Mat-DB: A Web-Enabled Materials Database to Support European R&D Projects and Network Activities

By *H. H. Over,* E. Wolfart, W. Dietz, L. Toth*

Fast access and exchange of materials data between research, design and manufacturing teams working on different sites worldwide is a challenging issue to be addressed during the product cycle in materials engineering.[1] Another imported issue is safeguarding high investments made into materials research, which means that experimental data must be properly conserved, easily be located and quickly be retrieved. Materials databases (MDBs) are powerful tools to address these problems. Various categories of MDBs exist for different requirements, for example containing standards data on metallic alloys[2,3] and plastics[4] or more complex database applications needed for the design analysis.[5] MDBs are also basic elements for establishing knowledge based and expert systems.[6]

With the emergence of the Internet, the capability of MDBs has further increased. Web-enabled MDBs provide a more centralized management and conservation of the data. Finding and accessing the required data is much faster than to search for them in a traditional manner, e.g. from handbooks or EXCEL files. In particular the dissemination of public research results has improved significantly, as the data are accessible over the World Wide Web. However, only few web-enabled materials applications exist at present on the market. Examples are the database materials databases of NIMS (National Institute for Materials Science) in Japan,[7] which offer a lot of data but their interface guidance is still very limited. Currently, acceptance and use of (web-enabled) MDBs is still hindered by the following problems:

Many organizations use proprietary MDBs, which are customized to their requirements and internal practices. The structures of the databases are not standardized and therefore interoperability and data exchange between different organisations is difficult.

Data entry and validation are necessary but time-consuming tasks in order to ensure high-quality data. Often, scientists do not invest the required time to store the data in MDBs, instead they keep them in simple EXCEL sheets or other customised formats.

Materials data from publicly funded R&D projects are not sufficiently made available in electronic format. Therefore a immediate access to free, public data sets is limited.

Industrial companies often hesitate to make their experimental data freely available; publications often contain limited information (e.g. on material processing details) and experimental information on product specific features is difficult to retrieve.

The JRC is addressing these problems with the aim to establish a European data network for materials data and analysis routines to be used in industry, research and education.

It is the objective of the paper to describe in detail the present status of JRC MDBs and planned activities to establish a European data network.

Database description and structure: The JRC has been developing two material databases for safeguarding and managing its experimental materials data resulting from in-house research some 20 years ago:[8,9] Alloys-DB and Corrosion-DB. Alloys-DB covers mechanical and thermo-physical properties data of engineering alloys at low, elevated and high temperatures for base materials and joints.[10] It includes irradiation materials testing in the field of fusion and fission, tests on thermal barrier coating for gas turbines and mechanical properties testing on a corroded specimen. Corrosion-DB refers to weight gain/loss data of high temperature exposed engineering alloys, ceramics and hot isostatic pressed powder materials and covers corrosion tests such as oxidation, sulfidation and nitridation. The extension to other types of corrosion is under consideration. Alloys-DB and Corrosion-DB have been merged to Mat-DB. The database structure of Mat-DB has continuously grown and the application developed from the initial mainframe database without graphical user guidance, over stand-alone PC and client/server applications to the new web-enabled application. All current applications use an identical database structure simplifying data exchange between the JRC and its external MDB partners. Alloys-DB and Corrosion-DB are being used as stand-alone PC or client/server applications by a number of European industry and research organizations to manage their in-house experimental test results. Updates and further developments are presented and discussed during annual user meetings with these customers.

Mat-DB is designed for experimental data, which is delivered by the laboratories in defined formats and quality. The emphasis is on data from tests, which comply with existing or pre-normative standards. The data can be entered, stored and accessed with typical database routines and can be evaluated with integrated analysis tools.

[*] *Dr. H. H. Over, Mr. E. Wolfart*
Joint Research Centre of the European Commission
Petten, The Netherlands
E-mail: hans-helmut.over@jrc.nl
Mr. W. Dietz
Consulting Metallurgist / MECS
Lindlar, Germany
Prof. L. Toth
Bay Zoltán Institute for Logistics and Production Systems
Miskolctapolca, Hungary

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In order to conserve as much information as possible, the database contains detailed meta-information and entry of many fields is mandatory to increase data quality (see Tab. 1). Thesauri are provided for many text and image fields facilitating and improving data entry and retrieval. All entities contain additional fields (customer internals), which can be used for company-specific purposes. In addition to the numerical and alphanumerical information, any type of binary files can be stored within the database, for example final reports of R&D activities, drawings or large amounts of raw data (unfiltered curve data, basic output of strain gauge measurements).

In total, the database structure for base materials contains more than 130 tables and 1850 fields, which are grouped into logical entities: *data source*, *material*, *specimen*, *test condition* and *test result* (see also Tab. 1). The entities are linked within a relation table. For tests on dissimilar joints, e.g. weldments a *joining* and also a second *material* entity are added. The entity *'test result'* is divided into different areas, which contain tables for storing test type specific mechanical (23) and thermo-physical (10) properties and corrosion data (see Tab. 2).

Manuals for using the databases and the analysis tools including e.g. descriptions of image and text thesauri, curve file structures, definitions of the test types are available for Mat-DB users from the ODIN portal (On-line Data Information Network: **http://odin.jrc.nl**).

Web-enabled Mat-DB: The emergence of the Internet created new opportunities for materials databases. Therefore the JRC has recently ported Mat-DB to the Internet. The objective of the web-enabled application is two-fold:

Facilitating data management, exchange and dissemination within European R&D projects

Providing a data pool which contains public and restricted data for use in industry, research and education

The final goal of JRC is to provide the full cycle of data entry, retrieval and analysis over the Internet as it is available in the PC and client/server applications. Furthermore it is planed to network with partners in order to increase both, the amount of available data and the tools for analyzing the data.

Table 1. Description of Mat-DB entities.

Entity	Meta-information for e.g.
Data Source	Organization, laboratory, scientist, R&D project
Material	Material characterisation, chemical composition, heat treatment, process data, microstructure
Specimen	Sampling, orientation, geometry, coating layers
Test condition	Test environment, mechanical or thermal pre-exposure, irradiation
Joining	Process method, joining parameters, joining geometry, filler metal
Test result	See table 2

Table 2. Mat-DB test result entity.

MECHANICAL PROPERTIES	• IRRADIATION
• CRACK GROWTH & FRACTURE	Irradiation creep
Creep crack growth	Swelling
Cyclic creep crack growth	• TENSILE
Fatigue crack growth	Compression
Fracture toughness	Multiaxial tensile
Impact	Uniaxial tensile
• CREEP	Small punch tensile
Cyclic creep	**THERMO-PHYSICAL PROPERTIES**
Multiaxial creep	Density
Torsional creep	Electrical resistivity
Uniaxial creep	Emissivity
Small punch creep	Linear thermal expansion
• RELAXATION	Poisson's ratio
Multiaxial relaxation	Specific heat
Uniaxial relaxation	Shear modulus
• FATIGUE	Thermal conductivity
High cycle fatigue	Thermal diffusivity
Low cycle fatigue (load control)	Young's modulus
Low cycle fatigue (strain control)	**CORROSION**
Thermal fatigue	High temperature corrosion
Thermo-mechanical fatigue	

Also, multi-national organizations and customers are interested in using the web-enabled Mat-DB, as they can make confidential data accessible to authorised employees at different sites via their Intranet. Furthermore it eases the life of the local database administrators since installations at the client PC are not necessary anymore. The following sections describe in detail the features of the web-enabled Mat-DB.

Data entry and exchange: Currently, Mat-DB clients enter data by using the user-interface of a stand-alone PC or client/server application. After data validation they export the data as a SQL file using Mat-DB administration tools. Then they transfer the file (e.g. by email) for upload onto the Petten Server. Since all the different Mat-DB applications are based on the same database structure, the JRC can directly import the file into the web-enabled Mat-DB. From that point onwards, the data are accessible by all authorized users via the Internet.

However, this data entry and transfer concept is only an intermediate solution; the aim is direct web-enabled data entry from the machine into Mat-DB for all European project and network partners (see Fig. 1) by using XML (eXtensive **M**ark-up **L**anguage). XML is an established standard to exchange data over the Internet between organisations having dissimilar structured databases or between machines and databases. Data are not only

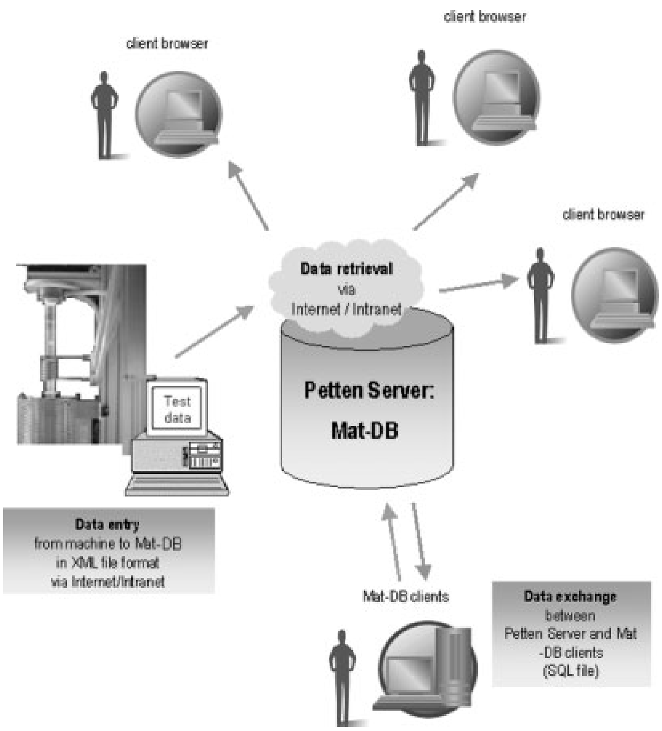

Fig. 1. Data flow from machine into Mat-DB.

assigned by their values but also by their names and units. The nomenclature of the field names within Mat-DB is compatible with the standard MATML (www.matml.org), a library developed by the international materials society and maintained by NIST (US: **N**ational **I**nstitute of **S**tandards and Technology).

Post processing tools of the machines, which are extended to export into the defined XML format, can transfer the test data in a random order into Mat-DB because the application recognises and applies the data to the assigned database fields. Source, material, specimen, test condition and joining meta-information can be completed within separate steps. The whole data sets can be checked, updated and validated before they are uploaded into the relational database part and released for clients. Such an XML based data entry procedure[11] with a user-interface similar to the PC client is pilot tested within the running European R&D project "TMF-Standard".[12]

Data retrieval and analysis: The user interface for web-enabled data retrieval follows the lines of the well-established stand-alone PC and client/server applications, although it is slightly less sophisticated due to the limitations of the HTML protocol.[13] It allows constructing a query to retrieve the test results in three sequential levels. The first level starts with mandatory selections on *source*, *test type* and *material* following a hierarchical order. Data retrieval can then be continued with optional selections of a so-called *combined material*, which characterizes special features of the material such as service exposed, irradiated, low carbon, etc., *batch identifier*, *specimen* (type) and (test) *environment*. Retrieval can be finished with optional selections on test type specific fields such as *time at rupture*, *test temperature*, *elongation* in the case of *uniaxial creep*.

After the mandatory fields have been specified the *Generate report* button is active allowing the user to create an overview report on the selected material tests. The report contains links to detailed information on e.g. source (including documentation), heat treatment, chemical composition, raw data sets or numerical and graphical curve information. Furthermore the report screen allows exporting the selected test data to pre-defined EXCEL charts or starting routines for analysing the test data.

Mat-DB contains a number of the test-type specific analysis routines, which allow a fast evaluation of the retrieved data. The evaluation programme library (see Tab. 3) contains mathematical models, constitutive equations, parametric expressions and regression functions. The analysis routines allow a comparison of data sets against each other. Database customers often use the analysis results for their publications and reports.[14] For the web-enabled application the analysis routines are re-programmed and implemented as Java applets, i.e. the analysis routines together with the selected data are downloaded onto the client PC and then run locally as fast and highly interactive desktop programmes. They allow user specified extrapolations and interactive manipulations to add or delete data points. Currently, only the Larson-Miller analysis routine is implemented. Within 2005 most of the other analysis routines shown in Table 3 will be implemented into the web-enabled Mat-DB as Java applets. The materials parameters calculated by the analysis routines are necessary for inelastic analysis calculations of high temperature exposed components. Figure 2 shows a 2nd order polynomial Larson-Miller extrapolation. Triangular symbols belong to the dissimilar welded joint X10 CrMoVNb9 1/ X20 CrMoV12 1 – dj, the rectangular symbols to the similar welded joint X10 CrMoVNb9 1 – sj.

In addition to the existing database analysis routines, the JRC is currently integrating **Fitit**, - proprietary software of the Fraunhofer Institute in Germany designed for the calculation of

Table 3. JRC Petten MDBs evaluation programme library.

Creep	Fatigue
Creep relations: Norton creep law, Prandtl creep law, Soderberg creep law, Monkman-Grant relation, Dobés-Milîcka relation	Ludvik law, Manson-Coffin relation, Basquin analysis, Frequency modified Manson-Coffin relation
Extrapolation methods: Larson-Miller, Manson-Haferd, Manson-Brown, Orr-Sherby-Dorn, Spera, Minimum commitment method	**Crack growth**
	ASTM compliant creep crack growth analysis, Creep crack growth plot, Fatigue crack growth analysis
Constitutive creep equations: Theta projection, Mc Vetty equation, Kachanov equation	**HT Corrosion**
Interpolation routines: Polynomial creep curve fit, Polynomial stress dependence, Isochronous & isostrain determination	*Weight gain/loss analysis:* Power law, Power law-time, Parabolic □m^2, Parabolic $t_{1/2}$, $K_P(t)$, Breakaway

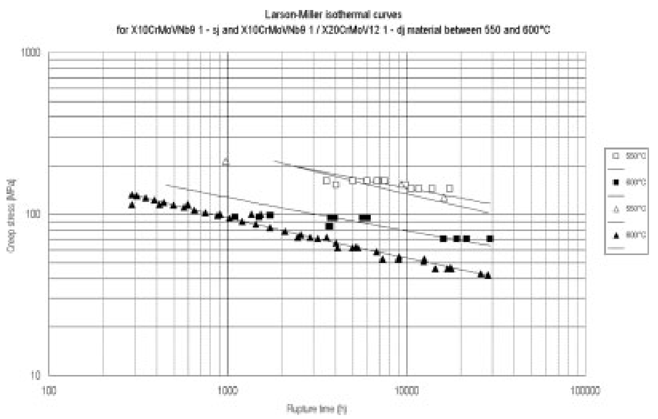

Fig. 2. Larson-Miller extrapolation of a Siempelkamp data set: Similar (X10 CrMoVN b9 1 – sj: triangular symbols) and dissimilar (X10 CrMoVNb 9 1/ X20 CrMoV 12 1 – dj: rectangular symbols) welded joints.

complex material models. **Fitit** can be used for models defined as a set of differential equations and analytic functions, e.g. Chaboche and Kachanov. Data selected within the web-enabled Mat-DB can be sent to **Fitit**, which then fits the data to a selected model. Once the model parameters have been calculated, they are returned to Mat-DB and the user can apply them for Finite Element (FE) lifetime calculations of high temperature exposed components with commercial codes like ABAQUS or ANSYS,[15] which improves safety and reliability and saves costs.

JRC data network policy: The web-enabled Mat-DB is deployed to the ODIN portal, which provides access to various web-enabled database applications for engineering and nuclear safety. It also hosts a web-enabled document management system (DoMa), which can be used to store the whole project documentation of R&D projects including minutes of meetings, final reports and the links to the relevant data in Mat-DB. The applications share fast cabling, firewall, secure connection, redundancy to guarantee high availability, central data and user management, professional hard- and software infrastructure in order to facilitate maintenance and further development, ORACLE as a powerful RDBMS and professional database servers with high capacity Raid Arrays for the storage of data and documents. They are continuously maintained and updated.

The web-enabled Mat-DB provides access to public, restricted and confidential materials data from former and current European R&D activities and from extensive material programmes, e.g. the German High Temperature Reactor Programme.[16] Public and restricted data sets are released only after agreement by the data owner, confidential data sets are accessible by the project participants only. The quality of validated data is the responsibility of the laboratory where they have been generated. JRC does not take any liability for the data.

The intention of the JRC as a supra-national institution is to increase the amount of public materials data available on the ODIN server. It currently contains a pool of public and restricted data with approximately 20000 materials tests.

As one way in achieving this goal, the JRC offers Mat-DB to European R&D activities as a free tool to manage and exchange their experimental data. The participants, who are partly supported by public funding, are encouraged to release their data for public access at the end of the project. Thus, the project benefits from a sophisticated web-enabled database for the management and conservation of materials data and related documentation. The European research community benefits from the availability of valuable data and analysis routines.

Another goal is to set up a European network with universities, research centres and associations, which uses Mat-DB as a common database. Students performing publicly funded experimental materials research within their graduation or PhD thesis should be encouraged to enter their data online into Mat-DB. These data have to be checked and validated by their supervisors. This materials data network would act as a 'club activity' to the benefit of all members in which data and analysis routines are shared by each other similar to the Japanese 'Data Freeway', which was set up to exchange data between several research centres.[17] In combination with background information on database structure, test type specifications and description of analysis routines it could also act as training instrument for students.

Free access to a wide range of experimental data and analysis routines for the European scientific society could act as a driving force to discover new relations and dependencies between material properties, which again could result in new types of material selection systems similar to the Ashby maps,[18] which not only show the differences of various material classes but more detailed the differences of material parameters within one material class and furthermore within various heats and batches. The DMD network could be the initiator for the design of new materials products.

However, often proprietary data are very sensitive and the data owners want to keep full control of the data. In such a case, the web-enabled Mat-DB could be installed on servers, which are under control of the data owner. Since all servers are using the same database structure it would be possible to create a data warehouse,[19] which would allow the user to search for the required data over all installations of Mat-DB while the data owner retains full control over its own data. The network could be joined by industrial organizations, which intend to sell restricted materials data sets over the Internet and by current client/server database customers who are interested in installing the web-enabled Mat-DB for internal use on their Intranet. In order to establish such a network, it will be necessary to obtain public funding on a European level.

Summary and Conclusion: Material databases (MDBs) are important and powerful tools for the conservation, exchange and dissemination of data. The potential has even further increased with the emergence of the Internet. The availability of experimental materials data in a defined and traceable quality is necessary for inelastic analysis calculations and complex modelling. In combination with FE calculations lifetime predictions can result in a much better use of high temperature exposed components, which improves safety and reliability and saves costs. Therefore the European engineering community should be very interested in an ever-growing data pool promptly accessible via the Internet.

The JRC has a long history of developing material databases and can offer a mature web-enabled Mat-DB to manage mechanical, thermo-physical and corrosion properties data. The database has a complex structure and includes detailed meta-information on the *material*, *test condition*, *data source* etc. Mat-DB and the related analysis routines are installed on a powerful and secure server within the On-line Data Information Network (ODIN: **http://odin.jrc.nl**). The application is offered at no charge to support European R&D activities for the management and conservation of their experimental materials data and the project participants are encouraged by the EU to release their data for public access at the end of the project. The JRC also intends to obtain data from other sources, e.g. universities and associations, which could be collected within a European materials data network where the members share their data and analysis routines with each other. Within this network Mat-DB could also be installed on different servers and networked together to form a materials data warehouse.

Since ODIN is a central portal to a series of its activities, the JRC intends to ensure a long-term continuation of the related applications including maintenance and further development of the web-enabled Mat-DB. The structure, for instance could be upgraded to include additional material groups such as polymers, ceramics and composites. New test types will be added as required. The web-enabled Mat-DB will be further developed to include the entire cycle of data entry from machine to database, data retrieval and analysis. Free access to a wide range of experimental data and analysis routines for the European scientific society could act as a driving force to discover new relations and dependences between material properties. A European materials data network could help to overcome the dispersion of effort and lack of coherence of EU research, which is due to inevitable fragmentation within and between the different countries and organizations. It is consistent with the ideas of the 7th Research Framework Programme of the European Commission: 'Building the Europe of Knowledge' and may contribute to the enlargement process through supporting and candidate country integration.

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[1] Special Issue "Materials and Process Selection", *Adv. Eng. Mater.* **2002**, *4*, 317–416.
[2] *Plantfacts Database of the German VDEh* (Verein Deutscher Eisenhüttenleute – German Iron and Steel Institute): http://www.vdeh.de/deutsch/arbeit/informat/plantfe.htm.
[3] *WIAM®-METALLINFO* database, IMA-Dresden: http://www.ima-dresden.de/deutsch/startde.htm.
[4] *Materials Databases of MBase*, Aachen, Germany: http://www.m-base.de/main/en/index.html.
[5] *MSC.Mvision* Databanks, USA: http://www.mscsoftware.com.
[6] *Wirtschaftswoche*, **2004** (*35*).
[7] Materials Databases of NIMS – *National Institute for Materials Science*, Japan: http://mits.nims.go.jp/db_top_eng.htm.
[8] R. C. Hurst, H. Kröckel, H. H. Over, P. Vannson, *The Use of Models in Materials Databanks*, Materials 88 – Materials and Eng. Design, The Institute of Metals, London **1988.**
[9] H. Kröckel, H. H. Over, *The Need for an European Approach to Materials Characterisation and Data Management,* International Symposium on Advanced Materials for Lightweight Structures, March **1994.**
[10] H. H. Over, J. H. Rantala N. Taylor, W. Dietz, *A materials properties database approach to cover welded joints*, 2nd International Conference on Integrity of High Temperature Welds, London, UK, 10th – 12th November, **2003.**
[11] M. Nagy, H. H. Over, A. Smith, *XML related Data Exchange from the Test Machine into the Web-enabled Alloys-DB,* 19th International CODATA Conference, "The Information Society: New Horizons for Science", Berlin Germany, 7th – 10th November **2004.**
[12] *Thermo-mechanical fatigue – the route to standardisation'*, CORDIS R&D project no. GRD2-**2000**-30014.
[13] H. H. Over, E. Wolfart, E. Veragten, *Data Retrieval and Evaluation within the Web-enabled Alloys-DB,* 19th International CODATA Conference, "The Information Society: New Horizons for Science", Berlin, Germany, 7–10 November **2004.**
[14] P. J. Ennis, *Candidate Materials for a Modular High Temperature Reactor Power Plant in Engineering Issues in Turbine Machinery, Power Plant and Renewables,* Maney, IoM3 Publications, Book Number B0800, ISBN 1-904350-20-8, **2003**, pp 1029–1037.
[15] Endbericht zum Verbund-Forschungsvorhaben des BMFT, *Auslegungskriterien für hochtemperaturbelastete metallische und keramische Komponenten sowie des Spannbeton-Reaktordruckbehälters zukünftiger HTR-Anlagen,* Teil B: Metallische Komponenten, KFA Jülich, August **1988.**
[16] R. Mohrmann, V. Denner, T. Hollstein, *'Zur Lebensdauervorhersage von Austenit-Ferrit-Mischverbindungen'*, Tagungsband FDBR Düsseldorf (**2003**) Teil 4.
[17] 15th *International CODATA* Conference, M. Fujita, Some Trials on WWW Servers in the "Data Freeway", Scientific Data in the Age of Networking 29 September – 3 October **1996**, Tsukuba, Japan.
[18] M. F. Ashby, *Materials Selection in Mechanical Design*, Butterworth-Heinemann, Oxford **1999.**
[19] Y. Li, *Adv. Eng. Mater.* **2004**, *6*, 92.