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Mössbauer spectroscopy database: past, present, future

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Abstract Mössbauer Spectroscopy is a useful tool for scientific research in many fields, lots of researchers benefited from this technology which discovered by Rudolf Mössbauer. Up to now, there are more than one million Mössbauer data records present in public papers and books, and the number is increasing. Most of these data records have been collected by Mössbauer Effect Data Center (MEDC) since 40 years ago, and now all these data records can be seen on the web of database. MEDC, as a part of Mössbauer community, is and always will be offering better service with the help of the entire community.

Keywords Mössbauer effect data center · Isomer shift · Quadrupole splitting · Mössbauer database

Mössbauer Spectroscopy is a research tool successfully utilized by scientists in various fields—physics, chemistry, geology, biology and others. More than 53,000 papers related to the subject were published since the famous discovery by Rudolf Mössbauer in 1958. During past 50 years, more than 50,000 scientists contributed to

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the development and application of the method. Currently, more than 3,000 scientists from about 1,000 institutions in more than 70 countries around the world benefit in their research activities from the use of Mössbauer spectroscopy [1–3]. Among them, one can identify 2,182 individuals from 756 institutions who are strongly connected to the application of the method [4]. Closer look helps to select a core group of the best specialists in the field of Mössbauer Spectroscopy – 875 scientists from 385 institutions [5]. All these researchers are known informally as Mössbauer Research Community, which is organized under the International Board on Application of Mössbauer Effect (IBAME).

Members of the Mössbauer Community are involved in various kinds of scientific work and publish their results in 910 different scientific periodicals and 144 books [6]. An enormous amount of research data was collected during the past 50 years. An acute demand for systematization of results, facilitating information dissemination, strengthening contacts between researchers was served for many years by the Mössbauer Effect Data Center (MEDC). Mössbauer spectroscopy is rather time-consuming type of scientific study. MEDC using the database can help to coordinate the research in the world to avoid unnecessary and expensive duplication. For example, 458 data records registered in the database under the absorber name Fe_2O_3, a-Fe_2O_3 and hematite, all extracted from various publications indicate certain redundancy in experimental activity.

MEDC, which had operated for 40 years in Asheville (USA), recently has been moved to Dalian (China). One of the activities of the Center is maintaining the Mössbauer Spectroscopy Database.

The idea of Mössbauer Spectroscopy Database goes back to Mössbauer Spectroscopy Index compiled by Muir and colleagues [7]. Further development of the concept was undertaken by the team of Mössbauer Effect Data Center led by John Stevens. The first generation of the Mössbauer Spectroscopy Database was established in 1979. It was created using RDB-VMS software and was running on DEC-VAX computers. The true innovation at the time was the concept of the spectral parameters—isomer shift and quadrupole splitting values along with other information being entered in the database. This information was extracted from the scientific publications by trained Mössbauer spectroscopists, who were digesting a vast volume of articles published in journals all over the world. A group of associate editors of the Mössbauer Effect Reference and Data Journal were contributing considerably to this process.

Technological advancements of the 1990's in computer hardware made possible a transfer of the database from mainframe computers to desktop machines. The whole database was moved to a desktop PowerPC Macintosh computer. The new 4D database software had been chosen for implementation of the new database design. At that time Mössbauer Effect Data Center made its first presence on the web and the database was made accessible worldwide.

Now the international Mössbauer Community has reached the new level of development and needs new services based on the web access database. Following the best achievements of the web development, it seems reasonable to accept the model of the database implemented on the platform of the open source products like Apache web server, MySQL database and PHP-based interface. This choice allows hardware platform independence of the solution allowing deployment of the system on Windows, Linux and Macintosh OS machines. This solution also opens

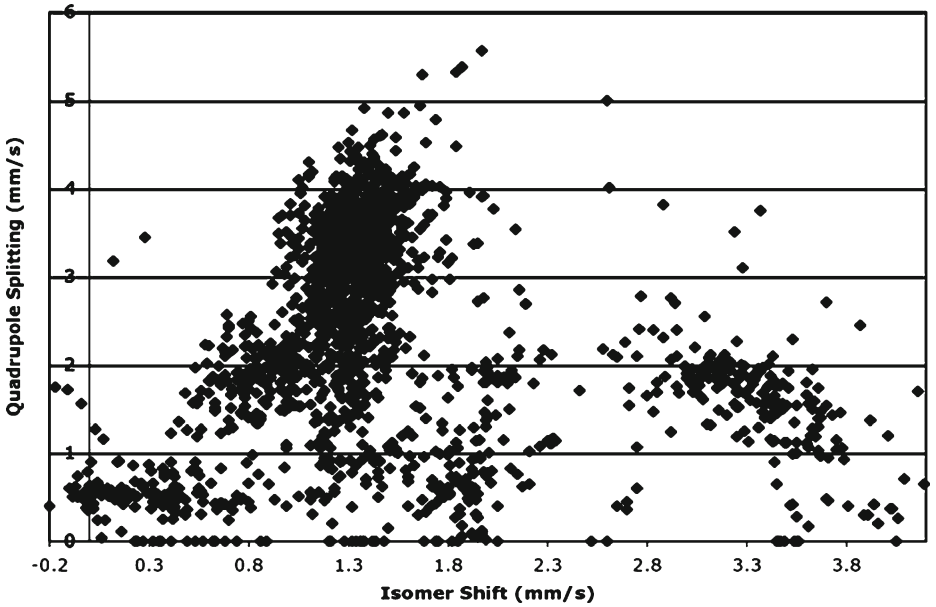

Fig. 1 ^{119}Sn Mössbauer spectral parameters from the MEDC database plotted on Isomer Shift – Quadrupole Splitting graph

the opportunity for making the future Mössbauer information system open source type one, allowing all members of the community to participate in development and improvement of the software.

Let's check out a possible database used by a researcher interested in ^{119}Sn isotope. Since the discovery of the Mössbauer effect, chemists appreciated the information obtained from the main spectral parameters—isomer shift (IS) and quadrupole splitting (QS). These values proved to be very sensitive to electron density and charge distribution in the atoms with resonant nuclei. For the past fifty years, thousands various substances were studied by using Mössbauer spectroscopy and a vast amount of experimental information was collected. For example, the observed values for ^{119}Sn isomer shift stretch over the span of more than 4 mm/s and the absolute value of quadrupole splitting values covers a 6 mm/s of Doppler velocity range. The distribution of the observed values shows some characteristic congregations (Fig. 1). If the results are plotted as distribution of observed isomer shift values, then a clear maximum is observed around 1.3 mm/s value (Fig. 2). One could inquire if the collected IS/QS data could be used for substance identification at least in the case of ^{119}Sn Mössbauer spectroscopy. The data plotted on Fig. 3 shed light on this question showing the distribution of quadrupole splitting values reported in publications having the isomer shift restricted to the mostly represented region around 1.3 mm/s. The distribution clearly shows that the number of observed results for a selected pair IS/QS stays below 1 for the all QS values except the region around 3.4 mm/s, were it does not exceed 2. This means that using a pair of values IS and QS, an inquisitive researcher will have no trouble of identifying the measured sample using the database of Mössbauer spectroscopic parameters.

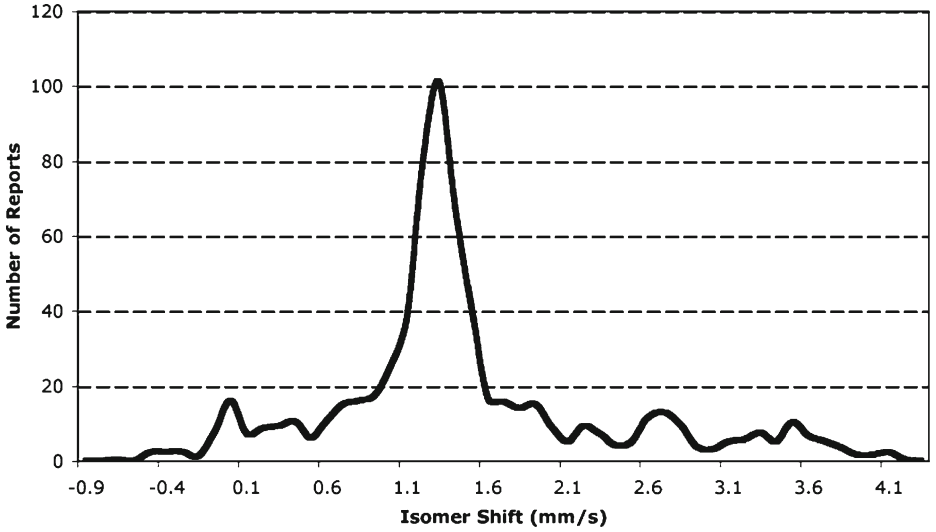

Fig. 2 Distribution of reported values of Isomer Shift for ^{119}Sn

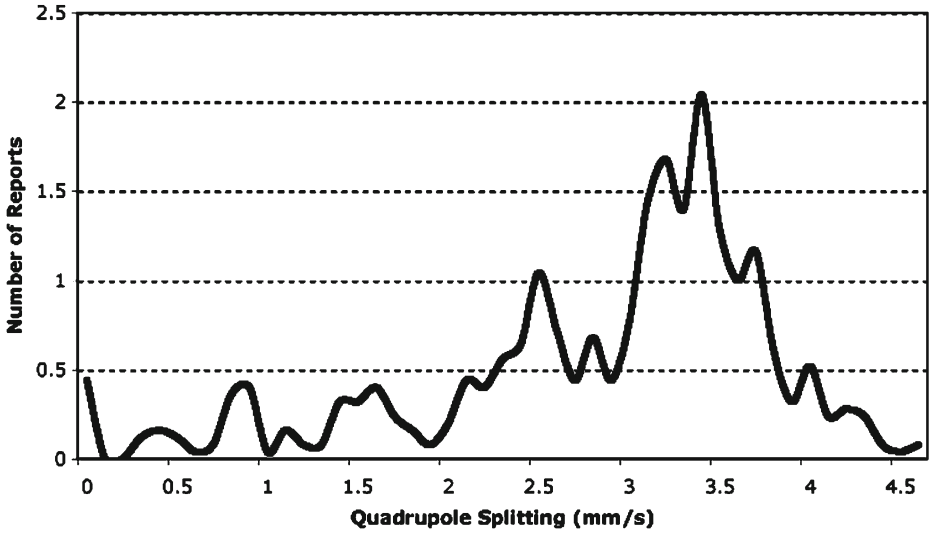

Fig. 3 Distribution of reported Quadrupole Splitting values for ^{119}Sn with Isomer Shift values between 1.3 mm/s and 1.4 mm/s

Mössbauer spectroscopists know how important is visual assessment of the spectrum. That is why it would be very helpful to create a tool that would allow visual comparison of a spectrum collected by anybody to as many appropriate results available. Currently, no such tool does exist. Popular fitting tools offer very limited capability of such kind even for a collection of spectra on one machine. Second feature any researcher would appreciate if the fitting tool equipped with a set of different models including dynamic effects, distribution of parameters etc. in addition

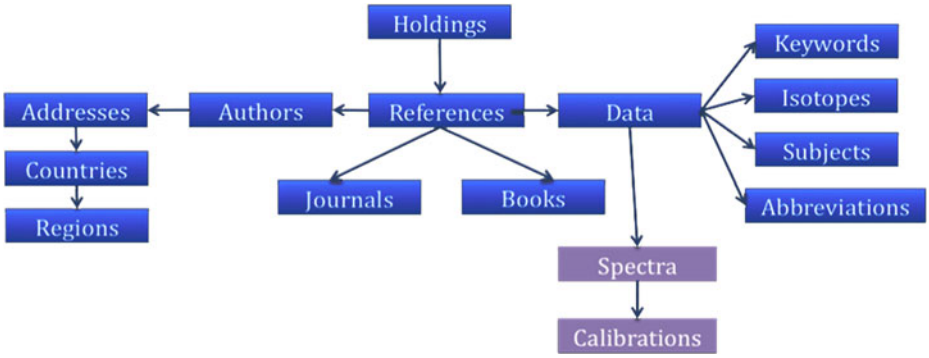

Fig. 4 Spectra and Calibrations tables added to the relational scheme of MEDC database

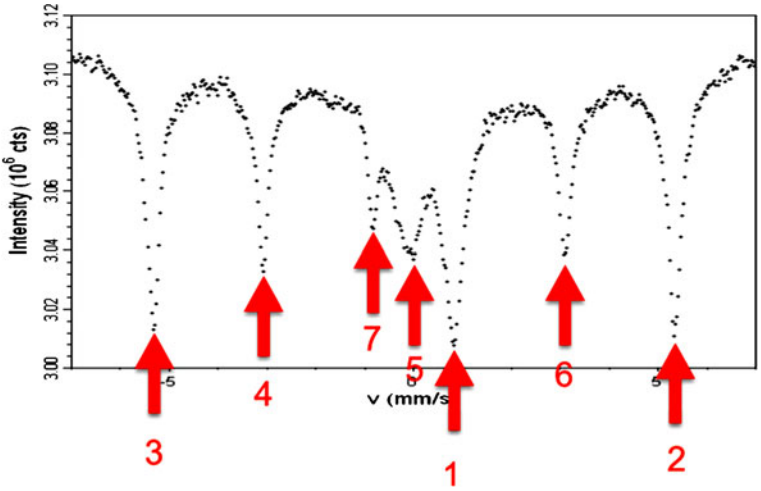

Fig. 5 Suggested scheme of indexing of the Mössbauer spectra for faster search in the table "Spectra"

to a regular lorentzian lineshape. These models can vary substantially and it is very difficult to expect them in the fitting package from one vendor. The modular solution based on open source ideology looks like a better solution, especially having in mind the problem of software support pertinent to any small company. Finally, only a fraction of MS measurements reach the stage of being published in a reviewed journal. It seems that the Mössbauer community could gain a lot by establishing a professional online publishing medium were any measured spectrum could be published and viewed by interested researchers.

We see the need of development of the next generation MS database capable of storing and managing not only spectral parameters, but also the whole original spectrum. This capability will open possibility for better use of the information collected in the measurement. Possibility for reevaluation of the spectra using different fitting models is also very helpful. The intrinsic digital nature of the Mössbauer spectra suggested this advancement long time ago, but only recently the development of

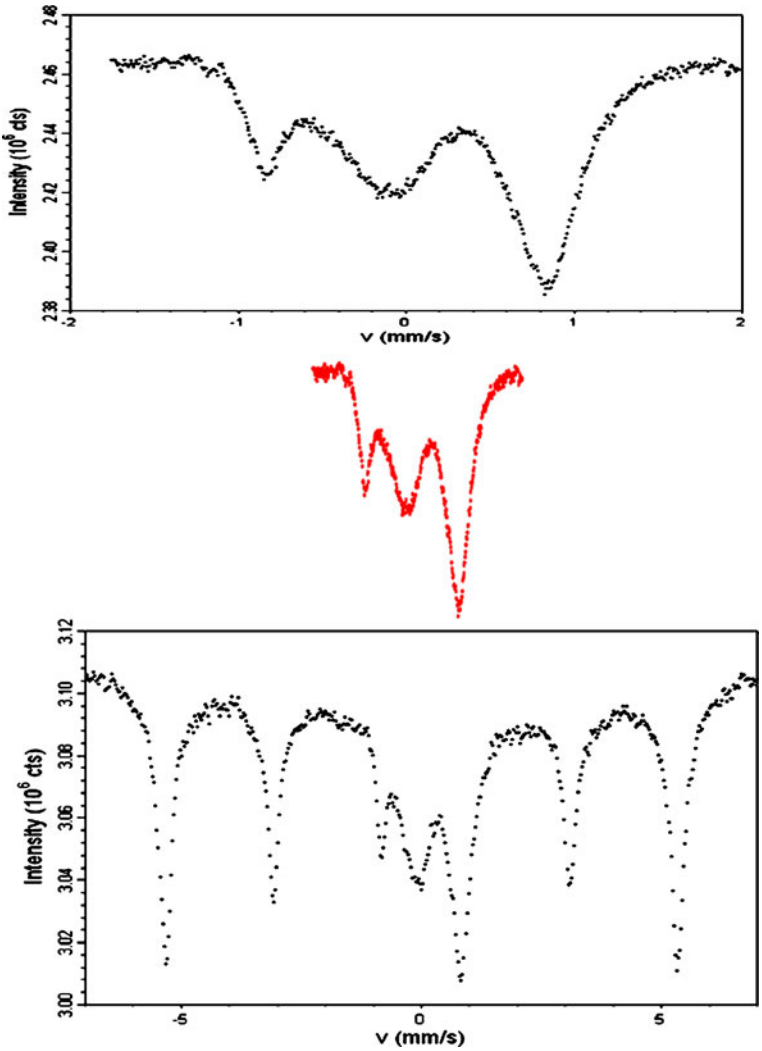

Fig. 6 The visual overlap comparison tool must perform absolute rescale of the velocity axis and relative rescale of the intensity axis

computer technology made it possible. The spectrum table of the database will fit naturally into the existing relational design of MEDC database (Fig. 4).

Each measurement is worthy only with proper calibration provided. That is why each stored spectrum must be linked to a file of calibration measurement, absolute or relative. An additional set of absolute calibration values for selected standard materials used for relative calibration must be provided in the system.

An additional methodology for fast searches in the database of raw spectra must be developed. A system of indexing based on positions and relative intensities of major resolved absorption (emission) peaks could be a solution that will allow fast

selection of relatively small set of spectra, which are presented for a human analysis or subjected to more detailed artificial intelligence analysis (Fig. 5).

Online graphical tool for comparison of two spectra will allow user to upload a spectrum with calibration, will perform calibration and scaling of the plot long x and y axis. The spectrum from the database will be overlaid for comparison using the same velocity scale. The relative intensity must be scaled as well to eliminate irrelevant difference in absolute statistics (Fig. 6).

A proper statistical criterion for comparison of two spectra must be developed so that in addition to subjective impression the user is provided with an objective criterion of similarity of two spectra under consideration.

The current stage of development of the Mössbauer database was achieved by MEDC staff and dedicated group of associate editors. More than 54,000 publications are entered in the MEDC database. More than 107,000 data records are created by processing the information published in these publications. About 1,300,000 keywords generated to facilitate searches in the database.

The realization of the next stage of development is possible only with the help, support and contribution from the entire Mössbauer community.

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2. Number of affiliation institutions in 2005 – 1,093; in 2006 – 1,045; in 2007 – 965; in 2008 – 940. (From MEDC database analysis)
3. Number of countries in connection to publications in 2005 -73 countries, in 2006 – 78, in 2007 – 79, in 2008 – 75. (From MEDC database analysis)
4. Criterion used for strong connection is 5 or more papers published in the last 10 years
5. Criterion used for a specialist is 10 or more papers published in the last 10 years
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