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Surface Chemical Analysis – Information Formats

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The VAMAS-Surface Chemical Analysis Standard Data Transfer Format (VAMAS Format) was approved by VAMAS Surface Chemical Analysis Community in July 1988. Since then, the VAMAS Format has been assessed by using the software named Common Data Processing System. The structure of the VAMAS Format is suitable for communication, but data storage for manipulation is quite separate matter from data communication. VAMAS Format has many terms to describe instrumental conditions, but it has almost nothing about sample information which is most imprtant part for the data storage. Therefore, information from the VAMAS Format is not enough to handle the data in the databases. The authors are the members of Japanese working group of SC3/WG1 of ISO/TC201, and have discussed the information formats which supplement the existing VAMAS Format. This format proposes three formats encoding information packages for (1) sample information, (2) calibration information, (3) data processing information.

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1. Introduction

The VAMAS-Surface Chemical Analysis Standard Data Transfer Format (VAMAS Format) was approved by VAMAS Surface Chemical Analysis Community in July 1988[1]. Since then, the VAMAS Format has been assessed by using the software named Common Data Processing System [2]. The Common Data Processing System is designed to be a program to assess the data processing procedures proposed by scientists, to calibrate a spectrum and to build a spectra and correction factor database. In this system, data format of a spectrum is converted from original structure to the VAMAS Format. VAMAS Format has been proposed as Surface Chemical Analysis - Data Transfer Format in ISO/TC201.

The structure of the VAMAS Format is suitable for communication, but data storage for manipulation is quite separate matter from data communication. VAMAS Format has many terms to describe instrumental conditions, but it has almost nothing about sample information which is most imprtant part for the data storage. Therefore, information from the VAMAS Format is not enough to handle the data in the databases. However, we believe the future compatibility is essential. New systems should be able to read from the old and vice versa.

This paper proposes four formats encoding information packages for (1) sample information, (2) calibration information, (3) data processing information. This format supplements the Surface Chemical Analysis – Data Transfer Format to enhance the usefulness of Surface Chemical Analysis Data stored in databases. The format is suitable for AES and XPS spectral data.

2. Description of the Information Formats

2.1 General

The information formats are inserted into the comment lines of VAMAS Format as packages. The existing VAMAS Format could be used without alteration as a carrier for the information packages; they could

occupy the experiment–comment line or block comment lines in the VAMAS Format.

In this modular structure the reading program utilizing those information packages can look for the format identifiers in either experiment comment lines, where they apply to all blocks, or in the block–comment lines, where they apply to the one block. Existing reading programs would simply retain these as text lines.

In this paper, the information packages other than Sample Information Format, Calibration Information Format and Data Processing Format are not clearly designed. However, the other Information packages may be added. It is fully modular and new–with–old compatibility is always maintained.

2.2 Additional rules

The all lines are written in ASCII code. The each line is followed by line discriminator code defined by each computer system.

2.3 The Formats

2.3.1 Structures

Sample Information Format = format identifier 1,
host material (popular name),
IUPAC chemical name,
chemical abstracts registry number,
host material composition,
bulk purity,
known impurities,
crystal structure,
form of products,
(form of products that the specimen is used for)
supplier,
lot number,
homogeneity,
crystallinity,
material family,
special material classes,
sample mounting,
ex situ preparation,
in situ preparation,
charge control conditions,
sample temperature
(not necessary to consider the temperature change by a primary beam flux),
comment on specimen information,

Calibration Information Format = format identifier 2,
energy scale calibration,
intensity scale calibration,
resolution calibration,

Data Processing Information Format = format identifier 3,
data–handling procedure,

2.3.2 Definitions of Formats

Sample Information Format
format identifier 1
= ISO Sample Information Format 1995 September 22
host material = text line;
IUPAC chemical name = text line;
chemical abstracts registry number = text line;
host material composition = text line;
bulk purity = text line;
known impurities = text line;
structure = text line;
form of products = text line;
supplier = text line;
lot number = text line;
homogeneity = text line;
inhomogeneous – inhomogeneous
homogeneous – homogeneous
unknown – unknown
crystallinity = text line;
single – single crystal
poly – polycrystalline
amorphous – amorphous
unknown – unknown
material family = text line;
metal – metal
inorganic – inorganic compound
organic – organic compound
polymer – polymer
semi – semiconductor

bio – biological material
composite – composite
super_conductive
– super conductive material
(others)
– (propose a new family;
each word must be
connected by "_")
special material classes = text line;
rod – rod or ingot
sheet
– sheet or foil
(without substrate)
film – thin film or coating
(on substrate)
sinter – sintered material
wafer – wafer
powder – powder
fiber – fiber
(others)
– (propose a new class;
each word must be
connected by "_")
sample mounting = text line;
mechanical
– mechanically mounted
using screw or spring or
etc
conductive_adhesive
– fixed by conductive
adhesive material
nonconductive_adhesive
– fixed by non–conducting
adhesive material
powder_compact _In
– powder compact in
indium foil, indium
pressure pad
powder_put_into
– powder put into a
conductive material(ex:
hole in copper block)
(others)
– (specify other method; each
word must be connected
by "_")
ex situ preparation = text line;
none – none
polish – polish
cleavage – cleavage
ion – cut by ion beam
powder_compact_steel_pad
– powder compact using
steel pressure pad
acetone – degreased by acetone
(others)
– (specify other method;
each word must be
connected by "_")
in situ preparation = text line;
none – none
ion – ion sputtering
together with ion gun
voltage, ion gun current
and ion species
cleavage – cleavage
heating – heating
scratch – scratch
(others)
– (specify other method;
each word must be
connected by "_")
charge control conditions = text line;
none – none
flood – flood gun
together with flood gun
voltage and flood gun
current
screen – screen
(others)
– (specify other method;
each word must be
connected by "_")
sample temperature = text line;
comment on specimen information
= text line;

Calibration Information Format
format identifier 2
= ISO Calibration Information Format

1995 September 22,
energy scale calibration = text line;
XPS_Cu_Au_Ag
- XPS using Cu, Au and Ag peak values from SIA 14,488(1989)[3]
XPS_Cu_Au
- XPS using Cu and Au peak values from SIA 14,488(1989)
XPS_Cu_Ag
- XPS using Cu and Ag peak values from SIA 14,488(1989)
XPS_Au_Ag
- XPS using Au and Ag peak values from SIA 14,488(1989)
XPS_Cu
- XPS using Cu peak values from SIA 14,488(1989)
XPS_Au
- XPS using Au peak values from SIA 14,488(1989)
XPS_Ag
- XPS using Ag peak values from SIA 14,488(1989)
AES_Cu_Au_Ag
- AES using Cu, Au and Ag AES peak values from SIA 15,293(1990)[4]
AES_Cu_Au
- AES using Cu and Au AES peak values from SIA 15,293(1990)
AES_Cu_Ag
- AES using Cu and Au AES peak values from SIA 15,293(1990)
AES_Au_Ag
- AES using Cu and Au AES peak values from SIA 15,293(1990)
AES_Cu
- AES using Cu AES peak values from SIA 15,293(1990)
AES_Au
- AES using Cu AES peak values from SIA 15,293(1990)
AES_Ag
- AES using Cu AES peak values from SIA 15,293(1990)
(others)
- (specify other methods; each word must be connected by "_")
uncalibrated - uncalibrated
intensity scale calibration = text line;
JSSS
- J.Surf.Sci.Soc.Jpn 15,376(1994)[5]
(others)
- (specify other methods; each word must be connected by "_")
uncalibrated - uncalibrated
resolution calibration = text line;
(others)
- (specify other methods; each word must be connected by "_")
uncalibrated - uncalibrated

Data Processing Information Format
format identifier 3
= ISO Data Processing Information Format 1995 September 22,
data-handling procedure = text line;
(specify)
- (specify data processing procedure sequentially)
(; each word must be connected by "_")
unprocessed - unprocessed

Annex A Example

Example 1

ISO Sample Information Format 1995 September 22
strontium chloride
strontium chloride
0476–85–4
SrCl2
99.9% checked by Nissan Arc
N:0.01%,O:0.02% checked by Nissan Arc
cubic fluoride crystal structure, a=6.98A
unknown
Johnson Matthey
No XYZ purchased 18 May 1993
homogeneous
poly
inorganic
powder
powder_compact_In
none
ion 2kV 10uA Ar
none
298K
(carriage return)
ISO Calibration Information Format 1995 September 22
Au
uncalibrated
uncalibrated
ISO Data Processing Information Format 1995 September 22
unprocessed

Example 2

ISO Sample Information Format 1995 September 22
stainless steel
unkown
unkown
Fe74–Cr18–Ni8
99.9% checked by Nissan Arc
N:0.01%,O:0.02% checked by Nissan Arc
face centered cubic, a=6.98A
unknown
Johnson Matthey
No XYZ purchased 18 May 1993
homogeneous
poly
metal
sheet
mechanical
acetone
ion 2kV 10uA Ar
none
298K
(carriage return)
ISO Calibration Information Format 1995 September 22
XPS_Au
uncalibrated
uncalibrated
ISO Data Processing Information Format 1995 September 22
unprocessed

References

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