The ESICMM Tsukuba topical seminar
Jointly organized by CMT/CMS seminar

Can materials data mining be of any use for the ESCIMM project?

Dr. Pierre Villars
Materials Phases Data System (MPDS), Switzerland

Date: 19th/Feb./2013 (Tue.) 16:15 – 17:00
Venue: The Seminar Room #811-812, NIMS Sengen site 8F

Abstract- One of the most challenging tasks in materials science is the design of new materials with tailored properties. Two different approaches are generally explored: The first one is by performing ab-initio calculations at the quantum-mechanical level on specific material to understand its properties at electronic structure base. We focus on the second approach, which remains at a more pragmatic level. Most of our knowledge in materials science has been collected empirically, by searching for patterns and regularities in large amount of observations. The data mining approach, however, depends on the availability of a sufficiently large amount of data of appropriate quality.
We have searched systematically with the help of a data mining technique to discover patterns within thousands of data sets of different compounds (materials). Here we show three most general valid patterns (always using the PAULING FILE data as data mining source) as the examples.
1)Compound Formation Maps; 2) Structure Maps; 3)Periodic Table – AET Maps for AxByCxz… compounds.
These relatively simple maps showing well-defined domains provide condensed overview of experimental data and offer some prediction ability which might take play the initial guidance for discovering new materials.
[2] An X-ray magnetic circular dichroism (XMCD) has become a universal tool for studies of magnetic materials. The most advantageous feature of XMCD is in its element specificity based on core-electron excitations, and the difference from a conventional MCD of visible light region is very clear. It is also very useful that the spin and the orbital magnetic moments are possibly obtained by magneto-optical sum rules in some case depending on the elements and absorption edges. Although this brief introduction is very common, but we need to know more about XMCD when we plan and perform XMCD experiments and analyses. In the seminar, I will start from a basic principle of XMCD, and will give overall views of XMCD with study cases as many as possible. The latter part will help us to consider what type of XMCD experiment is appropriate for our collaborations.

For contact: C. Mitsumata, e-mail : info-esicmm@ml.nims.go.jp