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Microbeam analysis — Hyper-dimensional data file specification (HMSA)

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Foreword

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This document was prepared by Technical Committee ISO/TC 202, *Microbeam analysis*.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

Most if not all commercial microanalysis systems acquire and store data in proprietary formats. This hinders the transfer of data between instruments and or between laboratories, such as might be required for multi-technique analyses, round robin studies or collaborations. It is possible that even software from the same manufacturer but for different generations of instruments does not store data in compatible formats. This makes the archiving of data extremely difficult beyond the lifetime of the supported system. The format in this document has been developed by an independent group of experts from the Microscopy Society of America (MSA), the US Micro-Analysis Society (MAS), and the Australian Microbeam Analysis Society (AMAS) to be fully transferrable and archivable. It is independent of instrument manufacturer, computer hardware and operating system.

An existing standard (ISO 22029) allows for platform independent transfer and archiving of simple x-ray spectral data, but the increasing capabilities of microanalysis systems to acquire multi-dimensional signals in parallel has made this standard insufficient to meet all current needs. This standard has been written to meet these expanded requirements.

Microbeam analysis — Hyper-dimensional data file specification (HMSA)

1 Scope

The MSA/MAS/AMAS hyper-dimensional data file specification (HMSA, for short) is a platform-independent data format to permit the exchange of hyper-dimensional microscopy and microanalytical data between different software applications. The applications include, but are not limited to:

— Hyper-spectral maps, such as electron energy loss spectroscopy (EELS), energy dispersive x-ray spectrometry (XEDS), or cathodoluminescence spectroscopy (CL).

— 'Hyper-image' maps, such as pattern maps using electron backscatter diffraction (EBSD) or convergent beam electron diffraction (CBED).

— 3-dimensional maps, such as confocal microscopy, or focused ion beam (FIB) serial section maps.

— 4-dimensional maps, such as double-tilt electron tomography.

— Time-resolved microscopy and spectroscopy.

In addition to storing hyper-dimensional data, the HMSA file format is applicable for storing conventional microscopy and microanalysis data, such as spectra, line profiles, images, and quantitative analyses, as well as experimental conditions and other metadata.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

No terms and definitions are listed in this document.

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at https://www.electropedia.org/

4 Overview

4.1 Design Considerations

The following requirements were considered in the design of this file format:

a) Modern experimental apparatus produce data with high dimensionality, such as spectral maps and 3D serial section maps. Therefore, this file format shall store data of high dimensionality.

b) High dimensionality data is necessarily very large, and consequently difficult and time consuming to store or transfer over networks. The file format shall therefore be as compact as is reasonably practical.

c) Many microanalytical techniques produce structurally similar hyperdimensional data. To simplify implementation of common tools, this file format shall use a common format to store data produced by different analytical techniques.

d) The data format shall preserve the scientific accuracy and meaning of the data. Therefore, the file format shall store data without loss of precision and include sufficient experimental parameters to permit the correct interpretation of the data.

e) To achieve the intended mission of being a widely supported exchange format, the file format shall achieve acceptance from instrument and software vendors, and from the microanalysis community. Consequently, the file format shall be useful, easy to understand, and easy to implement.

f) Furthermore, as the file format is intended for exchange, it shall be readable (and implementable) in any commonly available programming languages and environments. The format shall therefore be platform independent, and not require any proprietary or special software or hardware.

4.2 Binary and XML file pair

4.2.1 General

To satisfy the above requirements, the MSA/MAS/AMAS hyper-dimensional data file format uses a pair of files; a simple binary file to efficiently store the experimental data, and a text-based XML file to store the experimental conditions. The advantages of this dual format are:

— The structure of the binary file format is simple, unambiguous, and precisely defined in a human readable format within the XML file.

— High dimensionality experimental data is binary encoded for space efficiency, whilst also being easy to read and write programmatically.

— Experimental conditions are stored in a human-readable and self-descriptive format. Conditions are stored in a hierarchical structure to logically classify related settings.

— No special libraries are required to read or write HMSA/XML files. For convenience, XML libraries may be used, and are freely available on most programming environments.

4.2.2 HMSA general structure

The HMSA file is a binary file format consisting of an 8 byte (64 bit) unique identifier (5.4.4: The `UID` attribute), followed by one or more dataset objects. The location, size and layout of the binary dataset objects are described in the dataset definitions within the XML file (8: The `<Dataset>` element), and are not described within the binary HMSA file. The values contained within the HMSA file datasets cannot therefore be read or interpreted without the corresponding dataset definition within the XML file.

Blocks of arbitrary and proprietary binary or text data also may be placed in the binary HMSA file. These arbitrary data blocks may be used to store proprietary application-specific data, or ancillary experimental data that cannot be formatted as a HMSA data set object (8: The `<Dataset>` element). The formatting of these arbitrary data blocks in the HMSA file are not defined by this specification,