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Development of a Solid Spectroscopy Data Model

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Abstract

We describe the Solid Spectroscopy Data Model (SSDM) we are developing as a basis for the development of interoperable relational database infrastructures for solid spectroscopy.

1. Introduction

In the frame of the VAMDC European program (WP6) and the EUROPLANET RI European program (WP25 - IDIS) we are developing a general data model for laboratory spectroscopy of solids. A detailed and well structured data model is requisite to describe accurately the solid samples, the experiments, the spectra and their products in order to built relational databases that will be easily searchable and interoperable (among the various databases in this field, or from VO). We also develop such a generic database infrastructure for solid spectroscopy in the frame of Europlanet RI.

No solid spectroscopy data model covering a wide range of solids and spectroscopy techniques currently exists, contrary to gas phase spectroscopy. But on the other side this situation has the advantage that we can define now a unique data model to best fit our common purposes without having to deal with a heavy historical heritage. This will insure maximum interoperability between future databases.

2. Solid Spectroscopy Data Model

In this view we are including in the data model, up to some limited complexity level, the requirements of most of the European solid spectroscopy data producers. The spectral range considered is from UV to sub-mm wavelengths. All types of optical spectroscopies (transmission, reflection, emission, ellipsometry, ATR, Raman, fluorescence, microscopy, …) are considered.

At LPG during the last 2 years we have already developed the core of such solid spectroscopy data model (v0.2) in order to develop the GhoSST database service (http://ghosst.obs.ujf-grenoble.fr/) [1]. We started from this core data model, reshaped and expanded it to fulfil most of the needs of the producers of fundamental data in solid spectroscopy. For this aim we set a small expert group including representatives of different European solid spectroscopy data producers and a few laboratory data users of the astrophysical-planetary sciences communities. The aim of this group (*) is to advise on the necessary (and optional) improvements and extensions of the solid spectroscopy data model. It first meeting was held in Grenoble on 13th Jan 2010.

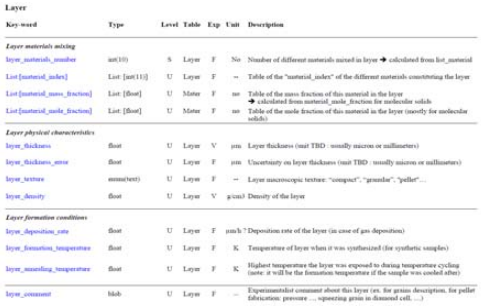
3. SSDM description

The SSDM has four major modules to describe the samples, the experiments, the spectroscopic data and the band list data.

3.1 Samples

The “Sample module” allows to describe them from macroscopic to atomic scales through different levels: layers, materials, constituents, molecules, and atoms.

A solid sample can have multiple *layers* added one on each other (films, granular layers, ...). The layers may have multiple *materials* mixed at grain or crystal level. The “simple” materials (natural or synthetic) are homogeneous collections (loose or compact) of grains, crystals, ... that are composed of *constituents* mixed inside each grain/crystal. “Complex” materials need a specific description (name, origin, formation). The constituents of individual grains or crystals of each homogeneous material are either several *molecules* or isotopes (or natural isotopic mix) mixed at molecular level, or several *minerals* organized at sub-grain level (heterogeneous polycrystal, coating, ...), or *molecules adsorbed* on the grain surface or absorbed in grain volume of *minerals.*



Layer

Key-word	Type	Level	Table	Exp	Unit	Description
Layer materials mixing						
layer_materials_number	int(10)	S	Layer	F	No	Number of different materials mixed in layer ➔ calculated from list_material
List [material_index]	List: [int(11)]	U	Layer	F	--	Table of the "material_index" of the different materials constituting the layer
List [material_mass_fraction]	List: [float]	U	Mater	F	no	Table of the mass fraction of this material in the layer ➔ calculated from material_mole_fraction for molecular solids
List [material_mole_fraction]	List: [float]	U	Mater	F	no	Table of the mole fraction of this material in the layer (mostly for molecular solids)
Layer physical characteristics						
layer_thickness	float	U	Layer	V	µm	Layer thickness (unit TBD : usually microns or millimeters)
layer_thickness_error	float	U	Layer	F	µm	Uncertainty on layer thickness (unit TBD : usually microns or millimeters)
layer_texture	enum(text)	U	Layer	F	--	Layer macroscopic texture: "compact", "granular", "pellet"…
layer_density	float	U	Layer	V	g/cm3	Density of the layer
Layer formation conditions						
layer_deposition_rate	float	U	Layer	F	µm/h ?	Deposition rate of the layer (in case of gas deposition)
layer_formation_temperature	float	U	Layer	F	K	Temperature of layer when it was synthesized (for synthetic samples)
layer_annealing_temperature	float	U	Layer	F	K	Highest temperature the layer was exposed to during temperature cycling (note: it will be the formation temperature if the sample was cooled after)
layer_comment	blob	U	Layer	F	--	Experimentalist comment about this layer (ex. for grain description, for pellet fabrication: pressure …, squeezing grain in diamond cell, …)

Figure 1: Extract from the SSDM dictionary (Layers)

The formation conditions, composition and physical characteristics of each sample level as well as a possible processing history (annealing, irradiation, …) are fully documented.

3.2 Experiments

The “Experiment module” describes global technique parameters common to a complete experiment. An experiment is first defined by an “instrument type” and a “measurement technique” as well as associated measurements parameters such as spectral, spatial, angular and source information. Sometimes source information (laser type, power) is also needed.

3.3 Spectroscopic data

The “spectroscopic module” describes the various spectral product levels (raw spectra, absorption coefficient, optical constants, …) and descriptive information on spectra processing. The spectra are stored by lines in a table with a wavenumber and the corresponding intensity value(s) which depend on the type of spectrum. For each value there is also a quality flag and an error bar, eventually asymmetric.

3.4 Band list

The “Band list” module gives detailed individual information on each absorption band of solid materials and the physical information of the corresponding solid. It is largely an autonomous data base and can include bibliographic data too. We currently limit this fundamental band list database to simple molecular solids (pure, simple mixtures, binary compounds, hydrates, clathrates, …) at different temperatures and in different solid phases. We intend to extend it to molecules adsorbed on, or trapped in, minerals.

Each band is linked to the molecule inside the solid which creates the band. Each solid material is defined in a simplified way as in the sample module. A few important physical conditions of the solid are also considered such as its measurement and annealing temperatures, as well as the gas in contact with the sample (for adsorbed molecules).

Each band is described by its position, its vibration type and transition mode. The parameters of the band are then given, such as the band width and its intensity in various units (normalized absorbance, absorption coefficient, optical constants) and in relative band strength, depending which one is available. For each of these band parameters an error (symmetric or asymmetric) is given, when possible. A link to spectra and publications in the data base is also given, when available.

3.5 Publications

The “Publications” annex data base gives all references to publications linked with the spectral data. Some additional information and link to spectra are also provided.

6. Summary and Conclusions

This data model should be finalized in july 2010. It is the building frame of the generic database infrastructure, query interface and tools for solid spectroscopy in development for the GhoSST database service (http://ghosst.obs.ujf-grenoble.fr/) within the Europlanet RI and VAMDC programs.

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