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The Solid Spectroscopy Data Model (SSDM) and the GhoSST database

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Abstract

The "Solid Spectroscopy Data Model" (SSDM) provides a data model allowing a complete description of spectral data of solid materials. It includes a detailed description of the solid samples through their layers, materials, constituents and species. Natural and complex materials are also included. The instruments and techniques used for the measurements are described. The spectral data are of two types: spectra and their various higher levels products (instrument specific) and band list. It is the base of the development of the GhoSST relational database infrastructure for solid spectroscopy.

1. Introduction

In the frame of the VAMDC European program (WP4&6) 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 build the GhoSST relational database infrastructure that will be easily searchable and interoperable (among the various databases in this field, or from any Virtual Observatory).

No solid spectroscopy data model covering a wide range of solids and spectroscopy techniques currently exists, contrary to gas phase spectroscopy. This situation allowed us to define a unique data model to best fit the common purposes of the solid spectroscopy community 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 have included in the data model, up to some complexity level, the requirements of most of the European solid spectroscopy data producers. An expert group (*) including different European solid spectroscopy data producers advised us on the necessary improvements and extensions of the solid spectroscopy data model. Its second meeting was held in Grenoble on 23-24th June 2011.

3.1 Description

The SSDM has four major modules to describe the solid samples, the experiments and instruments, the spectroscopic data and the band list data. The spectral range considered is from UV to sub-mm wavelengths. All types of optical spectroscopies (transmission, reflection, thermal emission, ellipsometry, ATR, Raman, fluorescence, microscopy, …) are considered.

3.2 Samples

The sample data model is the most complex part of the SSDM because it needs to describe the many different types of solid samples used in solid spectroscopy down to the atomic level, through a complete description of each of its layers, and of the materials (homogeneous collection of grains) constituting these layers and their possible mixtures and, for the simple materials, of the various constituents (crystals, phases, coating, …) making up these materials, and then of the species (molecules, minerals, atoms) that compose the constituents. All species are then described in term of atoms. For complex solids mostly a global description in terms of atoms is possible when an elemental analysis has been done. But we also let the possibility to partly describe them in terms of molecular functions.

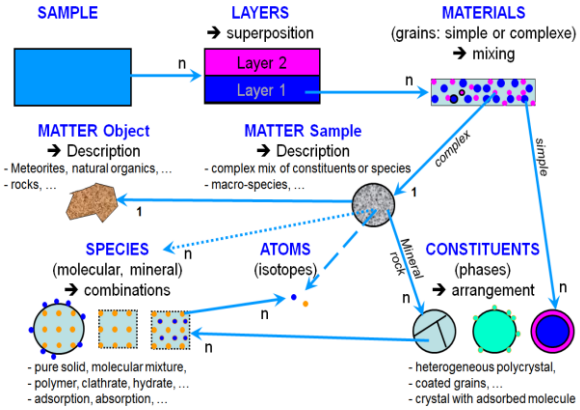

Figure 1: *Sample structure from layers to atoms*

Complex solids, natural and synthetics, as well as simple natural materials are called "matters" and are directly used as "materials".

At each level of the sample description there are parameters specific to this level (its physical characteristics, processing, …), and parameters describing how the next level is organized qualitatively and quantitatively in this level (e.g. organization of layers in a sample, of materials in a

layer, of constituents in a material, of species in a constituent, and of atoms in a species) in a relation "m sub-levels ‘n-1’ in one level ‘n’".

3.3 Experiment and instruments

An Experiment is defined as a series of spectrum measurements of a single sample with a unique instrument and only one of its techniques. The “Instrument module” gives all information relative to the spectroscopic instrument used, as well as on the specific technique implemented on it.

3.4 Spectroscopic data

The “spectroscopic module” describes the various spectral product levels (calibrated spectra, absorption coefficient, optical constants, …) and descriptive information on spectra and their processing.

3.5 Band list

A “band list” refers to all bands of one particular species in one well defined constituent. This module gives detailed individual information on each absorption band of solid constituents and its physical information. It is largely an autonomous data base and can include bibliographic data too. We currently limit this fundamental band list database to molecular solids and molecules adsorbed on, or trapped in, other solids (minerals, complex organics, …).

4. The GhoSST Database

SSDM is the building frame of the generic database infrastructure, query interface and tools for solid spectroscopy in development at IPAG. Its first implementation is underway for the GhoSST database service (http://ghosst.obs.ujf-grenoble.fr/) .

4.1 Data provider interface

The data provider web interface of GhoSST provides tools for data import (through xml import files) and management, data import and users consultation histories and data updates follow up.

4.2 User interface

The user web interface of GhoSST provides a guided step-by-step search, a full-query search, detailed information on the selected spectra, experiments and samples, spectra visualization with highlighted information, as well as data download options.

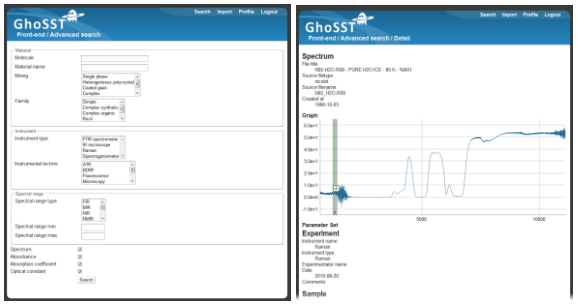

Figure 2: *GhoSST search and visualization interfaces*

A data user group from a few laboratories of the astrophysical-planetary communities has been set to give advices on the user interface and tools. Its first meeting was held in Grenoble on 30th June 2011.

5. Summary and Conclusions

A stable core of the SSDM data model and a prototype of the GhoSST database will be delivered in july 2011. The band list datamodel still need to have its vibration mode module fully developed. Several side modules describing different types of natural and synthetic matters (meteorites, minerals, tholins, …) will be also developed. The public release of GhoSST is planned for july 2012.

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