The Materials Digital Library: MatDL.org

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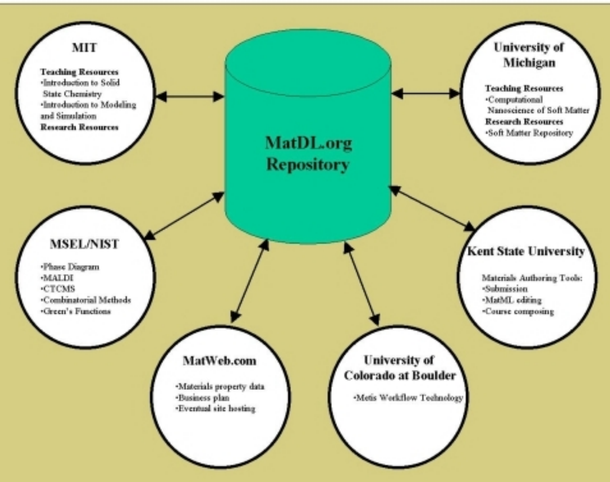
MatDL.org Materials Digital Library

Abstract

The Materials Digital Library (MatDL) project conducts research on the efficient delivery of a materials digital library to maximize opportunities to create and disseminate rich scientific content to researchers, educators and students using a three-pronged approach: (i) collection of materials content, with an emphasis on soft matter, (ii) use of materials content in a digital library, and (iii) construction of authoring tools for improved delivery. Submission, editing, and composing tools will enable experts and novices to characterize their contributions to MatDL, as materials scientists would, using metadata schemas and domain-specific markup languages, such as Materials Markup Language. Initial content of MatDL will begin with resources selected from the Materials Science and Engineering Laboratory at the National Institute of Standards and Technology. Students and faculty in "real world" MSE courses offered at MIT and the University of Michigan (U-M) will use and contribute to MatDL utilizing the domain-specific tools. Two courses are part of MIT's newly revised MSE curriculum and its OpenCourseWare Initiative. The first MIT course, *Introduction to Solid State Chemistry*, is a large freshman chemistry course with no lab component. The second MIT course, *Introduction to Modeling and Simulation*, is a multidisciplinary science course team-taught across seven engineering departments. The third course, *Computational Nanoscience and Soft Matter* taught at U-M, introduces students to cutting edge research on building new nanomaterials. The project's industrial partner, MatWeb, will work with the investigators to build a business plan and to eventually host MatDL as a sustainable enterprise.



MASSACHUSETTS INSTITUTE OF TECHNOLOGY

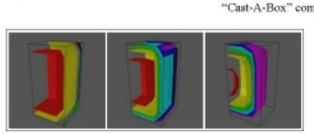
MatDL will be integrated into example courses as a reliable, up-to-date, and easy-to-use collection of materials resources described as material scientists would characterize them. Course work contributions to MatDL by undergraduate and graduate students and educators utilizing the collection will add further dimension and scope to the repository.

Initially at MIT, two OpenCourseWare courses will participate:

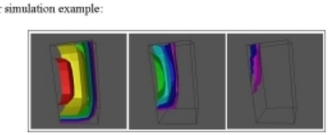
Introduction to Solid State Chemistry is a large freshman general chemistry course designed to give students the kernel of chemistry that will prepare them for engineering, science, architecture, management, and the humanities -- but within the framework of an analytical education. This subject teaches basic principles of chemistry and shows how they apply in describing the behavior of the solid state. The relationship between electronic structure, chemical bonding, and crystal structure is developed. Attention is given to characterization of atomic and molecular arrangements in crystalline and amorphous solids: metals, ceramics, semiconductors and polymers (including proteins).

Introduction to Modeling and Simulation is a multidisciplinary, team-taught, undergraduate science course involving ten faculty in seven departments across the MIT Schools of Engineering and Science. By covering basic modeling and simulation principles centered on materials, the course introduces techniques relevant to all of the participating departments, with the materials theme representing a core enabling technology for all engineers. The course spans a range of length and time scales and tools, from electrons and density functional theory to macroscopic structures and finite element and boundary element methods, with applications from mechanics to biology.

"Cast-A-Box" computer simulation example:



Simulation 1: The "cooler" dark blue contour covers the top of the box, indicating that the top has frozen over and a considerable amount of liquid is trapped inside, which will almost certainly lead to a casting defect.



Simulation 2: Heat is applied to the top surface, making it the last part of the box to solidify and preventing the casting defect which probably would have occurred in Simulation 1.

NIST
National Institute of Standards and Technology

Much of the initial content of MatDL will be supplied by the Materials Science and Engineering Laboratory at NIST. MSEL's contributions will be ongoing.

Resources to be provided:
Phase diagrams of binary and ternary solder alloys obtained from thermodynamic calculations, as well as a database file needed to perform the calculated diagrams, and software

MALDI, a database of methods for matrix-assisted laser desorption ionization mass spectrometry

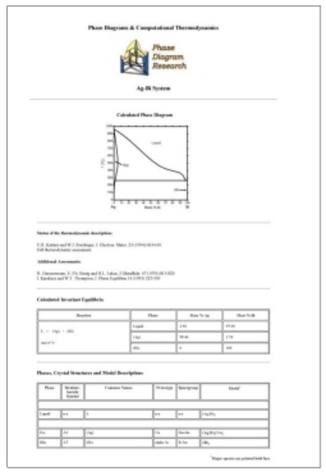
Combinatorial Methods Center online publications and presentations

Ceramics web book, a mature web-based project providing evaluated data, including a superconducting materials database, a structural ceramics database and other property data, a guide to other ceramics data centers and sources as well as links to other tools and resources

CTCMS archive of software modeling tools, a variety of codes for modeling such phenomena as microstructure evolution, deformation, crystal structures, and the performance of inhomogeneous materials

Multiscale Green's functions for nanostructures, computationally efficient techniques developed by The Materials Reliability Division for calculation of *multiscale Green's functions* for modeling nanostructures as well as their visualization on computer

Phase Diagram Example



MatWeb
MATERIAL PROPERTY DATA

MatWeb, MatDL's industrial partner, will work with the investigators to build a business plan and to eventually host MatDL as a sustainable enterprise.

MatWeb has successfully pioneered a freely accessible web-based material property knowledge base which attracts over 9,500 unique visitors daily. Over 35,000 users have registered at the site and regularly refer to its data. The searchable database of material data sheets includes property information on thermoplastic and thermoset polymers, metals, ceramics, plus a growing list of semiconductors, fibers, and other engineering materials.

Colorado
University of Colorado at Boulder

Metis Workflow Technology

The Metis approach makes use of event-based workflows to support the distributed nature of digital library workflow and employs techniques to make the resulting technology lightweight, flexible, and integrated with the Web.

Metis will allow MatDL to define a rather generic review process, while allowing each contributing organization to define specific review processes that match the needs of a particular type of resource.

UNIVERSITY OF MICHIGAN

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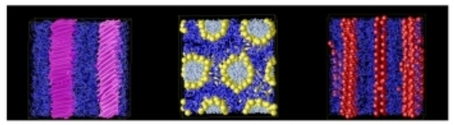
Initially At U-M, one course will participate:

Computational Nanoscience of Soft Matter is an undergraduate/graduate course designed to integrate research and education by introducing students to new approaches to materials design and fabrication through cutting-edge, simulation-based research in nanoscience and nanotechnology. Course topics span from ab initio to continuum methods, but emphasize molecular and mesoscale simulation tools used by computational materials researchers to predict morphologies of nanostructured and nano-assembled soft materials.

Nanostructures produced by the students and by members of the graduate-level Research Group, which focuses on the prediction of assembled nanostructures composed of soft matter and soft/hard hybrid nano building blocks, will be contributed to MatDL as part of the Soft Matter repository.

Examples of nanostructures of soft materials, including hybrid organic/inorganic materials, produced by computer simulations:



From left to right: (a) ordered sheets of nanorods in a polymer matrix; (b) tubes of gold nanoparticles surrounded by two species of polymer; (c) bilayers of tethered nanoparticles.

KENT STATE UNIVERSITY

Kent State University will contribute materials authoring tools including:

Submission Tool
The prototype materials user input tool will prompt the author for both learning metadata and domain specific description through an HTML form using server side scripting to create a valid metadata record using LOM and DC. The metadata generated will be made available for OAI harvesting.

MatML Editor
Materials Property Data Markup Language (MatML) provides detailed materials property information necessary for the exchange of materials science digital resources among users. A prototype MatML editor has been developed to assist authors in applying MatML to resources.

Course Composer Tool
A course composing tool will be built to help educators develop dynamic teaching materials for structured presentations of thematic concepts from massive collections. Constraint Resource Planning (CRP) based algorithms have been developed to layout a course based on delivery time constraint and depth optimizing criterions. The algorithms can enforce various pedagogical styles and goals, such as the linear approach, as well as iterative reinforcement.

Prototype MatML Editor