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De-MA: A Web Database For Electron Microprobe Analyses To Assist Electron Microprobe Lab Manager and Users

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Lab managers and users of electron microprobe (EMP) facilities require comprehensive, yet flexible documentation structures, as well as an efficient scheduling mechanism. A single on-line database system for managing reservations, and providing information on standards, quantitative and qualitative setups (element mapping, etc.), and X-ray data has been developed for this purpose. This system is particularly useful in multi-user facilities where experience ranges from beginners to the highly experienced. New users and occasional facility users will find these tools extremely useful in developing and maintaining high quality, reproducible, and efficient analyses. It also serves an educational purpose notably by a) providing a list of possible standards for each element to analyze, b) encouraging students to select appropriate x-ray lines to analyze by EMP based on line intensity, minimum critical ionization energy, and possible peak or background interference issues, c) providing default analysis setups, d) identifying unknown x-ray lines in a WDS scan or in an EDS spectrum, and e) recalculating mineral formula from EMP analysis results based on a fixed amount of oxygen or total cations.

This user-friendly database is available through the web, and uses MySQL as a database and PHP/HTML as script language (dynamic website). The database includes several tables for standards information, X-ray lines, X-ray element mapping, PHA, element setups, and agenda. It is configurable for up to five different EMPs in a single lab, each of them having up to five spectrometers and as many diffraction crystals as required. The installation should be done on a web server supporting PHP/MySQL, although installation on a personal computer is possible using third-party freeware to create a local Apache server, and to enable PHP/MySQL. Since it is web-based, any user outside the EMP lab can access this database anytime through any web browser and on any operating system. The access can be secured using a general password protection (e.g. htaccess).

The web interface consists of 6 main menus:

(1) “Standards” lists standards defined in the database, and displays detailed information on each (e.g. material type, name, reference, comments, and analyses; Fig. 1). More than one analysis obtained through different method or laboratory can be entered, and a preferred analysis set. Images such as an EDS spectrum or BSE can be associated with a standard.

(2) “Analyses” lists typical setups to use for quantitative analyses, allows calculation of mineral composition based on a mineral formula, or calculation of mineral formula based on a fixed amount of oxygen, or of cation (using an analysis in element or oxide weight-%); this latter includes re-calculation of H_2O/CO_2 based on stoichiometry, and oxygen correction for F and Cl. Another option offers a list of any available standards, and possible peak or background interferences for a series of elements. An export option of the complete standard for “Probe for EPMA” information is already available; other exportation formats (e.g. from JEOL or CAMECA software) are envisaged in the near future. An option for automatic importation of existing standard information from microprobe software is also planned.

(3) “X-ray maps” lists the different setups recommended for element mapping using WDS, and a map calculator to facilitate map setups and to estimate the total mapping time. This menu also

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allows the user to upload existing x-ray compositional maps and to calibrate the image with current stage position, which aids in navigation by providing EMP stage coordinates.

(4) "X-ray data" lists all x-ray lines for a specific element (K, L, M, absorption edges, and satellite peaks) using x-ray energy and wavelength data obtained from CAMECA (adapted from [1]) in terms of energy, wavelength and peak position. A check for possible interferences on peak or background is also possible (Fig. 2). Theoretical x-ray peak positions for each crystal are calculated based on the 2d spacing of each crystal and the wavelength of each line, and is entirely customizable by the EMP manager through the administration interface.

(5) "Agenda" menu displays the reservation dates for each month and for each EMP lab defined, and can include vacation/holiday time. It also offers a reservation request option, this request being sent by email to the EMP manager for approval.

(6) Finally, "Admin" is password restricted, and contains all necessary options to manage the database through user-friendly forms.

The installation of this database is made easy and knowledge of HTML, PHP, or MySQL is unnecessary to install, configure, manage, or use it. Two examples of this database are accessible at http://jeol.geoloweb.ch (JEOL-8600 microprobe) and http://cameca.geoloweb.ch (two CAMECA microprobes: SX-50 and SX-100). The database is still under development, although already fully functional, and suggestions are more than welcome for future development.

References:

[1] Bearden & Burr, Review of Modern Physics **39** (1967), p. 125-142.

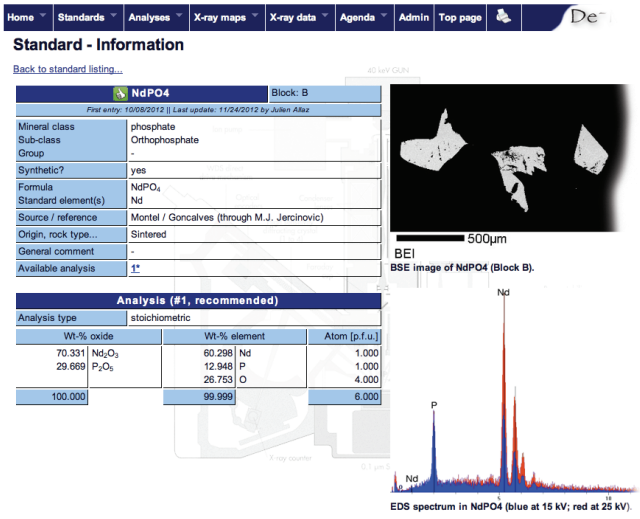

Figure 1 (top). Standard info page (example for $NdPO_4$) including two images: BSE of standard mount and EDS spectra.

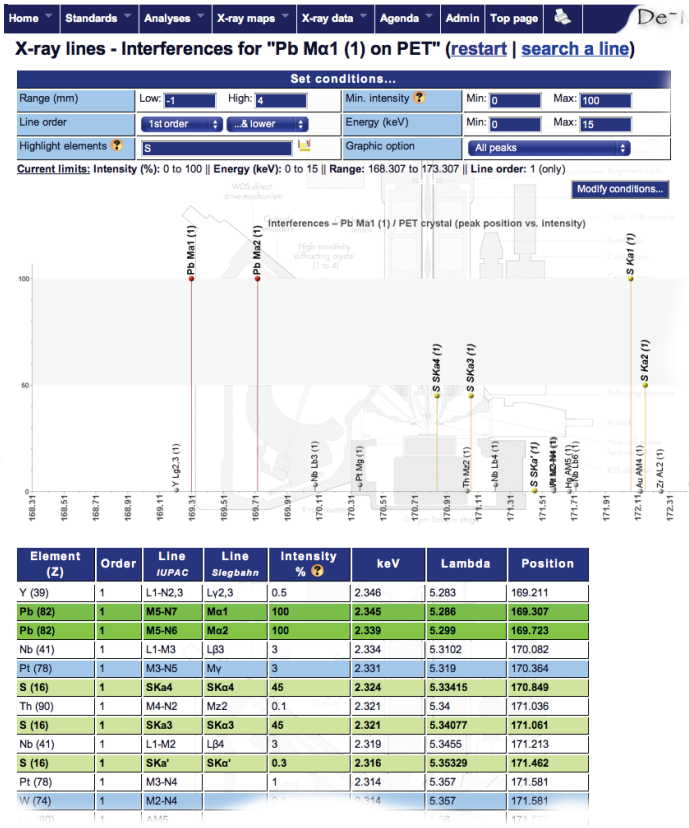

Figure 2 (right). Graphic and table display of x-ray lines (here Pb Mα) along a specific range of spectrometer positions, including various options for display, such as limited line orders, element to highlight, minimum intensity, and range of critical ionization energy.

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