materials design

WEBINAR

Materials Constitution Data in MSI Eureka – Fundamentals for Efficient R&D

Dr. Svitlana Iljenko and Dr. René Windiks
MSI GMbH and Materials Design

Materials Design Webinar Series

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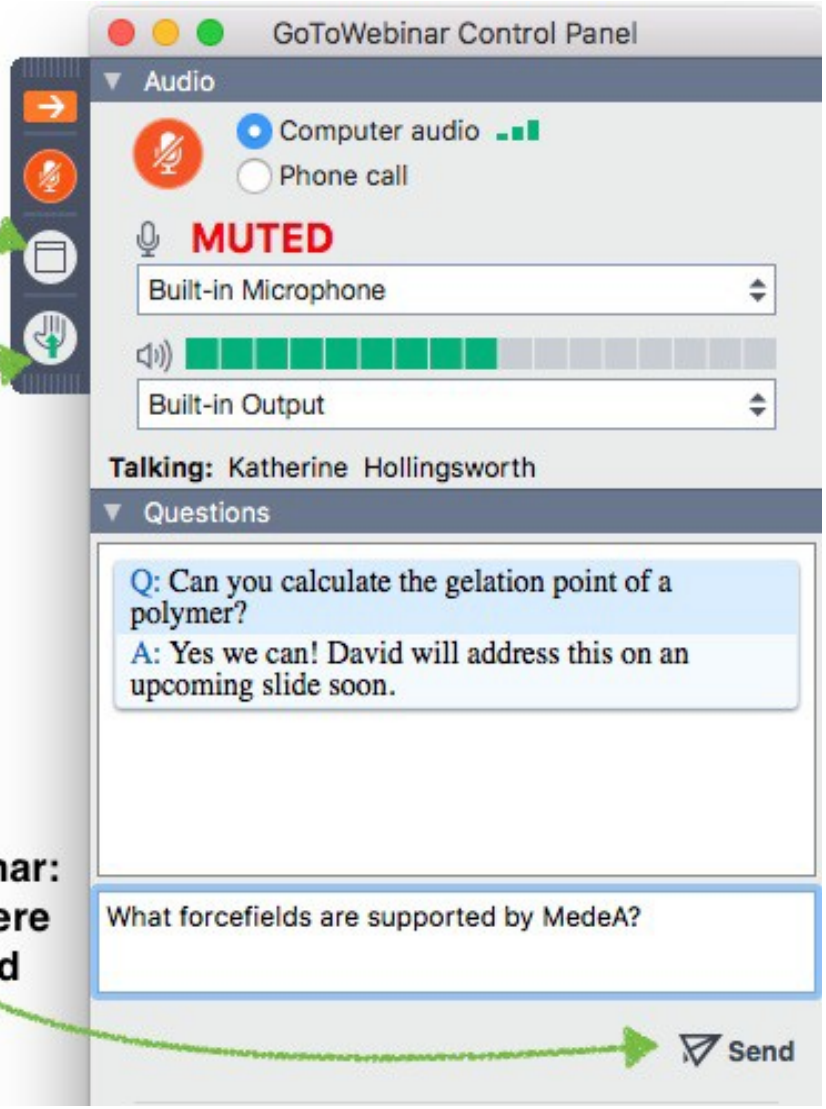
Please Ask Questions

full screen

during discussion:

Use the raise hand icon to bring attention to your question

any time during webinar: type your question here and then press Send



Webinar Speakers

Dr. René Windiks

Materials Design

Dr. Svitlana Iljenko

MSI Gmbh

Katherine Hollingsworth

Materials Design

An information platform for inorganic materials

- covers **Materials' Constitution**, completely
- monitors all publications and evaluates published data.
- integrates data: reducing data-flood and confusion.
- KEY subjects: phase diagrams, crystal structure, morphology, thermodynamics, properties

- Is designed to *understand* materials.

The global team, MSIT

Materials Science International Team is the world-wide group of scientists behind MSI Eureka. MSIT compiles and evaluates data, generates missing data, creates new knowledge, for over 35 years

The company, MSI

Materials Science International Services GmbH hosts the global team, markets MSI Eureka, participates in research projects, offers consulting services

The publisher:

1984 a global scientific team, MSIT, started from the Stuttgart Max-Planck-Institute for Metals Research.

Since 1990 MSI, GmbH gives office and guidance to MSIT.

Today MSI & MSIT form the largest network in materials constitution.

The team: MSIT

MSIT makes MSI EUREKA

~280 materials scientists collaborating remotely for over 35 years

- monitor all relevant publications
- evaluate materials systems
- create reliable knowledge
- execute joint research
- provide first-class tuition in Materials Chemistry – MSIT Winter School series.

Member Affiliations

GB Leeds; Sheffield; Manchester; Birmingham; Surrey
DE Stuttgart; Clausthal; Aachen; Jülich; Freiberg, Karlsruhe
NL Eindhoven
FR Lille; Montpellier; Rennes; Paris; Grenoble; Marseille
BE Leuven
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UA Kiev (Acad. Sci.); L'viv (Univ.); Chernivtsi; Kramatorsk
RU Moscow (Acad. Sci.); State Univ.; MISIS
CN Changsha / Hunan; Central South Univ.; Bejing STU
JP Tokyo (IT); Kyoto, Sendai
Malaysia Sains Univ. Tronoh
USA Cincinnati; Raleigh; Gainsville; Evanston; Gaithersburg
BR Campinas; Lorena; Sao Paulo, IPT; PUC Rio
South Africa Witwatersrand
India Chennai, Bhabha Atom. Center (Mumbai)
TR Istanbul

You know MSI & MSIT already

Authored by MSI & MSIT

None of them is updated

- "Ternary Alloys" book series of **20** volumes

  critical evaluation of materials systems; phase diagrams of ternary Al, Ag, As, Li, Mg systems; jointly with Wiley-VCH, later by MSI

- Landolt-Börnstein **17** volumes sub-series "Ternary Alloys Phase Diagrams"

  critical evaluation of selected materials systems; by MSI & MSIT, jointly published with Springer Verlag

- "Red Book" book series of **18** volumes

  extracts of constitutional data from the world publications, (now electronic only); jointly with VINITI, Russia

- "Metal-Boron-Carbide"

  author Peter Rogl, edited by MSI; jointly with ASM

- "Pressure Dependent Binary Phase Diagrams"

  author Yuri Lewinski, edited by MSI; jointly with ASM

With the coming of the digital information age, publication is continued electronically in "MSI Eureka"

MSI EUREKA

Objects

Inorganic Materials

- Alloys (metals, steels, bronzes, magnets, implants, electronic materials,…& more)
- Non-metals (ceramics, sensors, semiconductors,… & more)
- Composites (cermets, ceramic matrix composites, metal matrix composites & more)

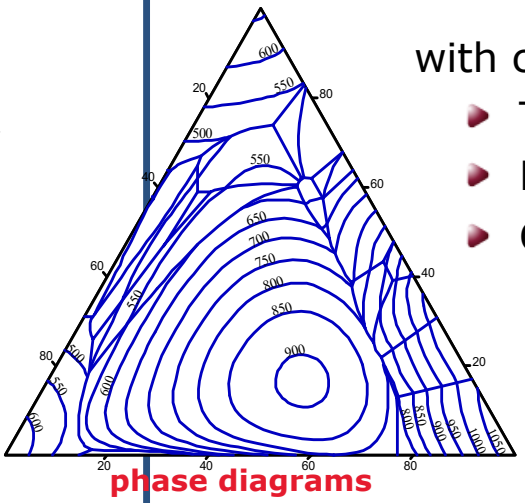
Subject

Materials Constitution

- phase configurations &
- phase transformations,

with changing

- Temperature
- Pressure
- Composition

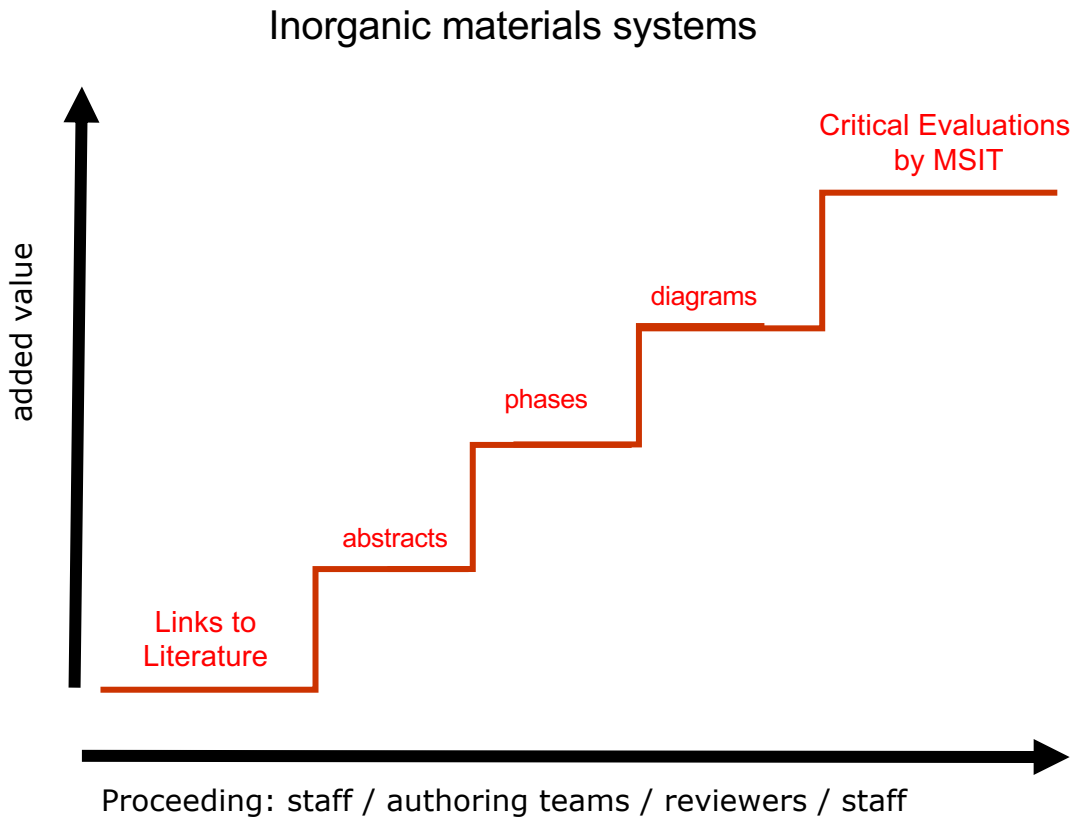


phase diagrams

road maps for materials R&D

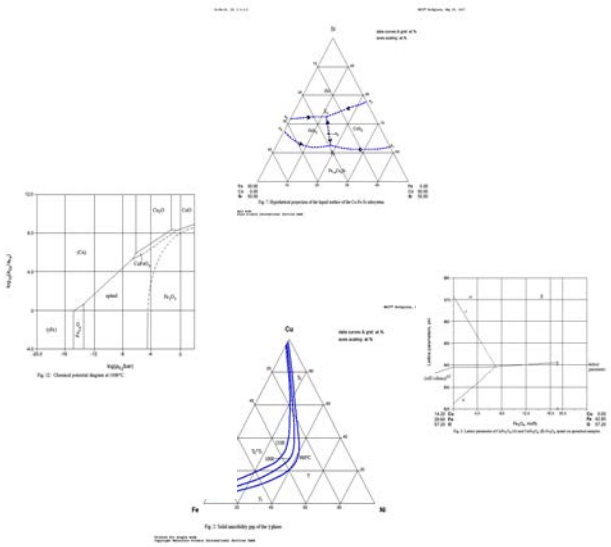
MSI EUREKA adding value

- monitoring all literature (MSI)
- supplementing data (MSI/MSIT)
- evaluating many literature (MSIT)

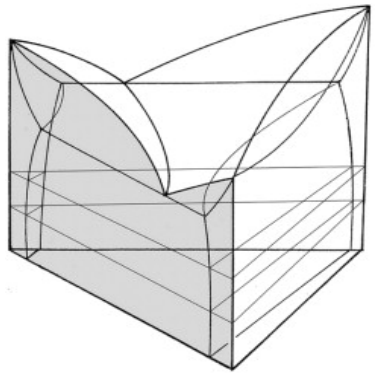


Critical Evaluation: Why to Evaluate?

- Published data are often conflicting
  - between different publications
  - within one publication
  - Different types of experiments (static/dynamic)
  - Different accuracy & precision
  - Different quality of starting materials
  - Poor experimental practice
  - Incorrect interpretation of data
  - Published data are often incomplete
  - Phase diagrams are not measured but concluded from experimental data –> to be evaluated



Data & conclusions are to be evaluated



to describe the entire system, consistently

So, which is the correct diagram?

- Users need a single diagram (or set) that they can trust
- These diagrams should come from a trustworthy source

Critical Evaluation Means

- **Find** conflicts
- **Point out** conflicts
- **Settle** conflicts (where possible)
- Give **arguments** for rejecting, accepting or amending data

Reliability of Data

- purity of initial materials
- sample preparation (suitability for particular material)
- conditions of heat treatment (suitability for particular material)
- experimental methods (suitability for particular material)
- compatibility with results/estimates from thermodynamics

Calphad modelling

Might be useful to help resolve data conflicts, but it is not required. Evaluation is not concerned with modelling. It is concerned with the best set of observations.

Correctness, coherence and interpretation of data

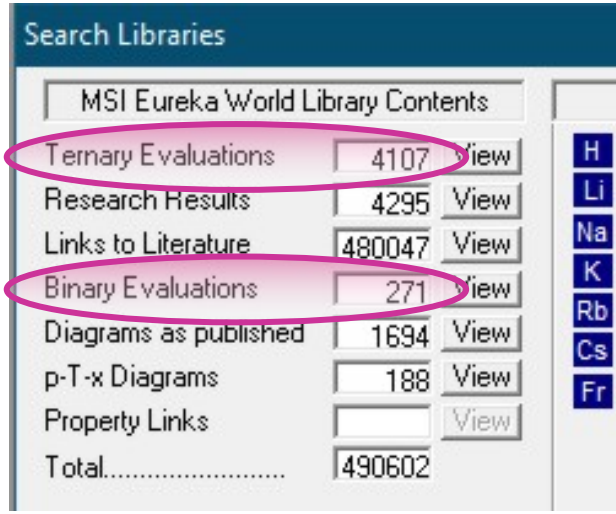
- correctness with respect to the rules of heterogeneous equilibria
- compatibility of binary and ternary data
- compatibility of intersecting e.g. isothermal *vs* vertical sections
- compatibility of consecutive sections/surfaces, e.g. isothermal sections at different temperatures

- interpretation of measured experimental values *vs* the author's conclusions
- depth of experimental details in the publication

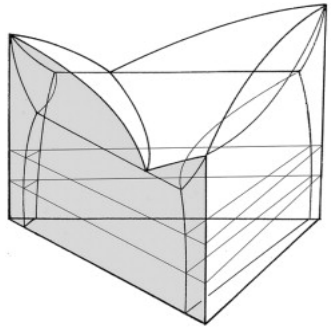
Output

Evaluation Report (system report)

- Considers all publications
- Describes the system as a whole
- Describes the steps/decisions taken in the evaluation process
- Presents best set of self-consistent information about the system (diagrams, tables & text)
- Generate consistent diagrams from many scattered data
- **All articles are peer reviewed**



Data & conclusions are to be evaluated



to describe the entire system, consistently

Category: Reference Diagrams

- Diagrams from the original publications
- Redrawn as published
- supplemented with crystallographic data of solid phases
- NOT evaluated

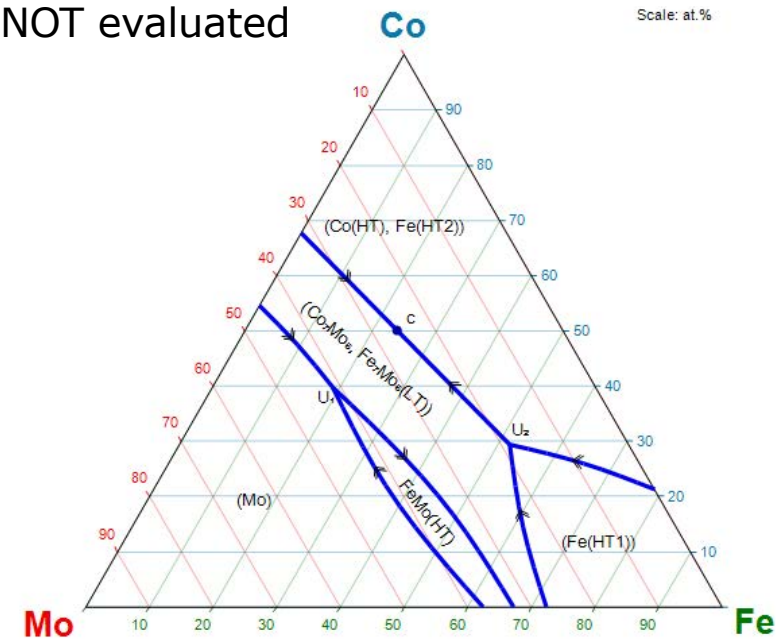


Fig. 1: Liquidus projection; after [1988Koe]

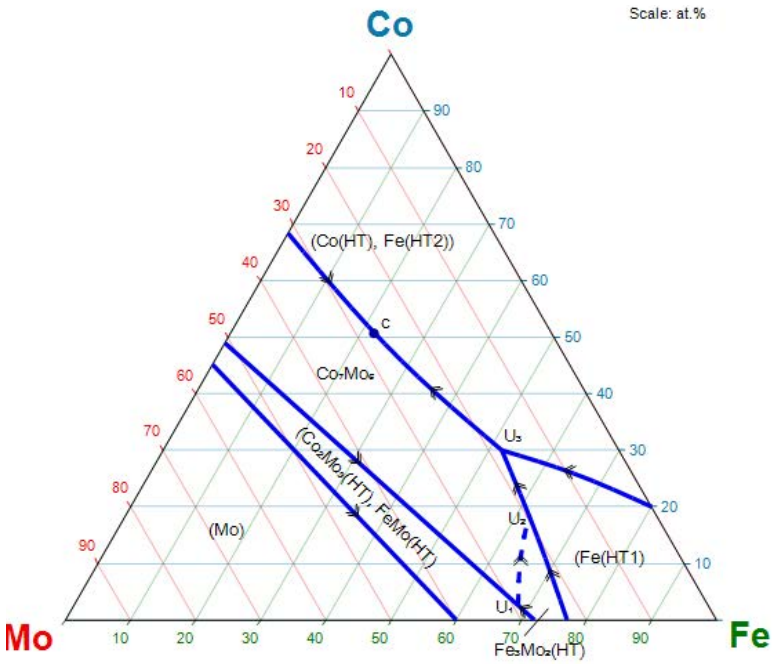


Fig. 2: Liquidus projection; after [1988Ray]

MSI EUREKA who does it serve

- Scientists & Engineers (academic & corporate; R&D professionals, educators & students)
- Information Managers (librarians; information professionals)
- Science Managers (program officers; project managers)

Faculties and Disciplines:

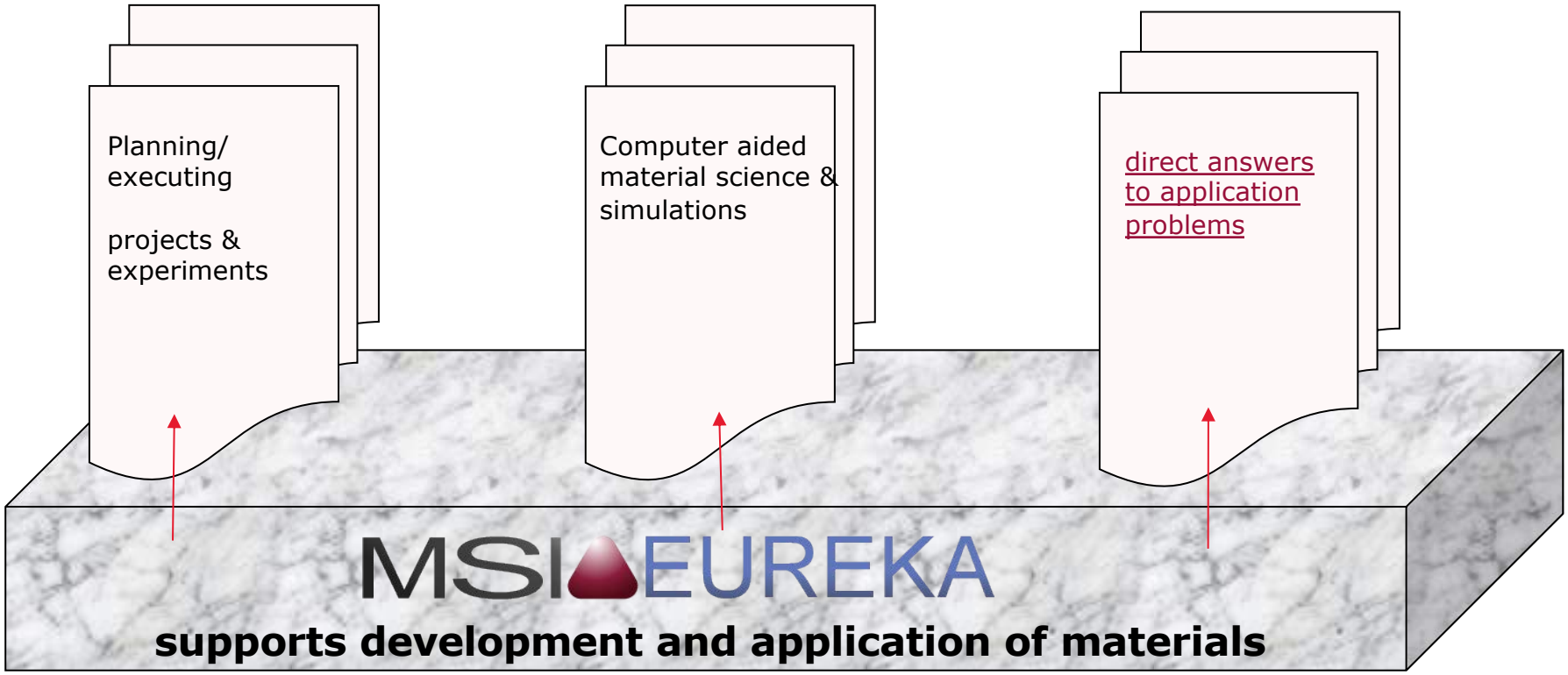
- Physics
- Chemistry
- Engineering
- Materials Science
- Metallurgy
- Crystallography
- Thermodynamics
- Crystal Growth
- Materials Design
- Mineralogy
- Magnetism
- Alloy Development, etc.

Multiple interdisciplinary industries:

automotive, aerospace, space, nuclear, heavy industry, manufacturing, energy technology, renewable energies, environmental technology, micro and nanotechnology, electronics, microsystems technology, medical materials, sensors, biomaterials, surface engineering, machine construction, magnets, etc.

Objects: **Inorganic engineering materials**
Alloys
Non-metals
Composites

MSI Eureka,
what does it serve



Answers from MSI Eureka: Brazing/Solidification

CASE 1: Electronic devices; Ag15-80Cu-5P alloy as self-fluxing braze in an automated brazing process.

QUESTION (**1**)
Does this alloy offer *melting temperatures* that our devices can stand, i.e. lower then 800°C?

ANSWER (**1**):
FROM Ag-Cu-P, Fig. 2:

Yes, *melting temperature* of this alloy is about 770°C

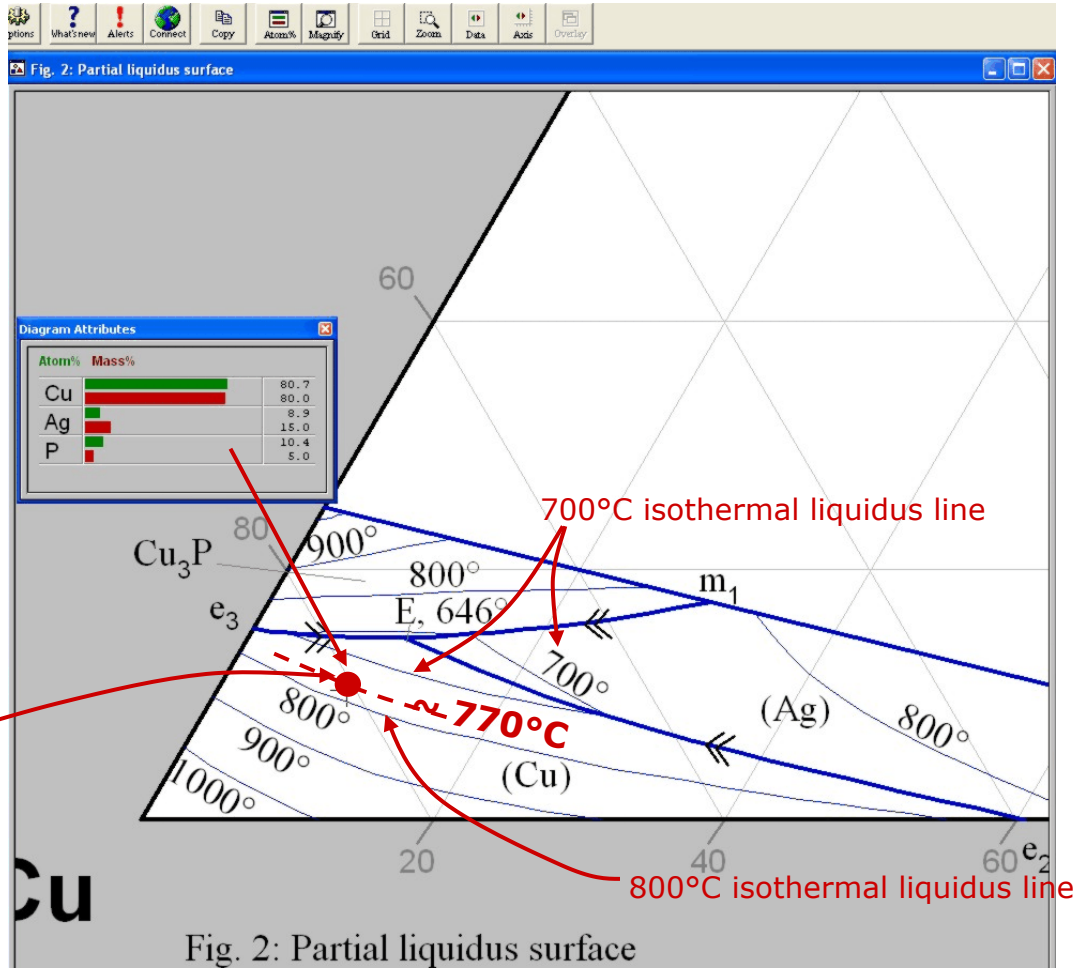


Fig. 2: Partial liquidus surface

Answers from MSI Eureka: Brazing/Solidification

CASE 1: 1st answer was favourable, case continued:

QUESTION (**2**)
How critical will the temperature control be during the continuous joining process, i.e. how large is the *melting range* that this alloy offers?

ANSWER (**2**):
from System Report Ag-Cu-P, Fig. 2 and chapter Invariant Equilibria:
Melting range of the Ag15-80Cu-5P alloy is ~770 to 646°C

Conclusion: temperature control is not that critical

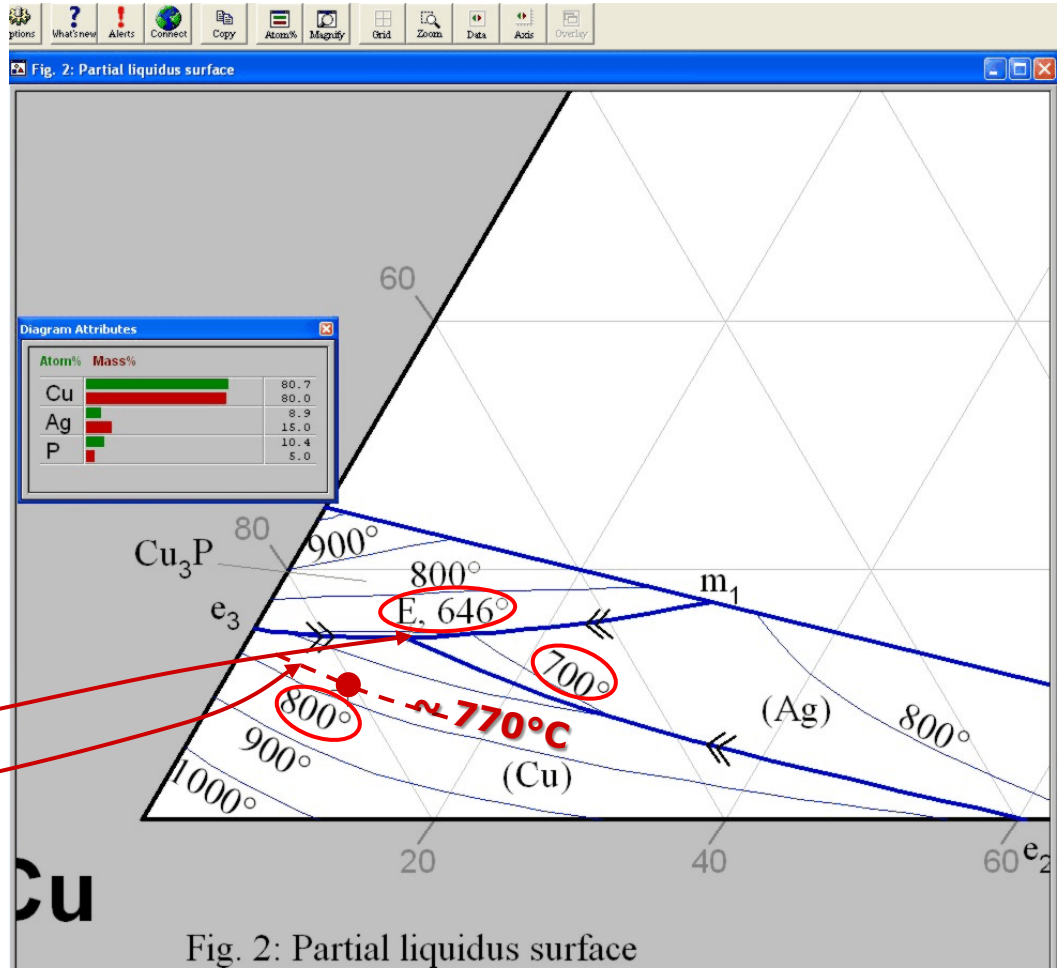
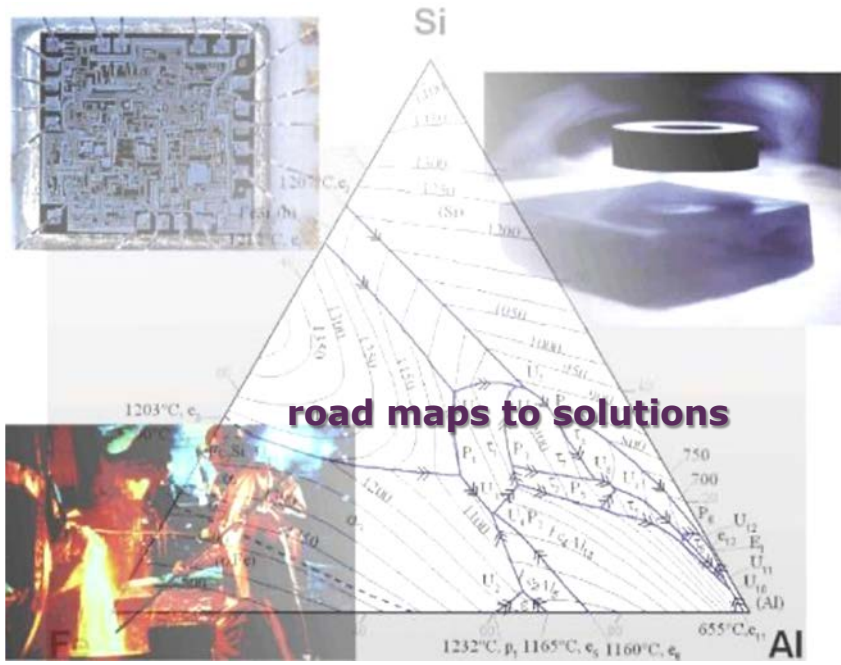


Fig. 2: Partial liquidus surface

Benefits for Engineers

Developing / applying new materials & processes



Problem

- fundamental information is missing
- leads to unnecessary experiments
- "mission impossible" may come too late

Solution with MSI Eureka

- you get additional expert brains into the company
- you minimize number of experiments
- you save resources and reach the targets faster

5th MSIT Winter School

2 – 6 May 2021
ONLINE

The aim of the MSIT Winter School series is to provide first-class tuition in a selection of subjects closely associated with the study of phase equilibria in Materials Science. The course, which is spread over three full days, comprises 5-6 'modules' on topics such as Phase Equilibria, Crystallography and Computational Thermodynamics.
Each module involves lectures, demonstrations and practical exercises, written and given by members of the MSIT who are world experts in their respective fields.

REGISTRATION OPENED

The Programme includes:

Principles of Chemical Thermodynamics
Phase Diagrams and Phase Equilibria (basic and advanced level) with „hands-on session"
Experimental Determination of Phase Diagrams
Crystallography with „hands-on session"
Experimental Methods in Thermodynamics with „hands-on session"
Application of Density Functional Theory in the Context of Phase Diagram Modelling
Computational Materials Thermodynamics
Calphad Method (with hands-on session)

MORE...

Organised by

Dr. Svitlana Iljenko / **MSI**, Materials Science International GmbH, Germany

Prof. Andrew Watson / **Coventry University**, United Kingdom

Dr. Frank Stein, Dr. Martin Palm / **Max-Planck-Institut für Eisenforschung** GmbH, Germany

In the framework of the 35th MSIT Annual International Seminar on Heterogeneous Multicomponent Equilibria.

MSI EUREKA - phase diagrams in MedeA

Evaluation Reports:

- 4 380 evaluations of ternary & binary systems with
- 10 560 diagrams, citing app.
- 66 000 literature references.

Reference Diagrams:

- 1 694 documents with
- 2 011 diagrams (binary & ternary)

MSI EUREKA

made by scientists for scientists

www.msiport.com

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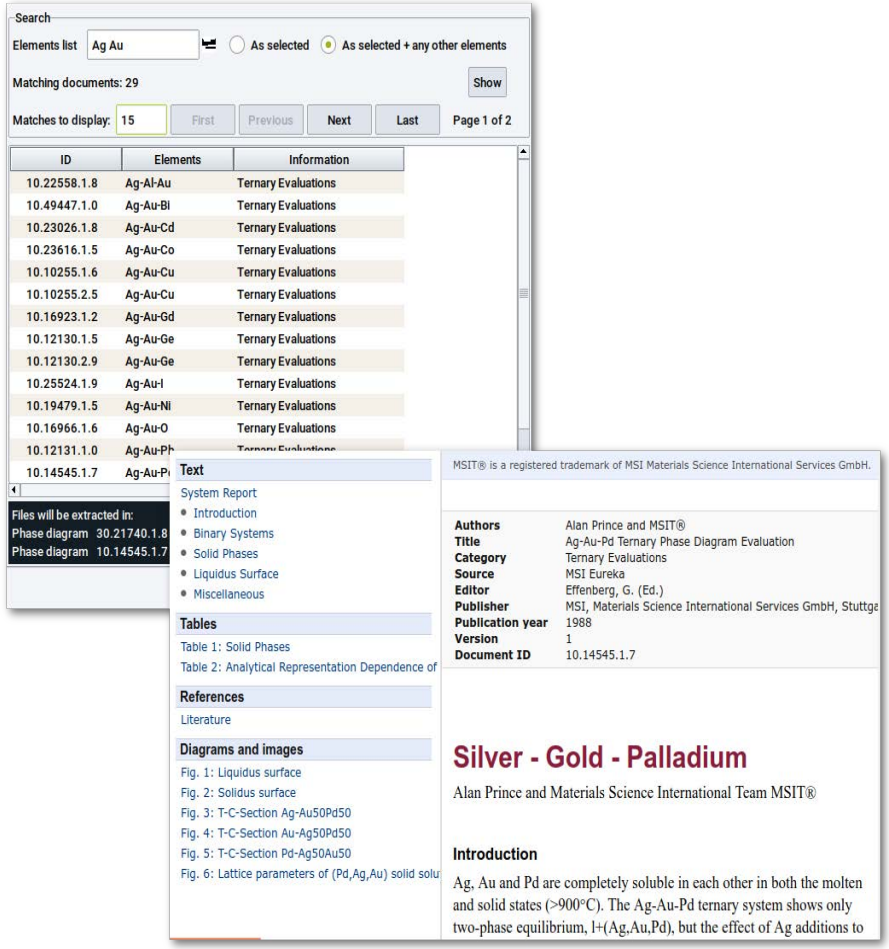
iljenko@msiport.com

MedeA MSI Phase Diagrams

Comprehensive Materials World Literature Search in *MedeA*

- MSI Phase Diagrams greatly enhances *MedeA*'s modeling capabilities for your materials discovery, design, and optimization projects

- Key benefits
  - Build your modeling strategy on expertly validated thermodynamic data
  - Swift access to factsheets and critical evaluation reports
  - Seamless integration with *MedeA*
- Key features
  - Full integration with *MedeA* provides on-disk, database search
  - Quick, efficient factsheet retrieval using an intuitive, menu-based query language
  - Complements *MedeA* builders, compute engines, and analysis tools



Comprehensive Materials World Literature Search in *MedeA*

- MSI Phase Diagrams greatly enhances *MedeA*'s modeling capabilities for your materials discovery, design, and optimization projects

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  - Build your modeling strategy on expertly validated thermodynamic data
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- Key features
  - Full integration with *MedeA* provides on-disk, database search
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  - Complements *MedeA* builders, compute engines, and analysis tools

- Required *MedeA* module
  - *MedeA* Environment with *InfoMaticA*
  - *MedeA MSI Phase Diagrams*
- Complementary *MedeA* structure databases
  - COD
  - Pearson's
  - ICSD
  - NCD
- Recommended *MedeA* modules
  - Vienna Ab-Initio Simulation Package (*VASP*)
  - *High-Throughput (HT) Launchpad*

Online Training and Demo

Advanced Atomic Model Building Based on Comprehensive Databases

Next Thursday, March 11, 2021
USA/EUROPE:
10:00 am PST/1:00 pm EST
7:00 pm CET

Register for the training:
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*Training open to everyone

Upcoming Webinar

Development of New Solvents for CO_2 Capture Using Molecular Simulations

March 23, 2021
8:00 a.m. PDT / 11:00 a.m. EDT / 15:00 GMT / 16:00 CET

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TOTAL

Dr. Erich Wimmer
Chief Scientific Officer,
Materials Design, Inc.

Dr. Frédérick de Meyer
R&D Leader for CO2 Capture,
Total S.E.

Question and Answer Session

Dr. René Windiks

Materials Design

Dr. Svitlana Iljenko

MSI Gmbh

MedeA Environment

- MedeA modules mentioned in today's webinar

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  https://www.materialsdesign.com/analysis-tools

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  MedeA MSI Phase Diagrams
  MedeA HT Launchpad
  MedeA COD
  MedeA ICSD
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  MedeA VASP
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  Katherine Hollingsworth
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Questions about the webinar

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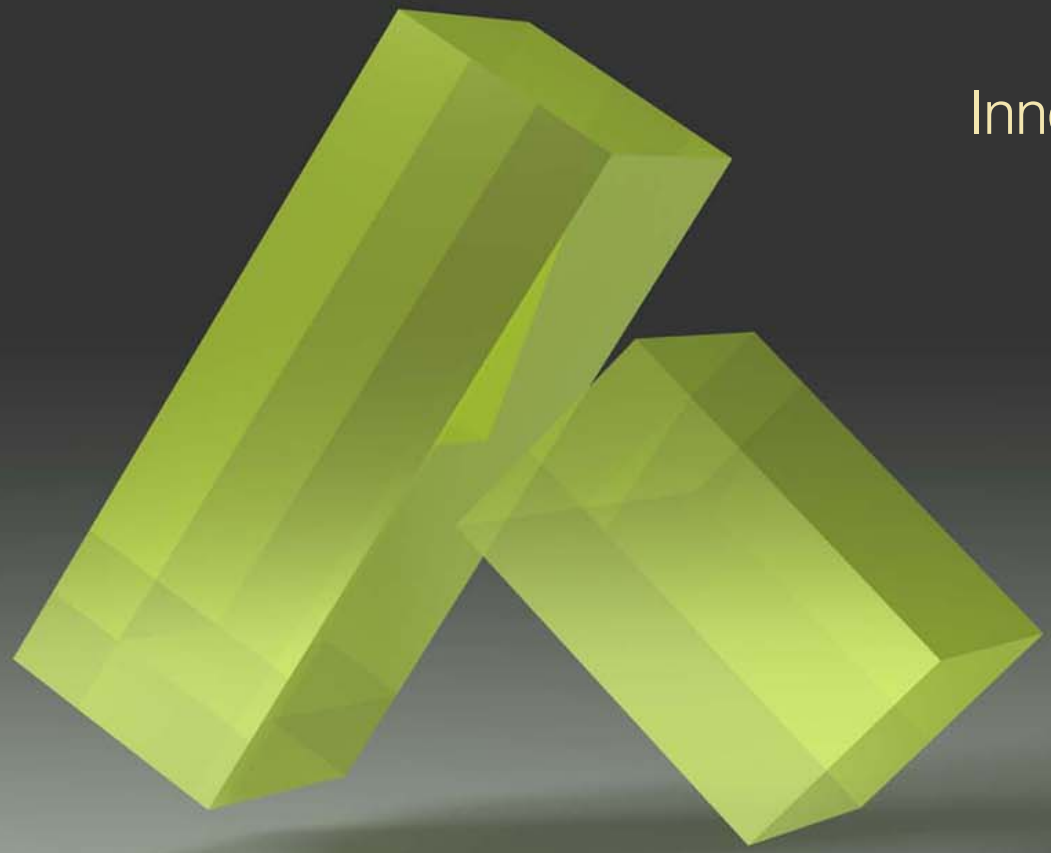

MedeA

Innovation by Simulation