MaiML: A Common Data Format for Measurement and Analysis and Its Application to an Autonomous Experimental System

Akira Aiba*[1] Shinsuke Inoue*[2] Hidemi Ohashi*[3] Kazuki Ito[1] Toshinari Tawara[1] Atsushi Ohbuchi[1] Satoshi Yamamoto[2] Tsuyoshi Morikawa[2] Kazuhiro Nakano[3] Keijiro Sakuramoto[4] Mitsunobu Yamamoto[4] Yoshihumi Sugihara[4] Hideki Yoshikawa[5] Shingo Ichimura[6] Takuo Yasunaga[7] Kazunori Nishio[8] Taro Hitosugi[8]

[1]Rigaku. Co, Matsubara-cho 3-9-12, Akishima-shi, Tokyo 196-8666, Japan
[2]Shmadzu. Co., Nishinokyo 1, Kuwabara-cho, Nakagyo-ku, Kyoto 604-8511, Japan
[3]JEOL Ltd., Musashino 3-1-2, Akishima-shi, Tokyo 196-8558, Japan
[4]Horiba, Ltd., Kanda Awaji-cho 2-6, Chiyoda-ku, Tokyo 101-0063, Japan
[5]NIMS, Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan
[6]National Institute of Advanced Industrial Science and Technology, Umezono 1-1-1, Tsukuba, Ibaraki 305-8560, Japan
[7]Kyushu Institute of Technology, Kawazu 680-4, Iizuka-shi, Fukuoka 820-8502, Japan
[8]The University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-0033, Japan

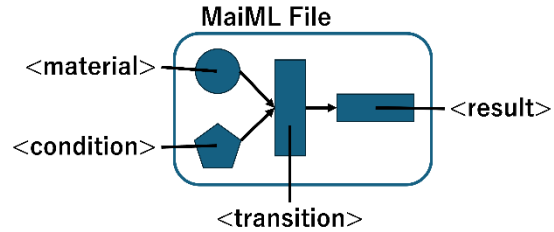
Correspondence to: Akira Aiba a-aiba@rigaku.co.jp

1. Introduction

AI-driven Materials Informatics requires standardized, machine-readable data formats to enable seamless integration and analysis. However, data obtained from different types of measurements and instruments manufactured by various vendors often lack interoperability, creating significant barriers to effective data utilization. To address this challenge and enable the seamless integration of measurement and analysis data from multiple sources—including environmental conditions— for comprehensive data analysis, a common data format, **MaiML (Measurement, Analysis, Instrument Markup Language)** [1.2], has been developed. This requirement is addressed under the published Japanese Industrial Standard JIS K 0200:2024. This JIS document is currently being prepared for standardization as an ISO standard, and a VAMAS round-robin test is also underway. Unlike conventional instrument-centric formats, MaiML explicitly represents experimental workflows, conditions, and results within a unified, machine-interpretable structure, enabling direct integration with autonomous control and optimization loops.

2. MaiML Overview

MaiML provides an extensible schema that unifies the description of experimental results and metadata, overcoming the limitations of conventional instrument-specific data formats. By adopting an XML-based hierarchical architecture, MaiML ensures both flexibility and interoperability, facilitating data sharing across heterogeneous platforms and supporting AI-driven post-processing and automation. This standardization enhances data integrity, traceability, and reproducibility, thereby playing a critical role in collaborative research and automated experimental workflows.




```
<maiml>
    <document>
        # Information about the document
    <protocol>
        <pnml> # Indicating workflow
        <template>
         # Template of material, condition,
           result node
    <data>
        <results>
            <material>
             # Sample (Material) informamtion
            <condition>
             # Experimental condition
            <result>
             # Result and anarytical data
    <eventLog>
        # Log data for operation
```

Fig. 1 MaiML uses an XML-based hierarchy to represent experimental metadata and protocols. A Petri net model describes the relationships among elements such as <material>, <condition>, <transition>, and <result>, enabling standardized data integration and AI-driven experimental workflows.

The core philosophy of MaiML is **"Independent Availability"**, which guarantees that all information necessary to understand and utilize the

data —such as sample details, experimental conditions, and workflows—can be retrieved directly from the file itself, independent of the original measuring device or proprietary software.

MaiML's further employs namespaces and ontologies to standardize technical terminology while remaining extensible enough to accommodate new measurement technologies and vendor-specific parameters. This interoperability is essential for material informatics, as it facilitates the aggregation of diverse datasets into "data lakes" for high-dimensional AI-driven analysis and automated experimental workflows. Ultimately, MaiML serves as a critical infrastructure for collaborative research and digital transformation in science, enabling reliable data sharing across global supply chains

3. Application and Implementation

The first implementation of a MaiML-based data format was realized in an autonomous experimental system for materials discovery, known as the **Digital Laboratory**, developed at the Institute of Science Tokyo and the University of Tokyo [3]. The Digital Laboratory integrates multiple autonomous measurement modules operating under closed-loop optimization, with all experimental processes recorded in MaiML. This unified data representation enables seamless interaction with robotic operations and optimization algorithms. However, practical deployment in real-world experimental environments revealed critical design considerations, particularly in balancing schema expressiveness with practical granularity for autonomous operation. These challenges indicate maturity rather than incompleteness.

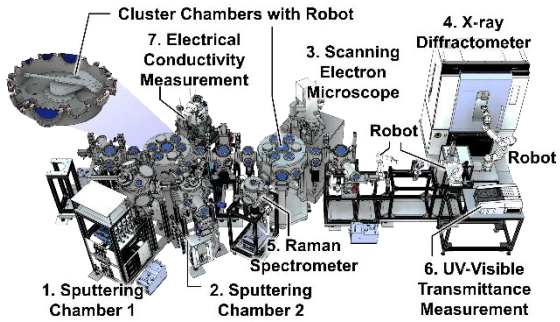


Fig. 2 Overview of the digital laboratory system for autonomous experimentation. Each experimental module operates automatically and outputs measurement data in the MaiML format. Adapted from Ref. [3] with permission from the Royal Society of Chemistry.

This work positions MaiML as a foundational data infrastructure for autonomous laboratories, enabling reproducible, interoperable, and AI-ready experimental workflows. This presentation introduces the concept and design principles of MaiML, demonstrates its application in an autonomous experimental system, and discusses the practical challenges encountered, along with future perspectives.

References

[1] Japanese Industrial Standard (JIS) K 0200:2024(J), **Common format for measurement and analysis data**.

[2] Japan Analytical Instruments Manufacturers' Association (JAIMA). **Comprehensive file format (MaiML) for the measurement and analysis**. https://www.maiml.org/index_en.html.

[3] Kazunori Nishio, Akira Aiba, Kei Takihara, Yota Suzuki, Ryo Nakayama, Shigeru Kobayashi, Akira Abe, Haruki Baba, Shinichi Katagiri, Kazuki Omoto, Kazuki Ito, Ryota Shimizu, Taro Hitosugi. **A digital laboratory with a modular measurement system and standardized data format**, *Digital Discovery*, **4**, 1734-1742, 2025.