



# Materials Constitution: The Need for Critical Evaluation of Data

# The publisher:



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

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

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



MAX-PLANCK-GESELLSCHAFT



# The team: **MSIT** MATERIALS SCIENCE INTERNATIONAL TEAM



~280 materials scientists  
collaborating remotely for  
**over 36 years**

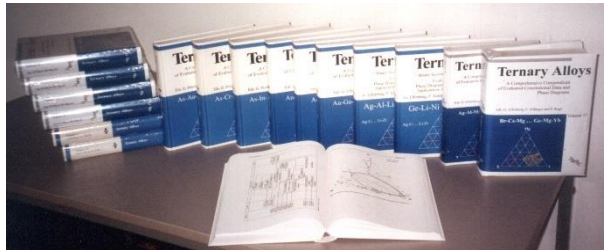
- ▶ monitor all relevant publications
- ▶ evaluate materials systems
- ▶ create reliable knowledge
- ▶ execute joint research
- ▶ provide first-class tuition in  
Materials Chemistry – MSIT Winter  
School & Advanced School.

## Member Affiliations

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

# 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)

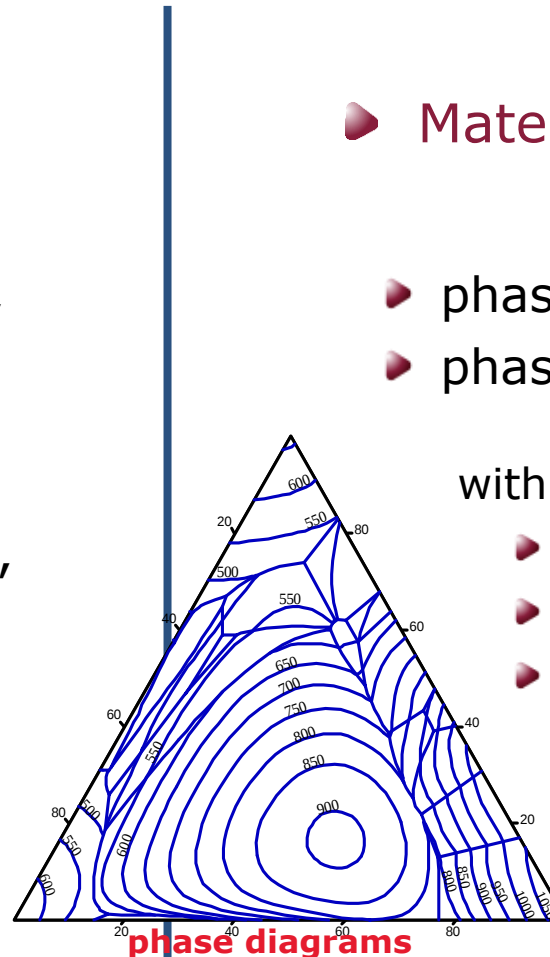
## Subject

### ▶ Materials Constitution

- ▶ phase **configurations** &
- ▶ phase **transformations**,

with changing

- ▶ Temperature
- ▶ Pressure
- ▶ Composition



**road maps for materials R&D**

# Critical Evaluation

Why do we do it?

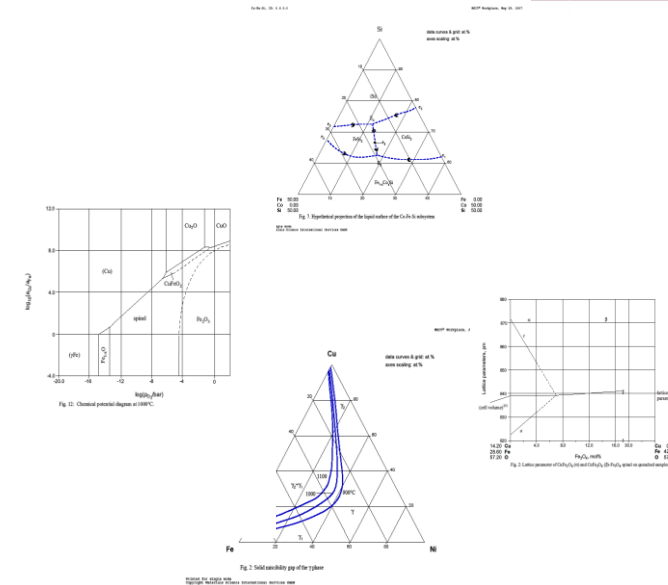
How do we do it?

# Critical Evaluation: Why to Evaluate?

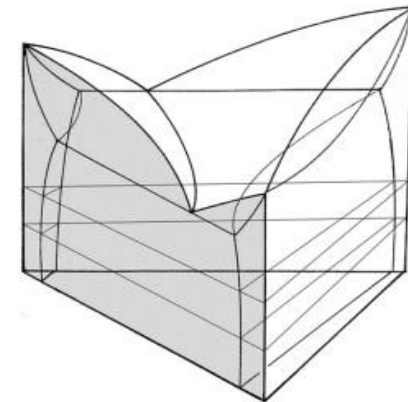
## ► Published data are often **conflicting**

- 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?*



...the solution...



*Users* need a *single* diagram (or set of complementary diagrams) that they can *trust*.

These diagrams should come from a *trustworthy* source

## ***CRITICAL EVALUATION***

## Critical Evaluation

*To produce in a concise and easily readable form a set of self-consistent phase diagrams and thermodynamic properties that represent the current (best) state of the knowledge of a particular system.*

- ▶ Careful consideration of all experimental and theoretical work carried out on the system in question.
- ▶ Thorough search of the literature
- ▶ Reviews
  - ▶ Useful, but *always* consult the original articles..... *trust no one.....*

*It is not making a list of the available literature*



## 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.*

## 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

## Intellectual Process

- ▶ Examine the literature

  - Phase equilibria

  - Crystal structure

  - Thermodynamics

- ▶ Check for consistencies and conflicts

  - Why do some data agree with each other and yet other datasets do not? Which are the best datasets?*

- ▶ Ternary data

  - Are the equilibria presented consistent with the accepted binary systems? If not, is it a fault with the ternary data...or the binary system?*

  - Do phase boundaries on isopleths and isothermal sections match-up?*

## Intellectual Process

- ▶ Check for gaps in the data

*What extra data are necessary? Is it possible to extrapolate to fill the gap in the knowledge?*

- ▶ Calphad modelling

*Might be useful to help resolve data conflicts, but it is not reported nor advisable.*

***Evaluation is not concerned with modelling. It is concerned with the best set of observations.***

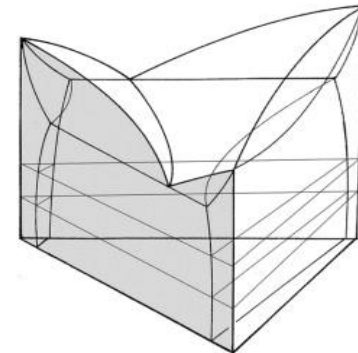
# Output

## 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 Evaluation Reports are peer reviewed**

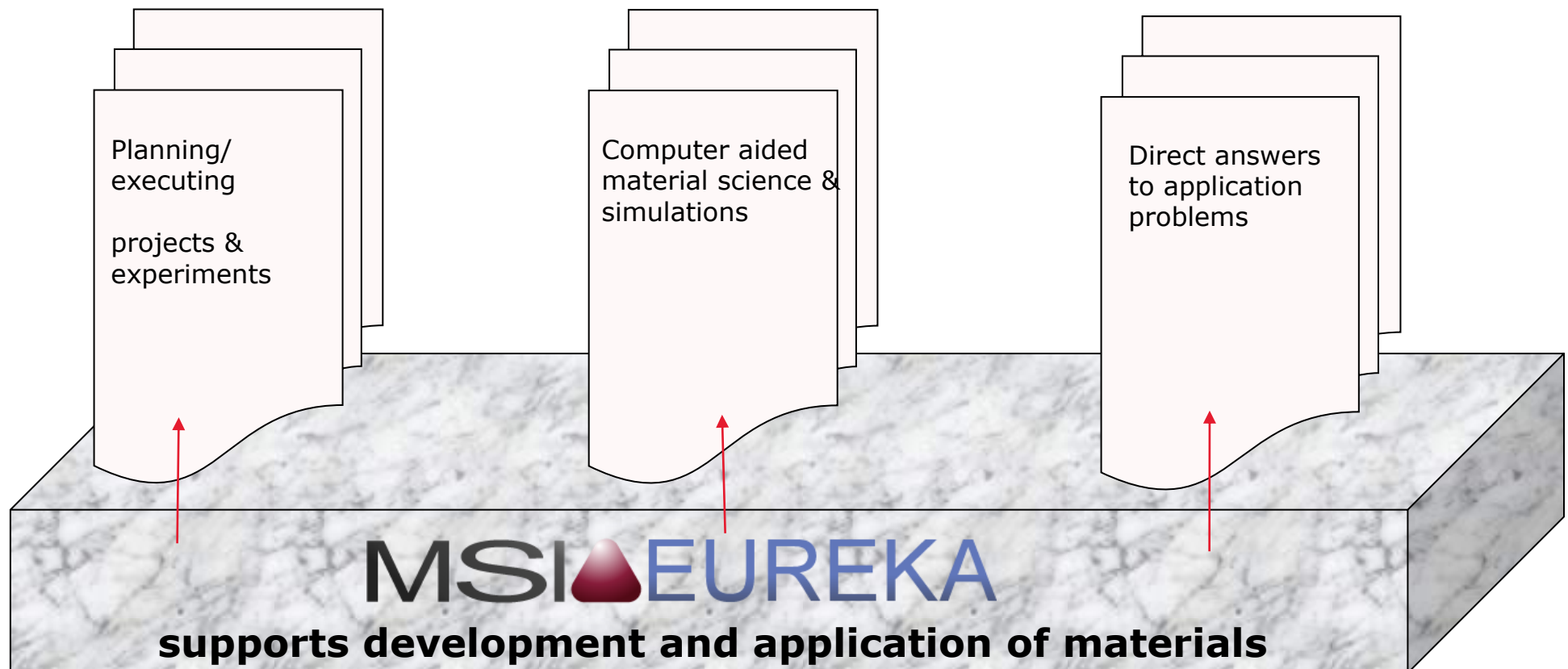
| Search Libraries                  |        |      |
|-----------------------------------|--------|------|
| MSI Eureka World Library Contents |        |      |
| Ternary Evaluations               | 4107   | View |
| Research Results                  | 4295   | View |
| Links to Literature               | 480047 | View |
| Binary Evaluations                | 271    | View |
| Diagrams as published             | 1694   | View |
| p-T-x Diagrams                    | 188    | View |
| Property Links                    |        | View |
| Total.....                        | 490602 |      |

Data & conclusions  
are to be evaluated



to describe the entire  
system, consistently

# MSI Eureka, what does it serve



# MSI

Science Simplified



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[www.msi-eureka.com](http://www.msi-eureka.com)