CHiMaD
Center for Hierarchical Materials Design

CHiMaD MATERIALS DESIGN TRAINING

Materials Design

A **disruptive approach** to design and development of new and improved materials for engineering applications **providing a competitive advantage** by integration of theory, experiment, computational tools and materials data.

Scope

The *CHiMaD Materials Design Training* aims to introduce and further the attendees' knowledge of the ***Materials Design*** **philosophy and framework through hands-on training** and exposure to practical design examples.

Format

••• 3-day virtual training [~ 10-hour commitment for each attendee]

- Lectures by CHiMaD design instructors
- Mini-plenaries by CHiMaD principle investigators
- Active small group training guided by CHiMaD design instructors

Content

••• Introduction to **Material Design and Materials Genome Initiative**

- Historical context • Vocabulary • Infrastructure

••• Introduction to Design Tools I: **System Design Charts**

- ***Employ*** *effective communication for interdisciplinary design teams developing complex high-performance materials using a dynamic and visual approach*
- ***Identify*** *team strengths, weaknesses, and system-related bottlenecks*
- ***Develop*** *a dynamic design strategy by understanding the Processing – Structure – Property – Performance relationships within a material system*

••• Introduction to Design Tools II: **Engineering Flow Diagrams**

- ***Recognize and rank*** *parametric design targets and constraints*
- ***Construct*** *a decision-making map using team-specific strengths, expertise and available resources*
- ***Design*** *a process flow using System Design Charts*

••• Active Learning: **Small Group Training** *(up to 10 attendees per group)*

- ***Discuss*** *real materials systems of interest to the Client*
- ***Demonstrate*** *integration of attendees' knowledge and individual expertise into the systems to provide a design team experience*
- ***Support*** *attendees' critical assessment of materials systems by developing System Design Charts from scratch, and/or identifying sub-systems*

Who should attend

CHiMaD's hands-on approach to design training is applicable to **<u>all</u>** types of materials and levels of materials expertise:

••• **Experimental and computational researchers** involved in design and development of engineering materials (all training)

••• **Managers** who are interested to learn about Materials Design and why it offers a competitive advantage (introductory lecture and mini-plenaries)

About

Center for Hierarchical Materials Design (CHiMaD) *is a NIST-sponsored center of excellence for advanced materials research focusing on developing the next generation of computational tools, databases and experimental techniques in order to enable the accelerated design of novel materials and their integration to industry, one of the primary goals of the U.S. administration's Materials Genome Initiative (MGI). CHiMaD, founded in 2014, is a Chicago-based consortium of Northwestern University (NU), University of Chicago (UC), Argonne National Laboratory (ANL), and QuesTek Innovations, a small-business, along with ASM Materials Education Foundation, a professional society. Designing novel materials of specific properties for a particular application requires simultaneously utilizing physical theory, advanced computational methods and models, materials properties databases and complex calculations. This approach stands in contrast to the traditional trial-and-error method of materials discovery. CHiMaD aims to focus this approach on the creation of novel hierarchical materials which exploit distinct structural details at various scales, from the atomic on up, to obtain enhanced properties. The center's research focuses on both organic and inorganic advanced materials in fields as diverse as self-assembled biomaterials, smart materials for self-assembled circuit designs, high-performance composite materials and advanced metal alloys. More information on CHiMaD research: chimad.northwestern.edu/research*

CHiMaD Materials Design Training

Example Agenda for Virtual Format

Day 1

Training

(1 hr)**Introduction to Materials Design and/or Plenary**
(10 min) *Break*
(1 hr) **System Design Charts (SDC) and Case Studies**
(10 min) *Break*
(1 hr + as needed) **In-class exercises (Materials Summary -> SDC)**

Small group training – Group 1 */ up to 10 attendees*

(15 min) **Team presentation of System Summaries**
(15 min) **CHiMaD team presentation of System Design Charts**
(1 hr) **Discussion & Revision**
(30 min) **In-class assignment (Identifying Subsystems and Lines)**

Day 2

Training

(40 min) **Mini-Plenary**
(10 min) *Break*
(1 hr) **Introduction to Engineering Flow Diagrams (EFD)**
(10 min) *Break*
(1 hr) **In-class assignment and/or Office hours**

Small group training – Group 2 */ up to 10 attendees*

(15 min) **Team presentation of System Summaries**
(15 min) **CHiMaD team presentation of System Design Charts**
(1 hr) **Discussion & Revision**
(30 min) **In-class assignment (Identifying Subsystems and Lines)**

Day 3

Training

(40 min) **Mini-Plenary**
(20 min) *Break*

Small group training – Group 3 */ up to 10 attendees*

(15 min) **Team presentation of System Summaries**
(15 min) **CHiMaD team presentation of System Design Charts**
(1 hr) **Discussion & Revision**
(30 min) **In-class assignment (Identifying Subsystems and Lines)**

Small group training – Group 4 */ up to 10 attendees*

(15 min) **Team presentation of System Summaries**
(15 min) **CHiMaD team presentation of System Design Charts**
(1 hr) **Discussion & Revision**
(30 min) **In-class assignment (Identifying Subsystems and Lines)**

Example*: In-class assignment for Day 1 (Hard Materials / Alloys)

**other examples used during the training include but are not limited to materials systems used in CHiMaD's research on hard, soft and functional materials*

Task 1 Constructing a Materials Summary and identifying the terms related to Processing, Structure and Property of a Material System

Scope

To define a Material System allowing for a clear identification of its significant building blocks within the Processing – Structure – Property – Performance design framework

Worked Example

Material Summary for Aluminum Alloy System*

**colored terms identified as being related to Processing, Structure or Properties of the Material System*

An aluminum alloy is prepared by ingot metallurgy. The process begins with ingot refining then deoxidation and then ingot solidification. During ingot refining, deoxidation, and solidification, Fe and other impurities form coarse inclusion or "constituent" phases such as Al_3Fe. In a final stage of solidification, finer scale "dispersoid" particles such as Al6Mn precipitate. These continue to form during hot working of the ingot. During subsequent solution treatment the dispersoids remain out of solution and pin grain boundaries. The alloy is quenched from the solution treatment and then aged to precipitate Cu G-P zones. The solution treatment, quenching, and aging processing stages effect the final matrix composition. Important properties governing alloy performance in service are the elastic modulus, yield strength, and fracture toughness. The modulus is determined by the final matrix composition, while the strength is determined by the G-P zone precipitation and grain size. Ductile fracture is controlled by primary void formation on the constituent particles as well as finer scale microvoid formation on the dispersoids.

Task 2 Developing a System Design Chart visually describing the Materials System and the relations between its Processing, Structure, Properties

Scope

To visualize the Materials System and clearly identify quantifiable and/or known relations/links between its Processing, Structure, Properties and Performance.

Worked Example

System Design Chart of Aluminum Alloy System