SEMINAR CUM MEETING REPORT: CODATA TASK GROUP FOR EXCHANGEABLE MATERIAL DATA REPRESENTATION TO SUPPORT RESEARCH AND EDUCATION

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ABSTRACT

On March 4-5, 2008, the CODATA Task Group for Exchangeable Material Data Representation to Support Research and Education held a two day seminar cum meeting at the National Physical Laboratory (NPL), New Delhi, India, with NPL materials researchers and task group members representing material activities and databases from seven countries: European Union (The Czech Republic, France, and the Netherlands), India, Korea, Japan, and the United States. The NPL seminar included presentations about the researchers' work. The Task Group meeting included presentations about current data related activities of the members. Joint discussions between NPL researchers and CODATA task group members began an exchange of viewpoints among materials data producers, users, and databases developers. The seminar cum meeting included plans to continue and expand Task Group activities at the 2008 CODATA 21st Meeting in Kyiv, Ukraine.

Keywords: Materials data, Materials research, Materials education, Data exchange, Data representation, CODATA task group

1 SUMMARY OF CONCLUSIONS

The first convening of the task group, bringing together materials data producers, researchers, and database developers, began useful discussions with good potential for productive activities and expansion. EU and Japan will begin discussions to unify their efforts on data representation for creep property. An updatable material information resource list on the Japanese National CODATA Committee (CODATA.JP) web site with distributed RSS technology will be made available with participation from India, Korea, EU, and Japan. The task group co-chairs will lead an effort to bring together international domain experts and data specialists actively engaged in research and education related to nanomaterials for a proposed workshop. Discussions about materials ontology will be expanded at the CODATA 2008 Conference in Kyiv.

2 RAISON D'ÊTRE OF THE MEETING

Increasing amounts of materials data and knowledge are being generated around the world. To utilize effectively these vast information resources for the development of new materials and for impact on material science education, it is exceedingly important to bring together multiple viewpoints of materials data evaluation.

To understand material behavior fully, data exchange and interoperability of material resources need the ability to integrate the complex information for multiple scales and multiple phenomena generated from observed phenomena, experiments, and computational simulations. To this end, there are many efforts to develop material databases, computational models, digital libraries, and data analysis methods, such as data mining and data visualization, to derive and disseminate knowledge about materials.

The CODATA Task Group for Exchangeable Materials Data Representation to support Scientific Research and Education was established at the 2006 20th International CODATA Conference to begin to address these vital issues. In today's global environment and economy, the international community is entering a new and rapidly evolving era of materials design research. Increasingly, researchers and product designers look to develop a material for a particular application rather than use an existing material. Examples range from such areas as traditional materials, such as metals, ceramics, and polymers, to biomaterials, where materials and composites are made to imitate human skin, muscles, bones, and neurons, to nanoscience for the design and control of self-assembled, functional nanomaterials. Coinciding with these developments is the rise of large-scale, government-funded, interdisciplinary materials programs across the international materials community that enable progress across a broad range of scientific disciplines and technological areas with dramatic impacts on society. Notable among such enterprises are:

In Asia
- National Institute for Materials Research in Japan
- Shenyang National Laboratory for Materials Science (SYNL) in China

In Europe
- EU Research Framework Programme (FP7) and its theme 'Nanosciences and nanotechnologies, materials and new production technologies'

In India
- Jawaharlal Nehru Centre for Advanced Scientific Research, Advanced Materials Research Laboratory

In US
- NSF's Materials Research Science and Engineering Centers (MRSECs)
- DOE's Nationals Laboratories in Materials Research

The overarching goals of the CODATA Materials Task Group are to foster collaboration and international cooperation for sharing expertise in materials research and education – especially among developed and developing countries – in order to advance scientific knowledge and to recruit, retain, and train the next generation of materials scientists, as well as to increase the numbers of highly skilled technical workers and materials scientists. Through its collective efforts, the Task Group seeks to contribute to the advancement of materials research and education through application of modern informatics, such as the use of distributed systems of hardware, software, information bases, and expert systems to complement the exponential growth in computing power, communication bandwidth, and data storage capacity.

The first convening of the CODATA Materials Task Group used the face-to-face meeting of researchers and developers to begin discussions on topics related to the interoperability of heterogeneous materials data representation. The seminar cum meeting addressed areas, such as system integration of factual databases and computer simulations for material development, multi-scale modeling, integration of material databases into material science education and, as their common infrastructure, development of material databases, and common representation for material data or common ontology for material knowledge. Further, the session considered the integration of materials data exchange into undergraduate and graduate education. Recent government studies have indicated that undergraduate students who participate in hands-on research are more likely to pursue advanced degrees and careers in science, technology, engineering, and mathematics (STEM) fields.

Membership in the CODATA Materials Task Group totals over 30 CODATA members with over 12 countries representing all corners of the globe and with increased participation anticipated at the 21st CODATA International Conference in Kyiv. Based on the response from task group members, a renewal from 2008 through 2010 has been submitted.

3 SUMMARY OF DISCUSSIONS

Task group members and researchers of material databases from six countries, four from Japan, two from Korea, three from EU, one from US, and two from India attended, making presentations about their activities and discussing issues in material data exchange and possibilities for international collaboration for material data dissemination. It was held as an NPL seminar, and about 30 NPL materials science researchers joined in the discussion. The various viewpoints of material data producers and users of databases were very informative for the task group members.

In this meeting, chairs listed the following four agenda items:

a) Identify online material database activities/material data resources,

b) Integrate material data representation and semantic issues,

c) Develop a commons for innovative reactors and sustainable energy resources, and

d) Integrate materials databases into materials science education for graduates and undergraduates.

Ten papers related to these topics were delivered and discussed along with the possibility for international collaboration.

All participants agreed that common material data and metadata representation is necessary for sharing scientific information and plays an important role in the infrastructure of competitive industries, a sustainable and reliable society, and scientific and engineering education. However, many difficulties exist when defining material data, as the concept "material" ranges from individual specimens to abstract substances such as “carbon steel.”

It was noted that several duplicate efforts in the definition of standardized data schema or other material data representations exist, and members agreed to form two task groups to coordinate two items requiring further discussions.

a) Professor Over's group (EU, JRC, Petten) and Prof. Monma's group (Kochi Univ. of Tech. et al.) are both trying to define data representation for creep property. They will start discussions to unify their results and to extend them to fatigue and other properties.

b) A second task group will continue discussions about material ontology introduced by Professor Ashino. Professor Hunter (Australia) is also doing research in this area, and her work will be included in the discussions at the CODATA Conference in Kyiv because she was absent from the New Delhi meeting.

Several countries and international organizations are attempting to establish national/international material data portal sites. Professor Ashino proposed utilizing distributed RSS with extensions as the international basis for a continuously updatable material database portal and creating an international material database portal on the codata.jp web site as the CODATA task group's activity.

4 LONGER DISCUSSION OF CONCLUSIONS

The March 2008 task group assembly at the National Physical Laboratory in New Delhi, India, convened an international group of developers, producers, and researchers for discussions to launch developments and expanded activities in preparation for the October 2008 21st CODATA International Conference in Kyiv, Ukraine. Work centered around four major areas: creep property data; materials information resource list; materials ontology; and the proposed satellite symposium.

4.1 Creep property

The creep property of a material is an important parameter in the material selection process for high temperature device design. Rising cost pressures and stricter environmental regulations in such areas as power-generation, petro-chemical, process and waste-incineration plants, and gas turbines and aircraft engines have heightened the need for reliable creep data. EU and Japan, along with other countries, have committed significant investment and effort to furthering technological developments to access and exchange creep data. Beginning discussions were launched at the task group meeting to join their individual accomplishments on data representation for creep property. The compatibility of mark up language elements and database structures will center on design and life assessment issues relating to creep and fracture in high temperature components. Progress on these collective efforts will contribute to support of the development of new advanced high temperature materials that can operate under more extreme conditions of temperature and stress.

4.2 RSS materials information resource list

An updatable materials information resource list on the CODATA.JP web site with distributed RSS technology will be made available with anticipated participation from India, Korea, EU, and Japan. “RSS” (RDF Site Summary) has become widespread in the information transmission of blogs and news sites. Though there are currently several versions of RSS, RSS 1.0 (Beged-Dov, et al., 2001) was adopted for use at the meeting. RSS 1.0 is based on RDF, so the data structure is easy to change as needs arise. There have been several trials to extend RSS distribution of metadata of scientific data in geoscience (Kubo, et al., 2006) and chemical science (Murray-Rust, et al., 2004; Rzepa, et al., 2006). A RSS module is proposed for material information, and a portal has been developed for transmitting information of material databases via networks. The portal consists of an “RSS reader” and “Registration function of available vocabularies in RSS module for material information”. An RSS reader is application software for obtaining RSS feeds. The implementer of each material database creates an RSS feed, which describes its database following the RSS extension. The RSS reader aggregates RSS feeds from the database sites. Because RSS does not define vocabularies of material properties or types, which are used to search and identify material databases, these features need to be defined in addition to RSS tags. An RSS module for material information defines only requisite elements when a user of the portal searches the databases’ metadata. The presented work uses class, type, name, composition, and property as important tags and fundamental concepts about a material database.

4.3 Materials Ontology

Discussions about materials ontology will be expanded at the CODATA Conference in Kyiv.

A standardized data schema for material properties in XML is under development to establish common and exchangeable data expression. The next stage toward knowledge management about material usage, selection, or processing is to define an ontology that represents the structure of concepts relating to materials, e.g., taxonomy, analysis, or properties of materials. Material selection for designing artifacts is a process of translating required material properties into a specific material substance. In order to manage knowledge of this process, definitions and rules of data analysis must be formalized in computer readable format. In this paper, an ontology structure for design process is briefly discussed using the example of the creep property of materials.

4.4 October 4, 2008 Satellite Symposium, Kyiv, Ukraine

The task group co-chairs will lead an international effort to bring together domain experts and data specialists actively engaged in research and education related to nanomaterials for a proposed satellite symposium coinciding with the 21st CODATA International Conference in Kyiv, Ukraine. The timing of the symposium will provide the opportunity for materials researchers to join their colleagues in astronomy, biological sciences, chemistry, earth sciences, and physics at CODATA in participating with their international counterparts. The purpose of the proposed symposium is to hold invited presentations and focused discussions about mining potential discoveries from the abundance of available data and bringing recent findings into the university classroom. Countries’ task group members, government standards agencies, including the US National Institute of Standards and Technology (NIST), materials researchers, and participants from countries such as France, India, Japan, the Netherlands, Russia, Korea, and the US are expected to take part in the symposium. The expected outcome of the symposium is the formation of an international pilot focused on the development of tools and software to improve use of data related to nanomaterials adaptable for undergraduate education and research experiences. The broader goals of the workshop are to enable researchers, faculty, scientists, and data specialists to exchange their experiences, ideas, and information, to establish collaborations with their counterparts in countries from Europe and Asia, and to promote nanomaterials and supportive data software and tools for the benefit of research and education in all of the involved countries.

5 ABSTRACTS

Ten papers were delivered during the task group meeting centering on four topics: a) Identification of online material data resources; b) Material data representation and semantic issues to integrate material and simulation; c) Nuclear data activities; and d) Integration of material data into materials science education.

5.1 Identification of online materials data resources

5.1.1 Mat-DB: Materials database for experimental mechanical and physical properties and corrosion

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The European Commission Joint Research Centre Petten has developed a Web portal for the Online Data and Information Network (ODIN). It contains engineering databases, document management sites, and other information related to European research in the area of nuclear and conventional energy. The objectives are: knowledge conservation of nuclear and non-nuclear energy-related R&D; management and exchange of data and documentation within European projects; dissemination of public data and information to the research community; and provision of data and documentation for training and education. The features are: container of public and restricted data; free-of-charge use to the benefit of European R&D; deployment of professional hard- and software infrastructure; provision of central, long-term maintenance of databases and applications; and an English user interface.

One of the databases is the JRC Petten Mat-DB that deals with materials testing purposes, covering mechanical and thermo-physical properties data of engineering alloys at low, elevated, and high temperatures for base materials and joints, including 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. The corrosion section refers to weight gain/loss data of high temperature exposed engineering alloys, ceramics, and hot isostatic pressed powder materials.

A major part of European R&D materials test data is stored in Mat-DB. A part of the European nuclear research activities and R&D projects contribute to the Generation IV International Forum (GIF). The Generation IV reactor systems are very important for the future to cover the whole fuel cycle from breeding to waste burning. The primary components operate from elevated up to high temperatures (1000° C). For reactor design, data sheets are necessary. These are not yet available for the materials taken into consideration, and extensive material programmes are necessary to establish these materials data sheets. This is associated with high costs, as one GIF partner is hardly willing to invest for all the considered GEN IV reactor systems. Data exchange of experimental data between partners is probably the easiest solution to reduce these costs.

Therefore, we are studying the possibility of becoming more standards compliant with the publication and interchange of our data, standards being XML technologies and the established MatML schema. Our aim is to complement the MatML schema with our own “Mat-DB schema," which means dealing with materials testing purposes. To achieve real life experience with these issues, we are working on defining the Mat-DB XML schema with necessary metadata included in the schema structures; implementing software to produce Mat-DB XML documents from our database and to import Mat-DB XML data into the database; mapping between Mat-DB and MatML contents; testing the suitability of XSL transformations in realizing this mapping; and studying the ways to extend MatML schema to sufficiently cover the contents of Mat-DB if that is needed.

5.1.2 NIMS MITS Materials Databases

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The Materials Database Station (MDBS) of the National Institute for Materials Science (NIMS) is playing an active role in the acquisition, collection, classification, and release of materials data and information. The NIMS Materials Databases system provides twelve databases: five concerning structural materials, five concerning physical properties, one for superconducting materials, and one for polymers. Theses databases are available on at http://mits.nims.go.jp/en. The cross search system MatNavi has been developed for retrieving information from these databases. By the end of February 2008, approximately 35,441 (26,069 in Japan, 9,372 overseas) users have registered NIMS Materials Databases from 110 countries and 10,293 organizations, and there are 700 new users register every month. The MDBS has wide international cooperation with other material information resources in the world. We have signed memoranda of understanding (MOU) with Matdata.net (Granta Desgin), MatWeb (Automation Creations Inc.), Springer Link (Landolt Börnstein), and the Metals Bank (Korea Institute of Materials Science). The cooperation includes hyperlinks between web pages, an integrated search engine, organization of international symposia, investigation of business models of materials databases, and establishment of standardized materials data formats, etc. Moreover, we have participated in activities of the World Material Research Institute Forum (WMRIF) and CODATA.

5.1.3 Materials Bank Project in Korea

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Several years ago, the Korean Ministry of Commerce, Industry and Energy (now the Ministry of Knowledge Economy) framed the policy for promotion of the compartment and materials industry in Korea. To further this policy, the Materials Bank Project was launched in 2007 with a five-year program as its first stage. The vision of the Materials Bank is to be the world's leading materials data bank as a national infrastructure. Its key roles are composed of the following three activities. First is the construction of a combined materials information system for the dissemination of user-oriented information. Second is international collaboration and networking to acquire advanced information on materials. The last is the education of materials specialists to secure R&D competence. The Materials Bank consists of 3 hubs for metals, chemicals, and ceramics respectively and is supervised by the Korea Materials and Components Industry Agency (KMAC, a subsidiary organization of the Ministry of Knowledge Economy to supervise national projects, such as budget affairs and estimation of research results). The Korea Institute of Materials Science (KIMS) manages the Metals Bank (www.metalsbank.com) as a hub, and several national institutes participate as spokes. The Korea Research Institute of Chemical Technology (KRICT) is constructing the Chemical Materials Information Bank, and the Korea Institute of Ceramic Engineering and Technology (KICET) is building the Ceramics Bank. We expect that the Materials Bank will act as a basis for international collaboration of materials data as well as the promotion of the Korean materials industry.

5.1.4 Centralized Indian Materials Database

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A project consisting of building a centralized Indian Materials Database for Scientists, Engineers, and Industries has been taken up. The importance of the common database was realized, as a great deal of data on creep, fatigue, tensile, fracture, and corrosion properties on different structural materials has been generated in Indian laboratories during the past four decades. Indian laboratories are now self sufficient in providing the vital data needed for the country's power, space, and chemical industries. There is also a large scope for Indian industries to use this database. In India, the availability of a materials database is of high relevance as a huge investment in energy, chemical and other sectors and new materials is being made. This database, once launched, would be available to the international scientific community. These data are uniquely authentic, as they have already been published. The main emphasis of the work is the compilation of the data from different laboratories, linking the laboratories for periodic updating of the data, and providing access to the data for scientists and engineers. The scope of the database centre extends to other materials properties. The Indira Gandhi Centre for Atomic Research (IGCAR) Kalpakkam, which has carved a special name for itself in the international community of metallurgists because of its contributions in the area of materials science, the Indian Institute of Metals (IIM), a professional body on metallurgical activities, and the Indian National Science Academy (INSA), a professional body for scientific activities in India, have been identified as the nucleators of the effort to set up a centralized materials database catering, at first, to materials and properties. In next five to ten years, the number of databases for this centre is expected to grow to about 500, and the volume of database may grow to a few terabytes.

5.2 Materials data representation/semantic issues to integrate materials & simulation

5.2.1 Material Data Exchange and Material Ontology

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We are performing several trials to develop material data schemas for material data exchange, but the schemas are for simple data structures. It is difficult to capture a complicated concept model for materials science. In contrast, ontology provides a network structure of concepts and their relationships. We have developed a material ontology for materials data exchange supported by NEDO (New Energy and Industrial Technology Development Organization in Japan) and tried to exchange thermal properties data between databases provided by three organizations. Our material ontology is divided into four core ontologies: "Substance," "Property," "Environment," "Process," and several peripheral ontologies, which represent physical constants or units of measurement. Also we designed an RSS extension for a metadata description of a material database in order to create a continuously updatable materials information resource list. It includes XML tags for material names, property types or expected applications, and definitions of vocabulary sets for each tag, which make the RSS list searchable. A material data portal site named IC4M (Information Commons for Material Science - http://www.codata.jp:8080/) is now online. IC4M provides RSS-based material information resource lists, as well as an aggregation function of distributed RSS entries that can be searched. Documents of specifications for RSS extension and Material Ontology, some examples of RSS entries, and material data exchange based on Material Ontology are also provided by IC4M.

5.2.2 Integrating Creep Knowledge and Material Databases

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Historically, creep and fatigue data have been some of the earliest implementations of computerized databases. Because of the cost and the time involved in obtaining long-time creep data, we have been able to use data systems from the Internet. In order to promote the sharing and exchange of these material property data, an international standard MatML, based on the markup language XML Schema, has been proposed. However, examples of MatML implementation are very limited. With funding from NEDO (New Energy and Industrial Technology Development Organization) in Japan, we have developed an extension of MatML, NMC-MatDB, and built a prototyping system of tensile and creep-rupture data with about 2000 specimens of 20 heat-resisting alloys. In this system we can query the XML database, and then by using TTP (Time-Temperature parameters) models, we can invoke data evaluation modules for creep-rupture curves. To access the database and the software see the Japanese CODATA TG site at: http://www.codata.jp:8080/. The database should be available soon.

5.2.3 Integrating NIMS thermal properties simulator & AIST thermal properties database

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Materials design by computer simulation has become an important approach for the development of new materials. CompoTherm is an Internet platform developed by the National Institute for Materials Science (NIMS) that enables a user to design the constitution and structure of a composite and predict its thermo-physical properties. In this presentation, we reported our recent work on data exchange between simulation software and materials database using a case study of data transport to CompoTherm from the AIST Thermo-physical Properties Database, an Internet materials database developed and maintained by the Japanese agency for Advanced Industrial Science and Technology (AIST). The procedure downloads the property data of a material as a data file from AIST's database and then uploads the file to CompoTherm so that the simulation system can use the data in calculations. Because the data formats used by AIST and NIMS are different, a common XML format designed under the cooperation of the University of Tokyo, NIMS, and AIST has been used as an intermediate data format. Other agreements between NIMS and AIST include a description of mathematical expressions and a coordination system for expressing thermal conductivity as tensors.

5.3 Nuclear data activities

5.3.1 Molten Salt Reactor (MSR) development including structural materials and components testing in the frame of the EURATOM activity in MSR Steering Committee of GIF

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Nuclear power is expected to become a source of energy for a significant part of the world demand in the future. However, its big disadvantage, the danger of the spent nuclear fuel, has to be solved. The Molten Salt Reactor (MSR) - SPHINX (SPent Hot fuel Incinerator by Neutron fluX) concept solves this principal problem of spent fuel treatment by means of so-called nuclear incineration (Hron, 2004). It burns the fissionable part of its inventory and transmutes other problematic radionuclides by use of nuclear reactions with neutrons in a MSR - SPHINX system. This reactor system is an actinide burner and a radionuclide transmuter. The R&D program of MSR - SPHINX contains physical, chemical (partitioning), and structural material parts of the reactor. In the physical section, computational analyses and experimental activities (Hron, 2005) are involved in the program, which serves to validate computer codes and, finally, to verify design inputs (Hron, 2006 & 2007) for designing a MSR-type demonstration unit. The molten fluoride salt demonstration unit is needed to show the operation and design performance for closing the nuclear spent fuel cycle for PWR or VVER reactors operated in the once-through cycle mode.

The experimental program has been focused, in its first stage, on a short-term irradiation of small size samples of molten-salt systems as well as structural materials proposed for the MSR blanket in the field of high neutron flux of research reactors. The proposed next stage of the program focuses on a large-scale experimental verification of design inputs by inserting MSR-type zones into the existing light water moderated experimental reactor LR-0, which may allow modifications to an experimental zero power salt reactor SR-0. One of the elementary modules has been arranged and adopted for an irradiation by a hard spectrum of neutrons generated by a neutron generator installed at the cyclotron accelerator in the Institute of Nuclear Physics of the Czech Academy of Sciences. All these experiments will generate a huge amount of primary data, which must be elaborated into corresponding databases. This data will help us to verify computational codes used and to recognize anomalies related to fluorides utilization.

5.3.2 Investigation methods and recent results on lanthanide halide systems

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Lanthanide halides have been the subject of investigations for many years. Their physicochemical properties as well as those of the compounds they form, for instance alkali halides, can be examined and correlated in a unique way because the lanthanides vary regularly along the series they form in the periodic table.

Lanthanide metal halides as well as the systems they form with alkali metal halides were recently the subject of focused and renewed interest. While lanthanide fluorides or chlorides and related systems have been investigated in the past in relation to different nuclear applications, they are still currently being investigated in the present context of pyrochemical separations (novel fuel cycles for future reactor systems, innovative waste management strategies, etc.) (Forsberg 2006). Very little information existed until recently on lanthanide bromides and iodides or on the systems they form with corresponding alkali halides. These systems are of technological importance in several fields, of which optical and scintillation devices and high-temperature energy-saving light sources (metal-halide lamps) are just a few examples. They also are characterized by several features making them challenging objects of fundamental interest. Several experimental techniques were used complementarily to acquire the corresponding physicochemical data (enthalpy/temperature of phase transition: heat capacity, electrical conductivity (Rycerz, 2008), standard potential and diffusion coefficients (Kuznetsov, 2007), and structure (Watanabe, 2005), which is also mandatory for process development. From there, a fascinating route opened from data acquisition to data correlation (Rycerz, 2008) and ultimately to data prediction (Gadzuric, 2006) for those still unknown compounds. This latter goal makes use of informatics tools and data mining techniques applied to large data sets in the molten salt database (Fuller, 2002) and of the above research results.

5.4 Integrating materials data into materials science education

5.4.1 Cyber-enabled learning & undergraduate materials education

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Undergraduates utilizing networking technologies in their learning activities serve not only as early adopters of emergent cyberinfrastructure but also as role models to motivate future students with the potential of cyberinfrastructure-enabled scientific inquiry and learning (NSF Cyberinfrastructure Council, 2007). The Materials Digital Library (MatDL http://matdl.org) currently serves as the Materials Pathway in the National Science Digital Library (NSDL http://nsdl Zia, 2002) to facilitate the integration of materials research and education with a targeted audience of undergraduates and above (Bartolo et al., 2006). Adhering to open standards and open access protocols (Hannay, 2007), MatDL leverages, implements, and maintains current, recognized, open source collaborative software, such as code versioning systems, wikis, and content management systems to connect distributed teams, promote resource exchange, and facilitate information sharing.

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