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

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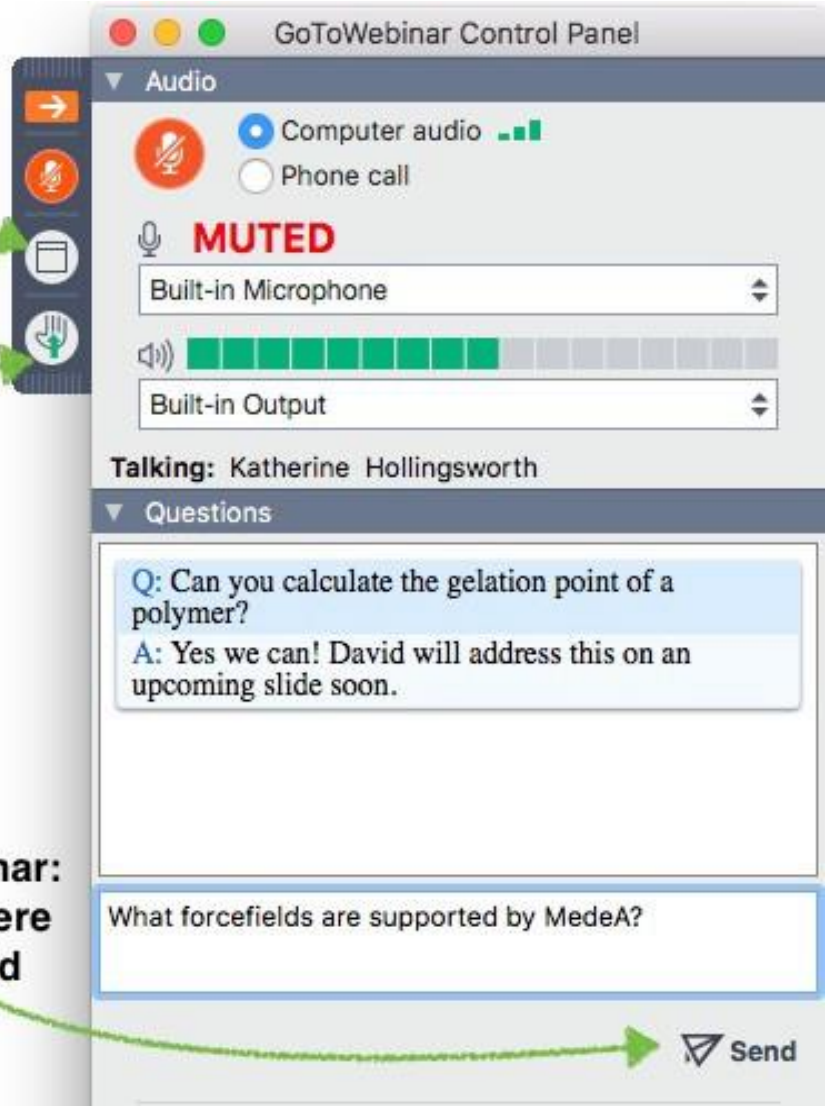


Webinar Speakers

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 MATERIALS SCIENCE INTERNATIONAL TEAM

MSIT makes MSI EUREKA

~280 materials scientists collaborating remotely for over 35 years

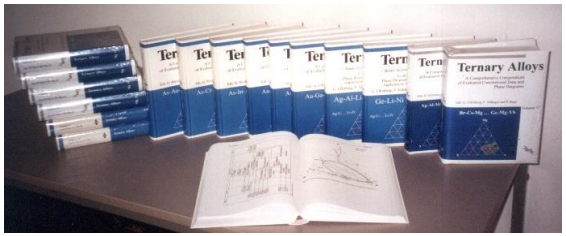
- monitor all relevant publications
- evaluate materials systems
- create reliable knowledge
- execute joint research
- provide first-class tuition in Materials Chemistry – MSIT Winter School series.

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
AT Vienna
IT Genova
GR Volos
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)

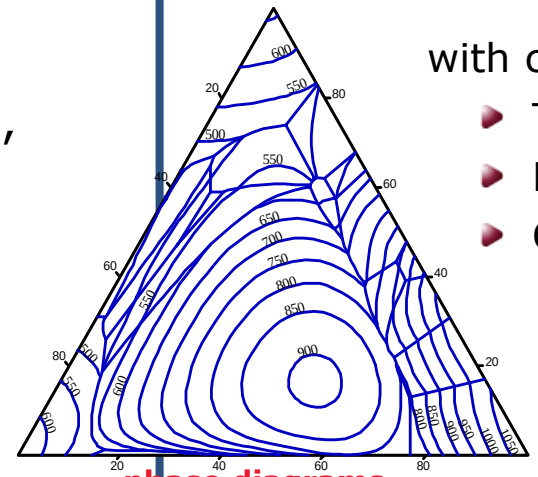
Subject

Materials Constitution

- phase configurations &
- phase transformations,

with changing

- Temperature
- Pressure
- Composition

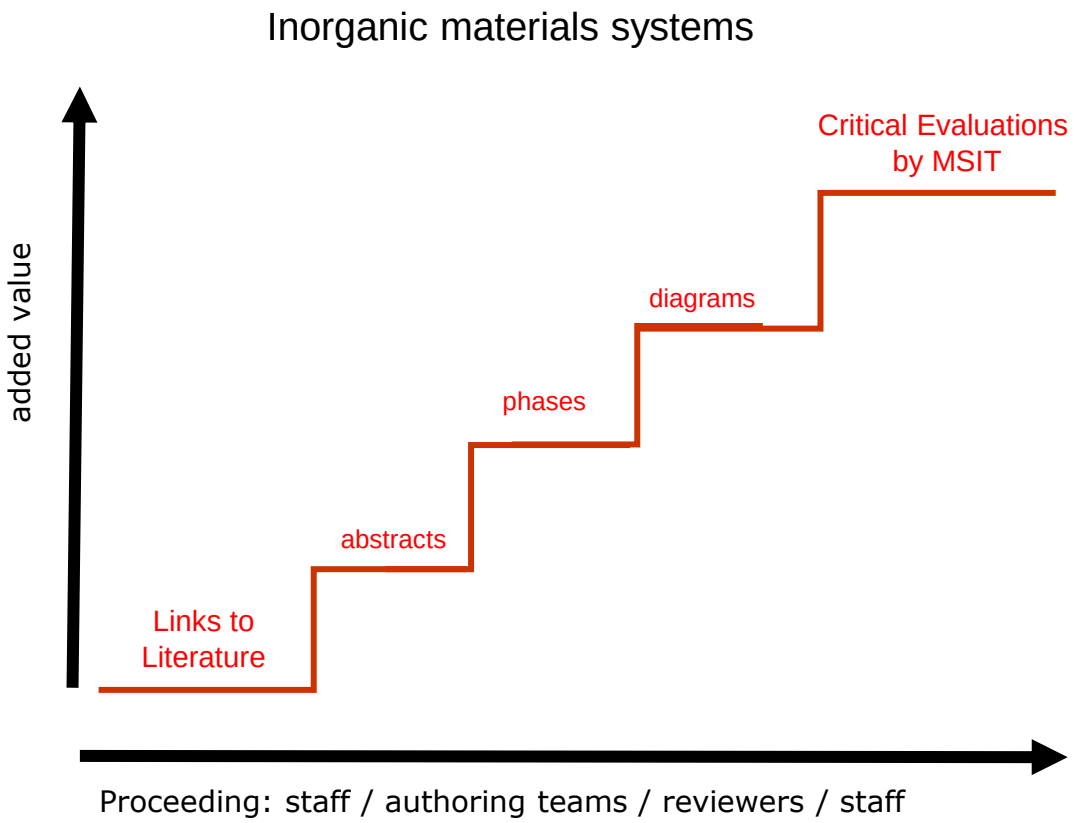


phase diagrams

road maps for materials R&D

MSI EUREKA adding value

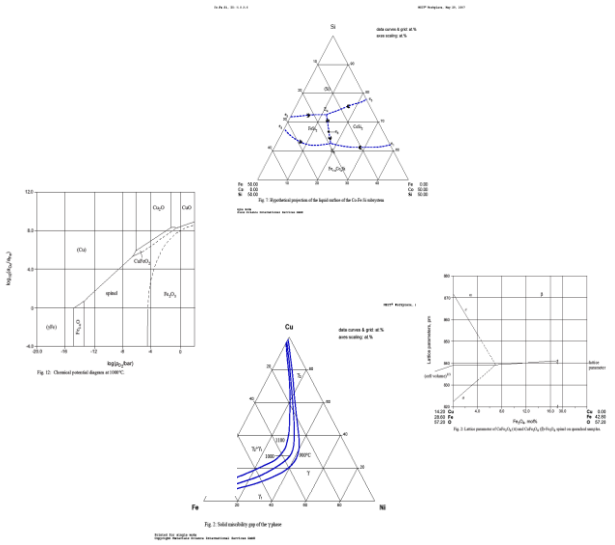
- monitoring all literature (MSI)
- supplementing data (MSI/MSIT)
- evaluating many literature (MSIT)



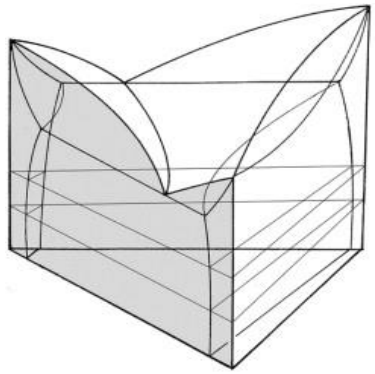
Critical Evaluation: Why to Evaluate?

- 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

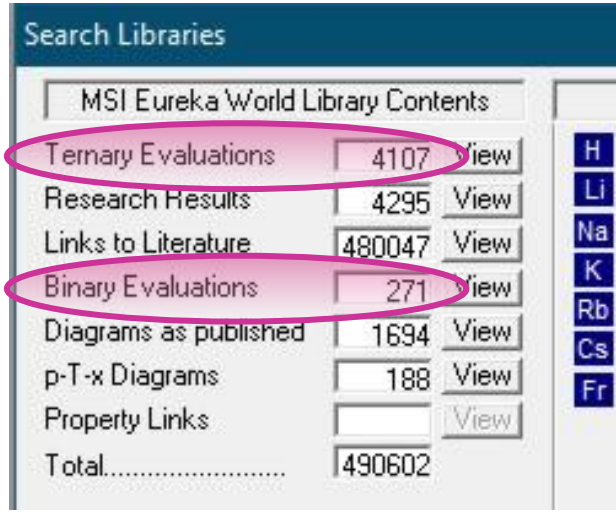
- correctness with respect to the rules of heterogeneous equilibria
- compatibility of binary and ternary data
- compatibility of intersecting e.g. isothermal *vs* vertical sections
- compatibility of consecutive sections/surfaces, e.g. isothermal sections at different temperatures

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

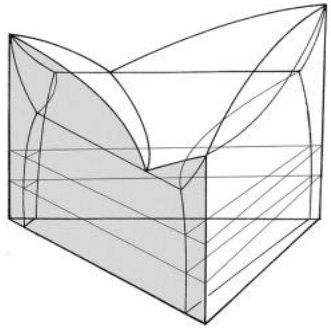
Output

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: Diagrams as Published

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

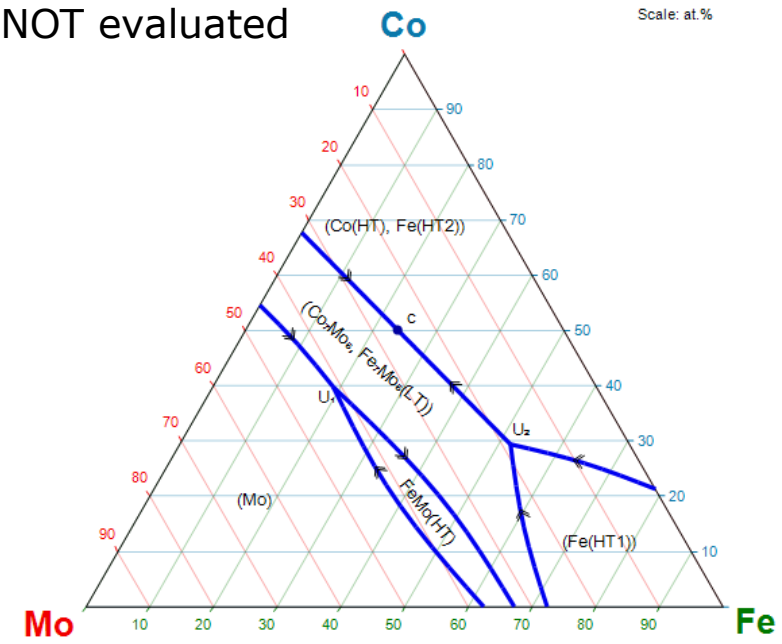


Fig. 1: Liquidus projection; after [1988Koe]

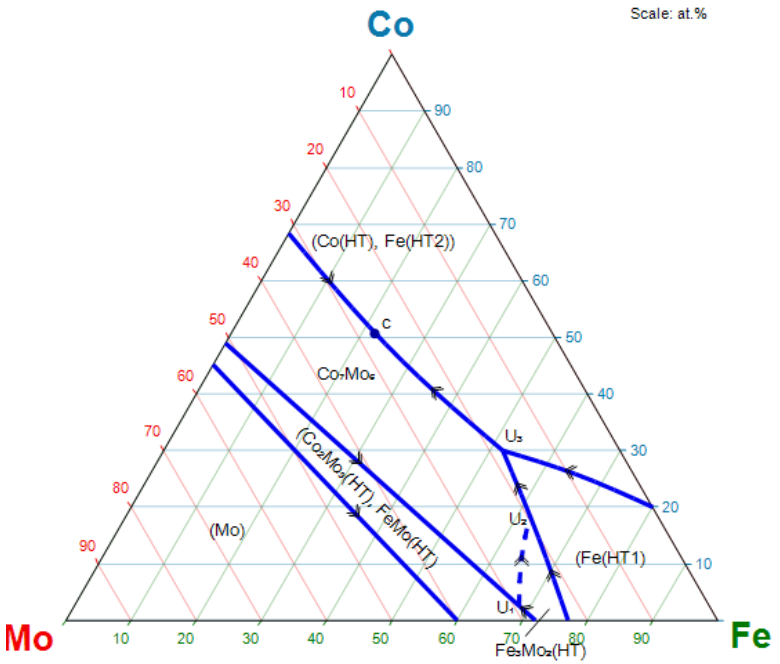


Fig. 2: Liquidus projection; after [1988Ray]

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:

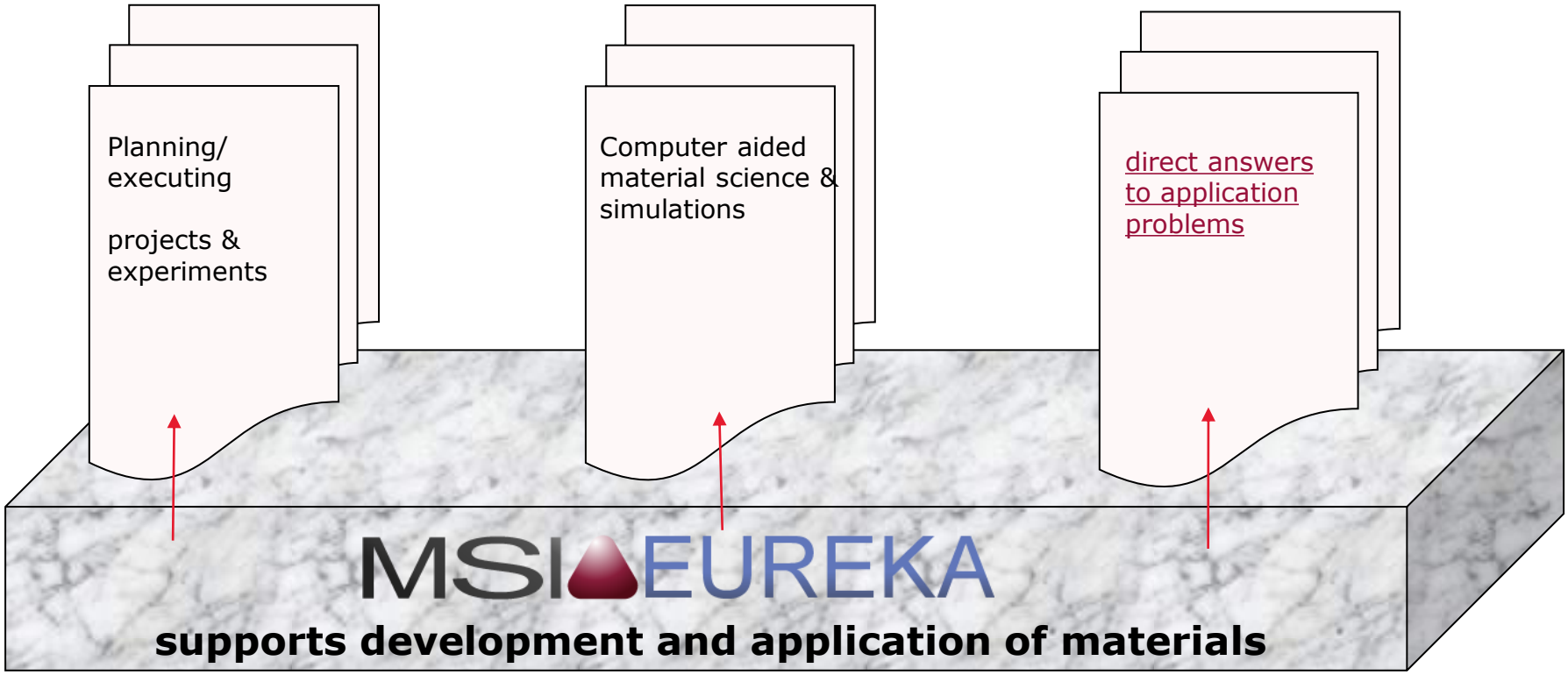
- Physics
- Chemistry
- Engineering
- Materials Science
- Metallurgy
- Crystallography
- Thermodynamics
- Crystal Growth
- Materials Design
- Mineralogy
- Magnetism
- Alloy Development, etc.

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

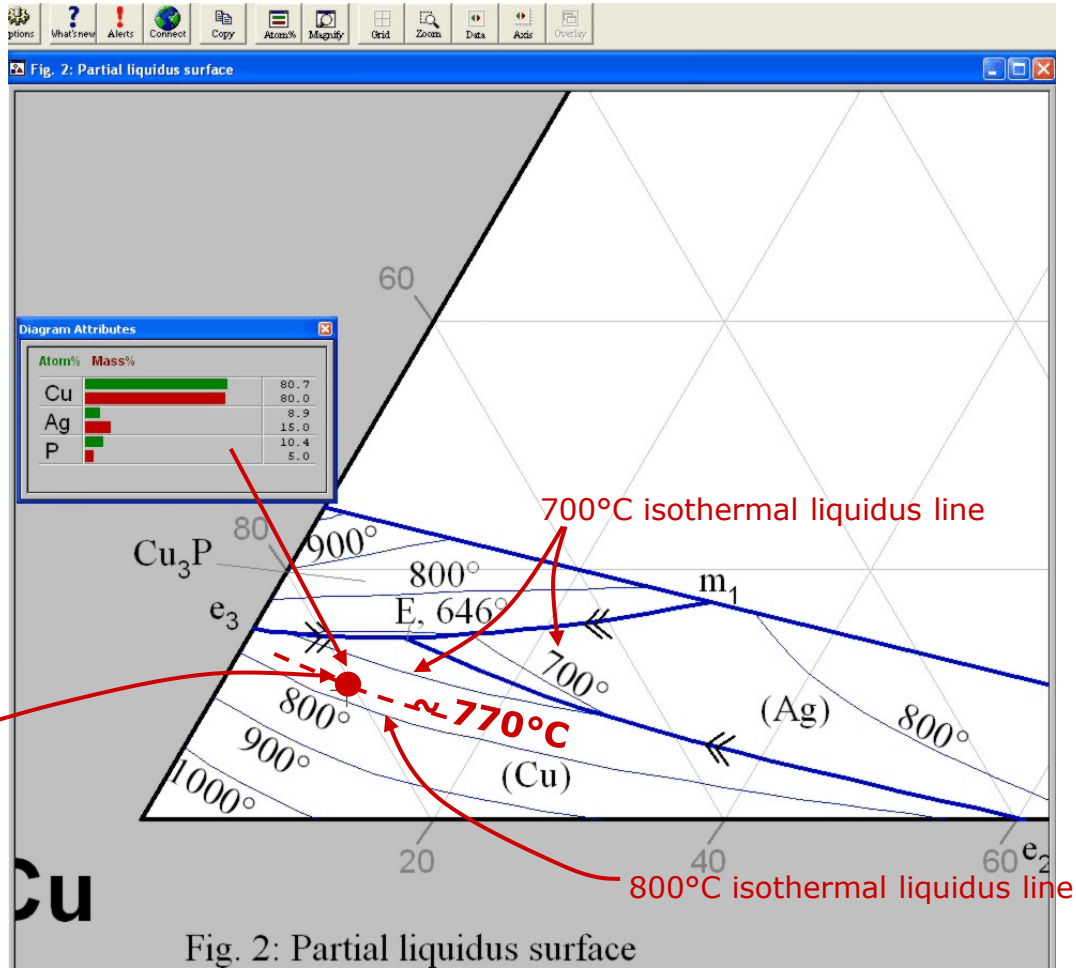


Fig. 2: Partial liquidus surface

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

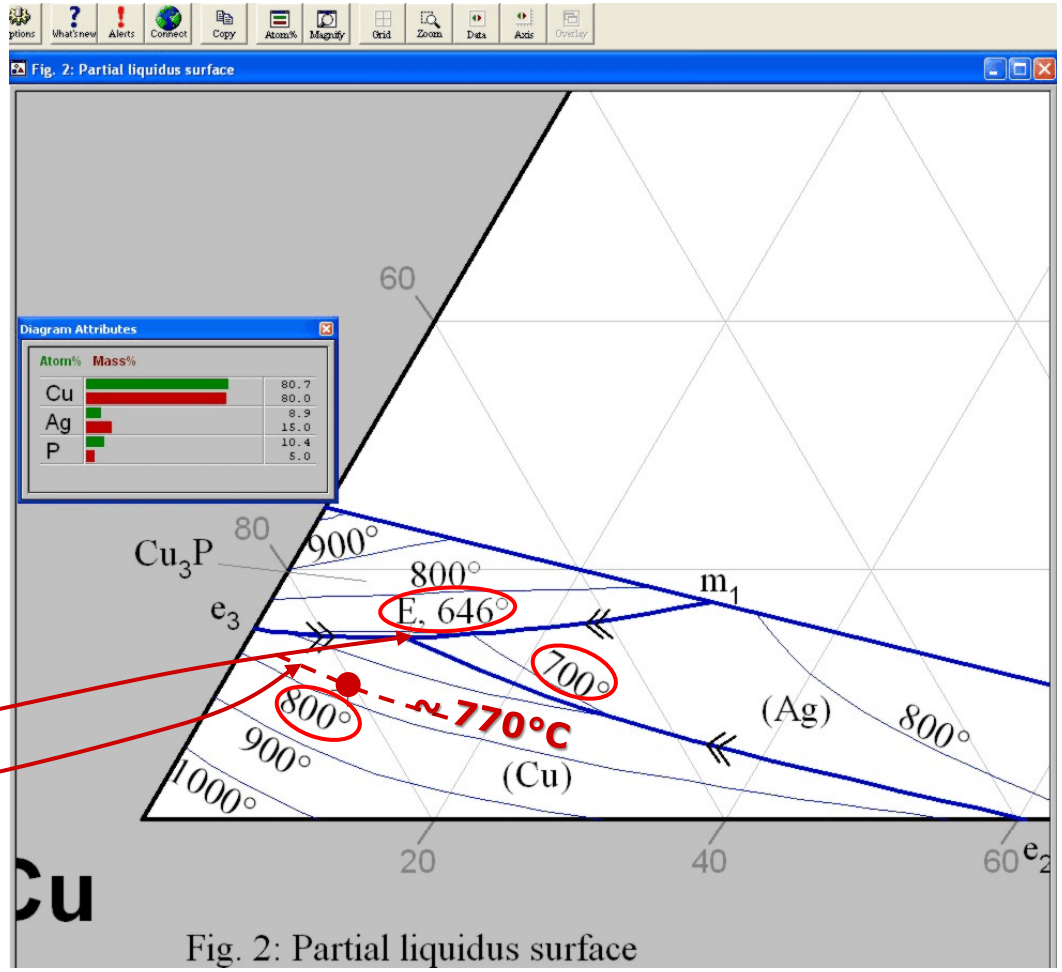
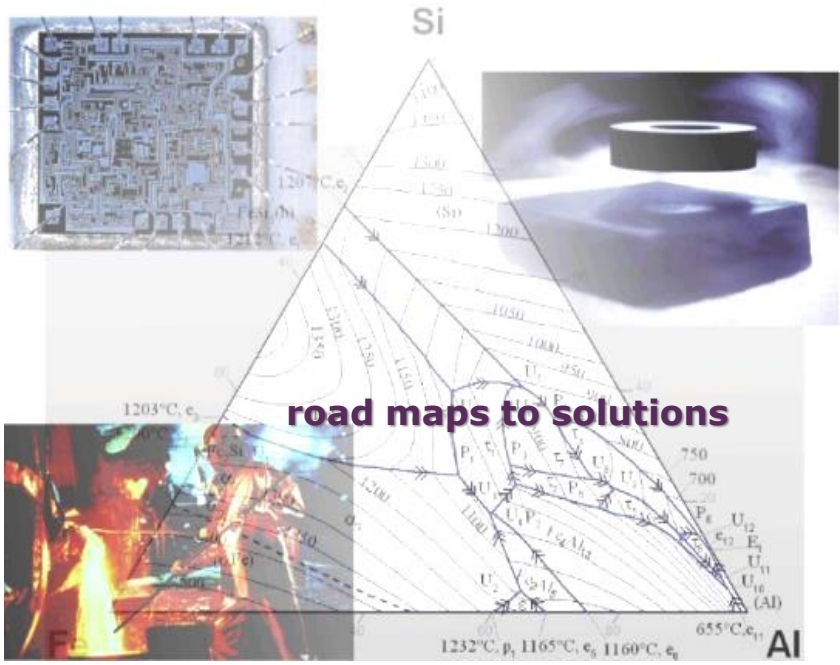


Fig. 2: Partial liquidus surface

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

6th MSIT Winter School on Materials Chemistry

3 – 7 April 2022

Castle Ebernburg, Germany

First-class tuition in a selection of subjects closely associated with the study of phase equilibria in Materials Science.

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 DFT in the Context of Phase Diagram Modelling
- **Computational Materials Thermodynamics**
- **Calphad Method (with hands-on session)**

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 ENDS in January 2022

Organised by

MSI, Materials Science International GmbH, Germany / Svitlana Iljenko

Hampton Thermodynamics, UK / Andy Watson

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

In the framework of the 36th MSIT Annual International Seminar on Heterogeneous Multicomponent Equilibria.

1st MSIT Advanced School

Diffusion in Materials – Fundamentals and Applications

The Programme includes:

- Diffusion theory;
- Diffusion couples: theory & practice;
- Simulations using DICTRA (hands-on training);
- Diffusion couples evaluation by EPMA and advanced methods;
- Diffusion couples in industrial practice;
- Examples from audience (ask experts for help).

REGISTRATION STARTS in January 2022

25 – 26 October 2022

Castle Ebernburg

Germany

Organised by:

MSI, Materials Science International GmbH, Stuttgart, Germany

Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

In association with:

Thermo-Calc Software AB, Sweden

MSI EUREKA - phase diagrams in MedeA

Evaluation Reports:

- 4 400 evaluations of ternary & binary systems with
- 10 780 diagrams, citing app.
- 67 110 literature references.

Diagrams as Published:

- 1 700 documents with
- 2 030 diagrams (binary & ternary)

number of documents as of October 2021

MSI EUREKA

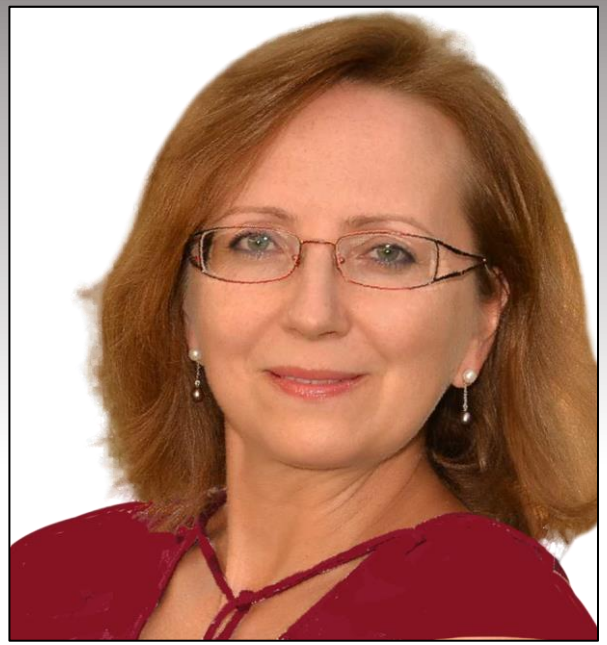
made by scientists for scientists

www.msiport.com

www.msi-eureka.com

iljenko@msiport.com

Question and Answer Session



Dr. René Windiks

Materials Design

Dr. Svitlana Iljenko

MSI Gmbh

MedeA Environment

- MedeA modules mentioned in today's webinar

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

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  MedeA MSI
  MedeA HT Launchpad
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Questions about the webinar

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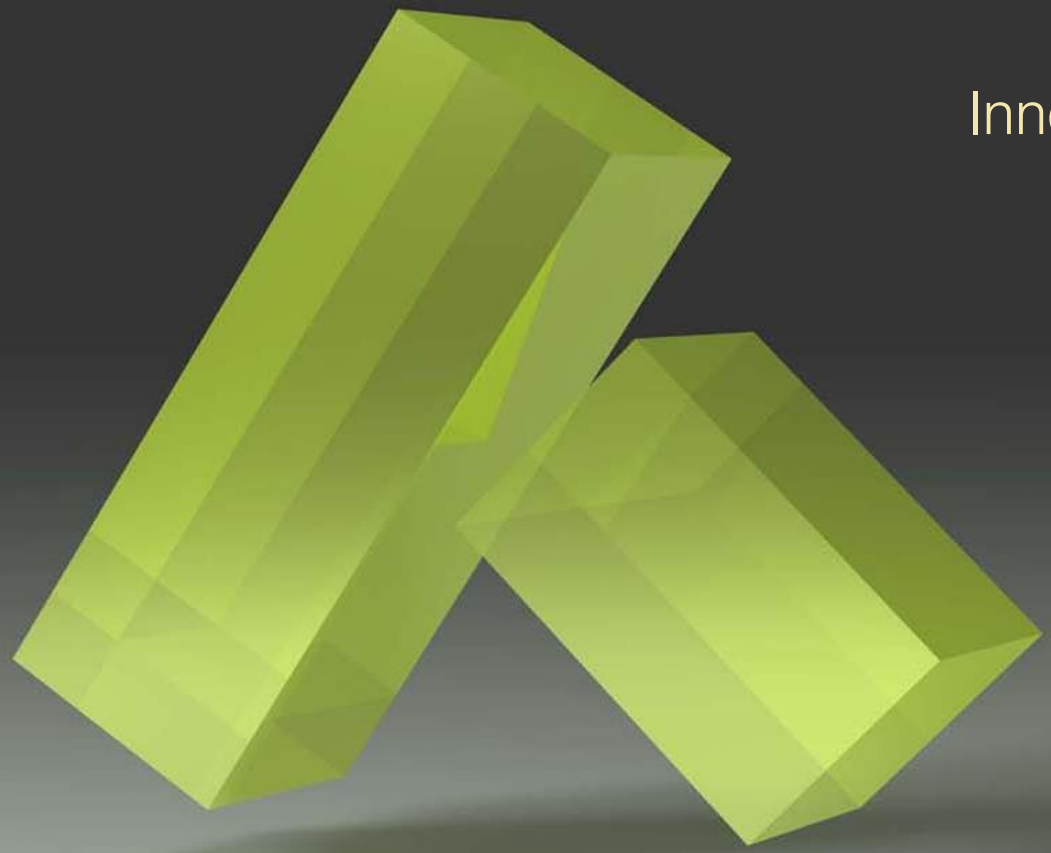

MedeA

Innovation by Simulation