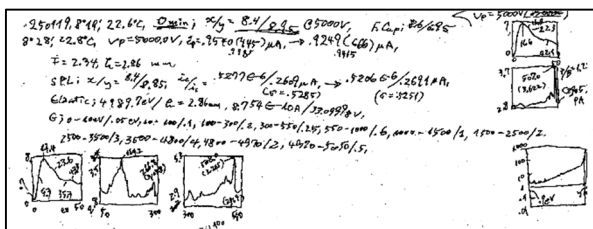Figure 3 shows a part of the ELN, corresponding to

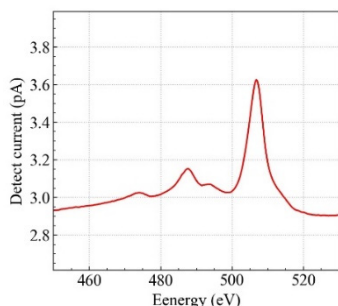**Fig. 1** Handwritten record for measuring an absolute Auger spectrum.

Fig. 2 Under the conditions described in Fig. 1, the AES spectrum of O KLL on Ta surface was acquired.

Fig. 3 A part of the view cut from the ELN data corresponding to the information described in Fig. 1.

Fig. 1. A set of these items includes all information in Fig. 1. It also includes the information that are not described in PLN on the primary electron beam and elastic peak conditions. Though here is not shown, we can add meta-information with ELN such like 2) in the chapter 2, leading to the easy searching process of the data of interest. As described 5) in the chapter 2, we can attach any electronic file to the ELN data, meaning the linkage of raw data like Fig. 2.

These shown data from Fig. 1 to 3 are just examples. We can apply this ELN system to any characterization measurements and materials processing to record parameter values in routine-like works. We have introduced about 15 templates of ELN sheets for 25 persons in NIMS for the beginning one month of the trial operation period as of June 20, 2019.

4. Summary

Advantages of ELN are (1) to be searchable by meta-information, (2) to link with an actual electronic data, leading to (3) to share contents exactly with collaborators in R&D sectors. We demonstrated them using the example of absolute AES measurements.

5. References

[1] K. Goto et al., *Surf. Interface Ana1*. **22**, 75 (1994).