# Materials Constitution:

# The Need for Critical Evaluation of Data

***Svitlana Iljenko***

*MSI - Materials Science International Services GmbH*

MSI EUREKA

## An information system 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.

MSIT MATERIALS SCIENCE INTERNATIONAL TEAM

## The global team, MSIT

Materials Science International Team is the wolrd-wide group of scientists behind MSI Eureka. MSIT compiles and evaluates data, generates missing data, creates new knowledge, for over 34 years

MSI Science Simplified

## The company, MSI

Materials Science International Services, GmbH hosts the global team, markets MSI Eureka

# The publisher:

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

Since 1989 MSI, GmbH gives office and guidance to MSIT.

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

# Our Mission

To make the world's collective knowledge

✓ Transparent and validated

✓ useful and usable

✓ accessible

– in an area that applies to all inorganic materials.

The MSI founder-
Günter Effenberg

**Mission achieved - and ongoing,
in MSI Eureka !**

# The team: MSIT

MSIT makes MSI EUREKA

~280 materials scientists collaborating remotely for over 34 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; Lyon
**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 18 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

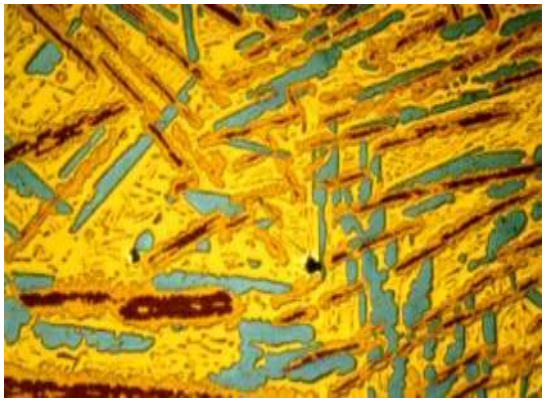
*With the coming of the digital information age, publication is continued electronically in "MSI Eureka"*

# MSI Eureka: engineering materials

- Alloys (steels, bronzes, magnets, electronic materials,… and more)
- Non-metals (ceramics, sensors, semiconductors,… and more)
- Composites (cermets, … and more)

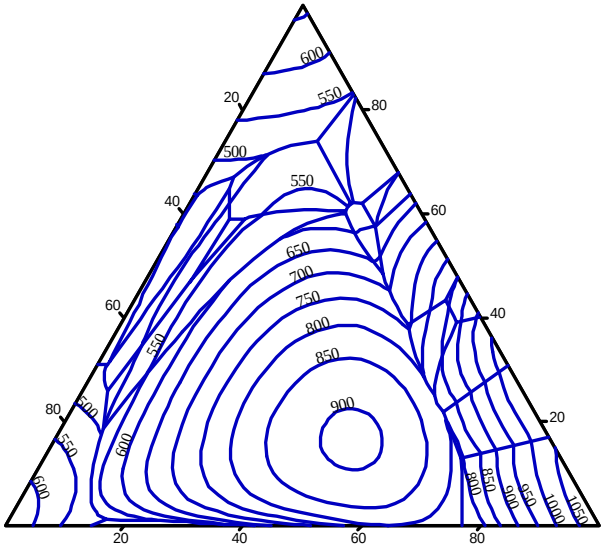
## Phase changes affect properties of engineering materials

microscope



multiphase, Ag-Cu-Sn solder alloy

MSI EUREKA gives the road maps for changes in materials!




**phase diagrams**

**road maps for materials R&D**

MSI EUREKA

## An information platform for Materials Constitution

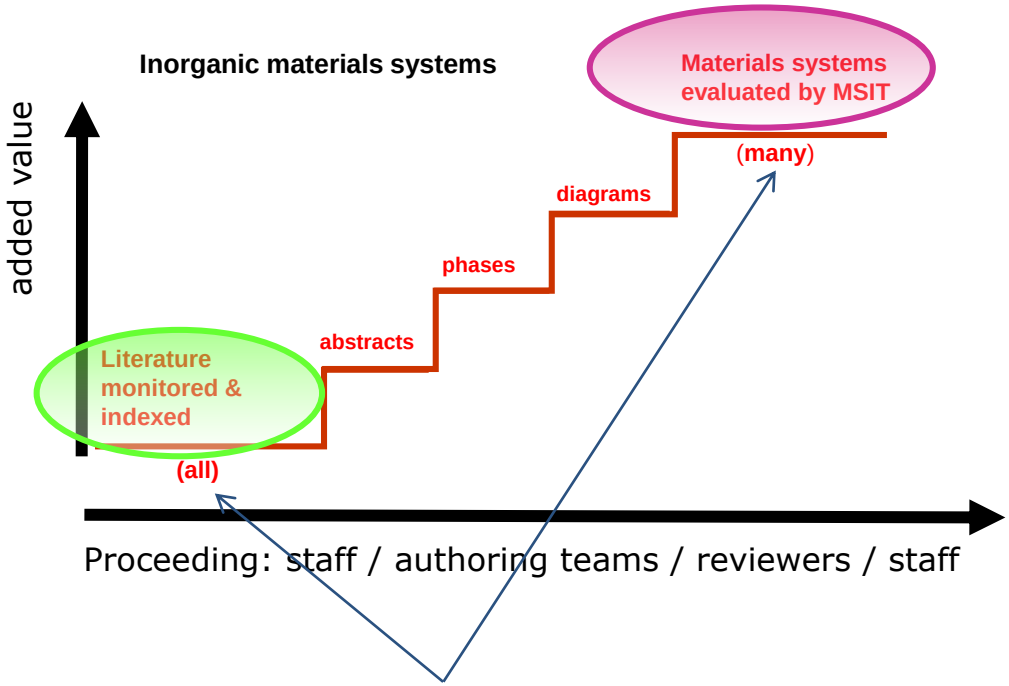
- covers materials' constitution of all inorganic materials, over 72000 systems.
- critically evaluates published data, provides Evaluation Reports for ca. 4500 systems
- integrates scattered data.
- explains by text, phase diagrams and tables
- provides information on structures, properties, thermodynamics & more.
- helps to *understand* the material.

MSI EUREKA

*by Scientists for Scientists!*

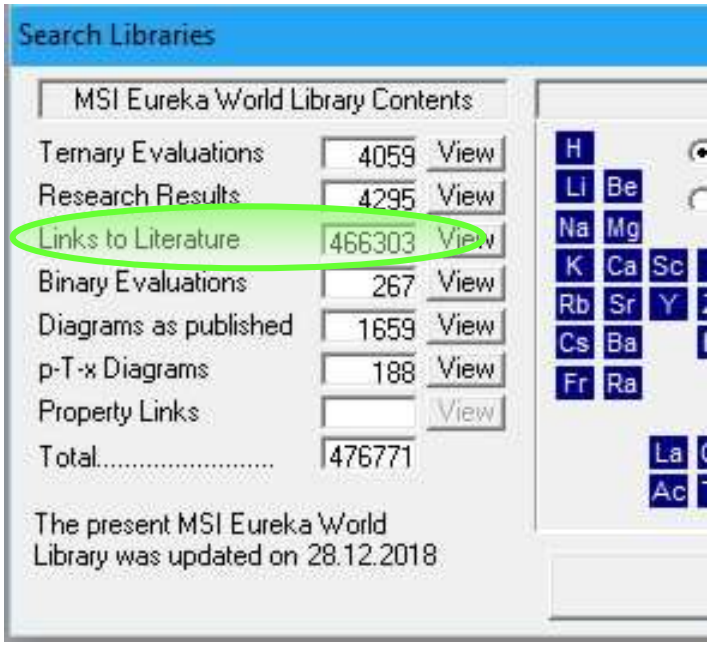
# MSI EUREKA adding value

- monitoring all literature (MSI)
- evaluating many literature (MSIT)




Key categories (next slides)

# Key Category - Links to Literature



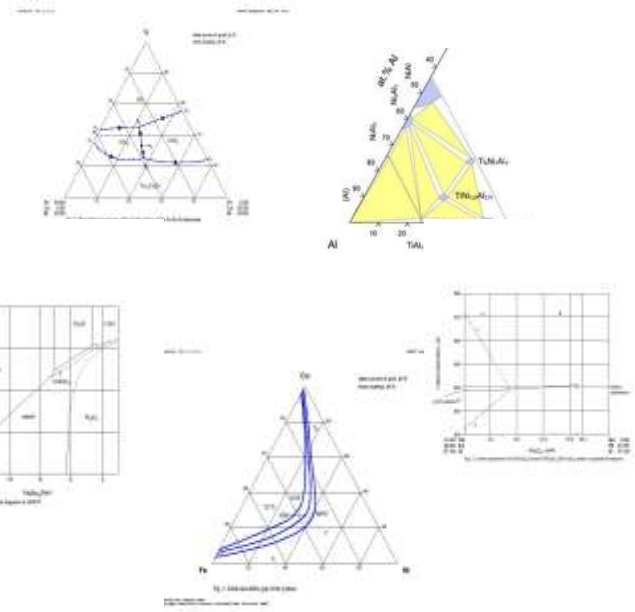

Bibliographic database & keywords, indexed by MSIT, Correlating materials with relevant publications

## Features

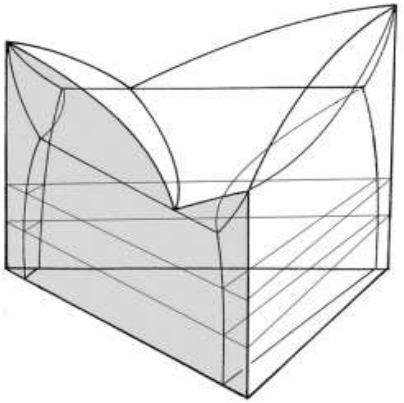
- simple search by periodic table of elements
- delivers relevant results only
- complete overview:
  - from the year 1830 to present
  - ~250 journals+books+grey literature monitored continuously
- 468,900 citations on 73,816 systems (as of June 2019)
- coverage of relevant literature better than anywhere else (*e.g. Inspec, Web of Knowledge, etc.)*

# Critical Evaluation: Why to Evaluate?

- Published data are often conflicting
  - between different publications
  - within one publication
- Published data are often incomplete
  - describing points or ranges of the entire 3D diagram
- Phase diagrams are not measured but concluded
  - from experimental data – to be evaluated

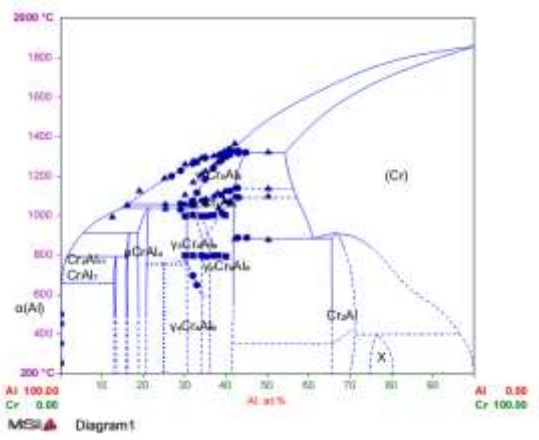


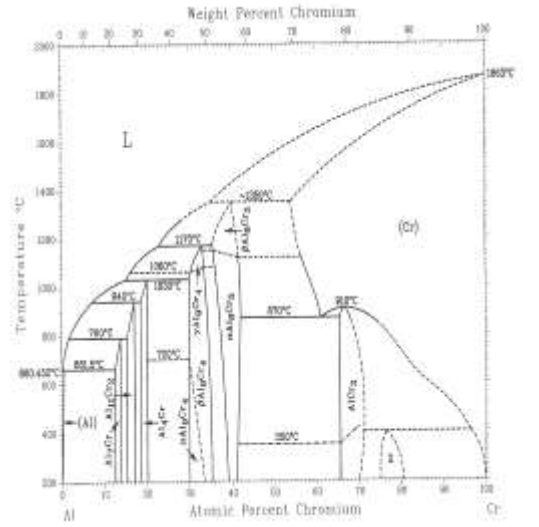
Data & conclusions are to be evaluated



to describe the entire system, consistently

# *So, why aren't all phase diagrams for a particular system the same?*




Different types of measurement

- Different accuracy and precision
- Static measurements
  - X-ray analysis, microscopy/SEM
- Dynamic measurement
  - DTA/DSC

Different quality of starting materials

Data missing

Poor experimental practice

Incorrect analysis of data

***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***

# *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

All articles are peer reviewed

# 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 cuts at different temperatures

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

- All articles are peer reviewed

# Materials Constitution: the Need for Critical Evaluation of Data

| | |
|---|---|
| **Authors** | Gautam Gosh |
| **Title** | Al-Fe-Si Ternary Phase Diagram Evaluation |
| **Source short** | MSI Eureka |
| **Source full** | MSI Eureka, Effenberg, G. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart |
| **Volume** | Ternary Evaluations |
| **Pages** | |
| **Publication year** | 1992 |
| **Comment** | Version 1 |
| **Document ID** | 10.14596.1.7 |
| **Cited references** | 138 |
| **MSIT keywords** | Amorphous, Assessment, Crystal Structure, Electrical Properties, Electrochemistry, Electronic Structure, Kinetics, Magnetic Properties, Mechanical Properties, Morphology, Phase Diagram, Phase Relations, Review, Thermodynamics, Transport Phenomena |
| **Language** | English |

Full text | Export RIS | Print version

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| **Pages** | |
| **Publication year** | 2013 |
| **Comment** | Version 4 |
| **Document ID** | 10.14596.4.9 |
| **Cited references** | 255 |
| **MSIT keywords** | Amorphous, Assessment, Crystal Structure, Electrical Properties, Electrochemistry, Electronic Structure, Interface Phenomena, Kinetics, Magnetic Properties, Mechanical Properties, Morphology, Nanomaterials, Optical Properties, Phase Diagram, Phase Relations, Physical Properties, Review, Semiconductivity, Thermodynamics, Transport Phenomena |
| **Language** | English |

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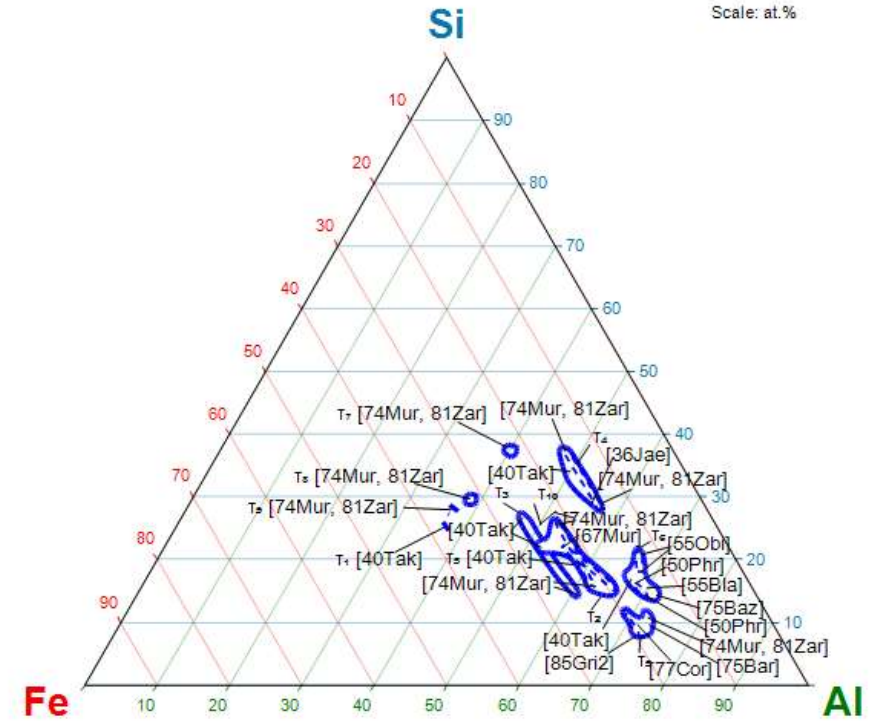
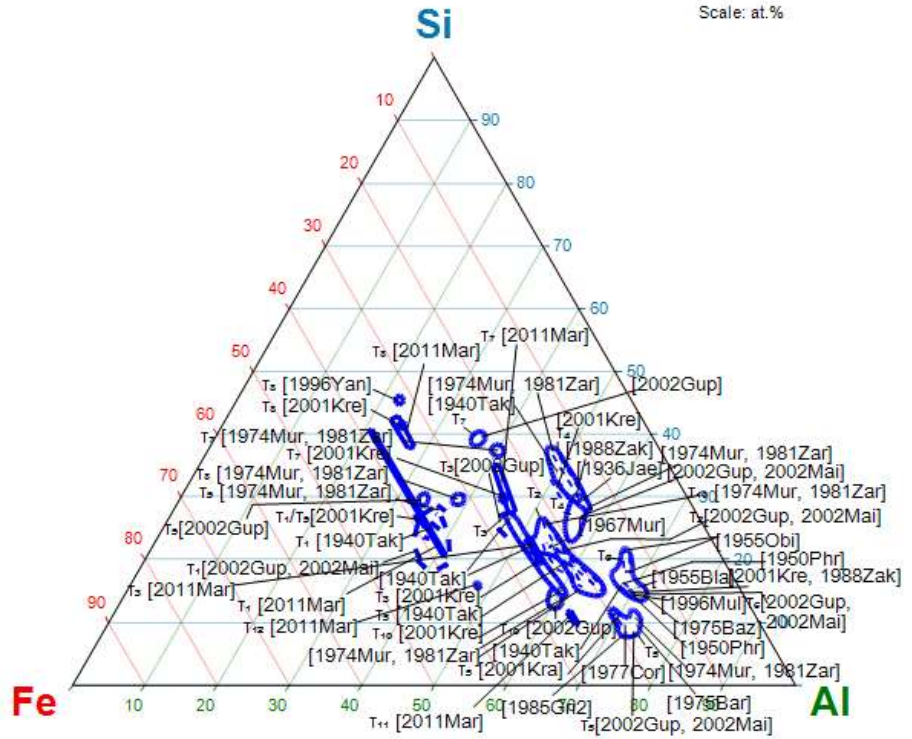
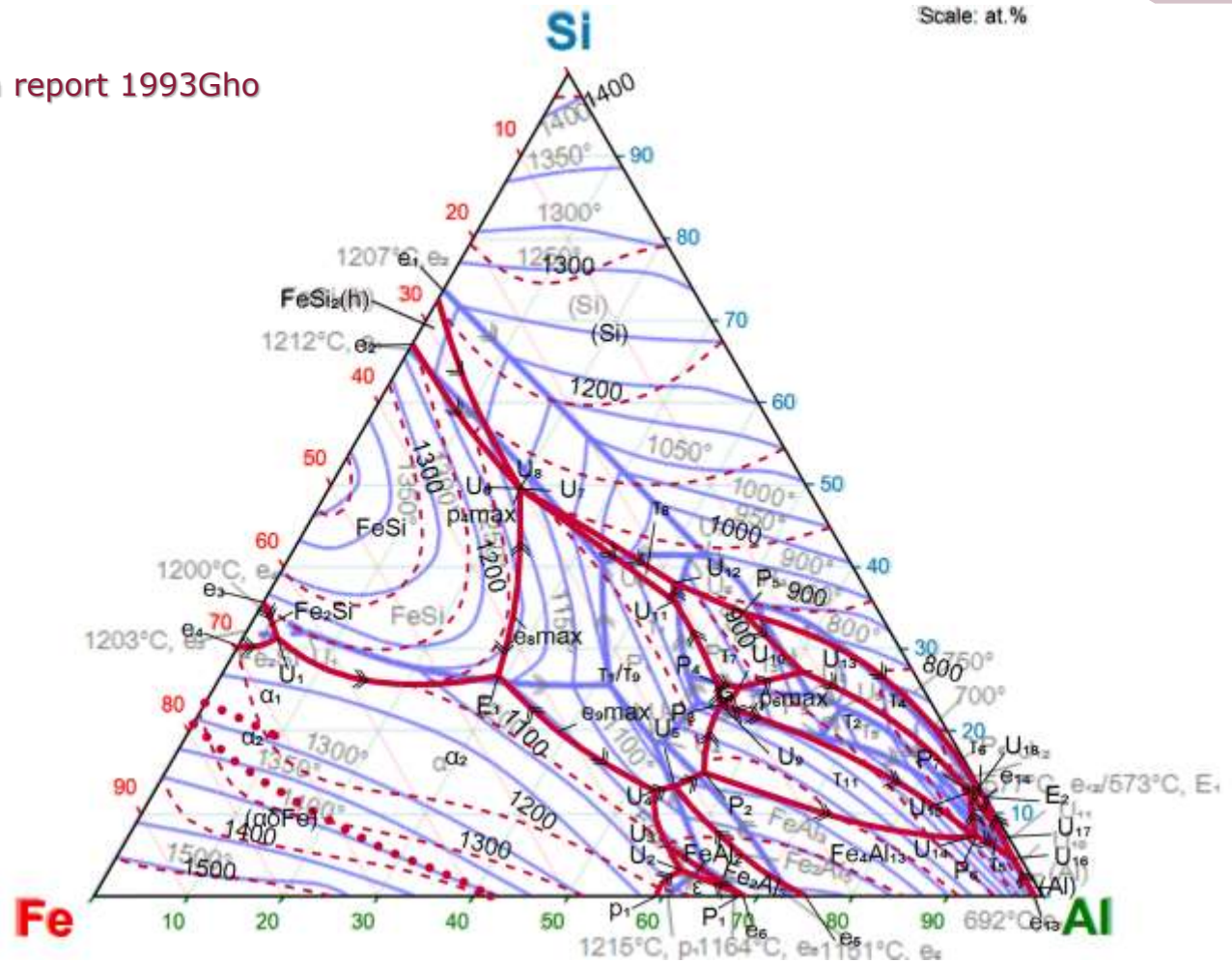



MSI **Fig. 1: Distribution of the equilibrium ternary phases in the Al-Fe-Si system, as reported by different authors as reported by different Autors.**




MSI **Fig. 1: Distribution of the equilibrium ternary phases, as reported by different authors as reported by different Autors.**

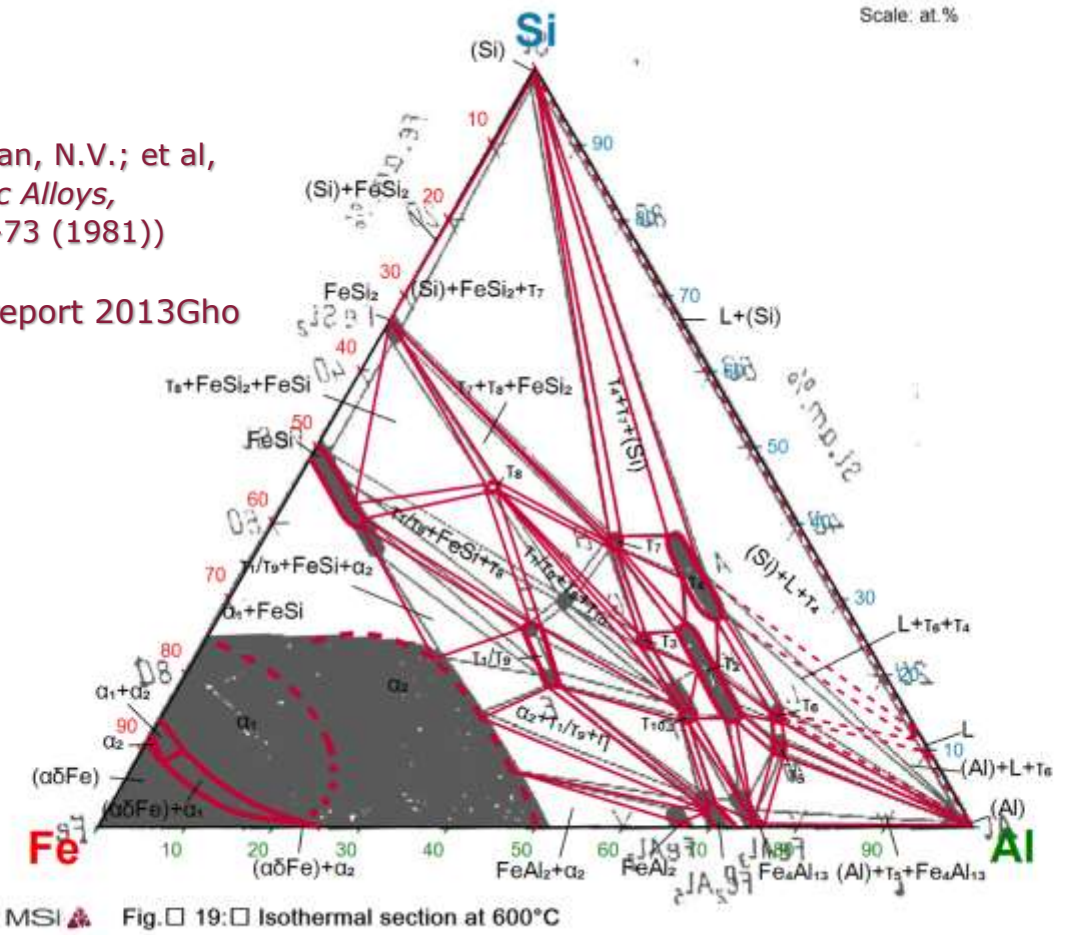
Blue lines – evaluation report 1993Gho
Red lines – 2013Gho




"Figure 10 shows the calculated liquidus surface of the whole Al-Fe-Si system as reported by Du et al [2008Du] with small correction according to accepted type of invariant reactions (see Invariant Equilibria section). It depicts at least 25 melting grooves separating different areas of primary crystallization. Overall, the calculated liquidus surface shows a good agreement with experimental results, and previous assessments [2005Gho, 2007Kre]. Experimental investigations [1933Nis, 1936Jae, 1937Ura, 1951Now, 1967Mun, 1987Gri1, 1988Zak, 2003Kha, 2004Pon1] have confirmed the topology of the liquidus surface."

Black lines – 1981Zar
(Zarechnyuk, O.S.; German, N.V.; et al,
*Phase Equilibria in Metallic Alloys,*
*Publ. Nauka, Moscow*, 69-73 (1981))

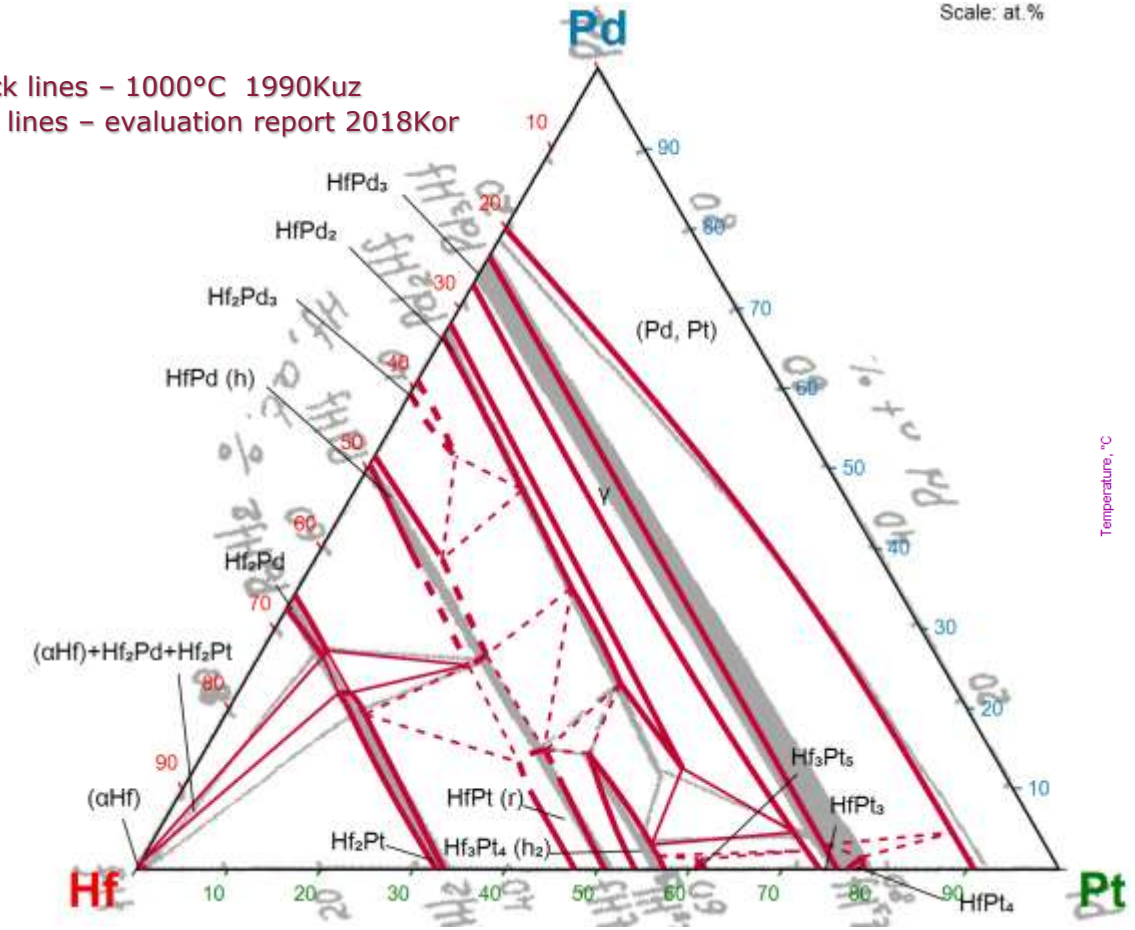
Red lines – evaluation report 2013Gho




MSI Fig. 19: Isothermal section at 600°C

"Figure 19 shows the assessed isothermal section at 600°C. The Fe corner involving the ordered phases is taken from [1982Miy, 1986Miy], but in certain composition ranges the ordered phase regions are still doubtful, and they are shown as dashed. The observation of three-phase fields τ2+τ4+τ6 and τ2+τ5+τ6 are consistent with the reaction scheme shown in Fig. 8. However, the isothermal section at 600°C reported by [1981Zar] has undergone several amendments. Previously reported τ1 and τ9 phases [1992Gho] are treated as one phase [2001Kre]. The composition of τ8 is accepted from [1996Yan]. Also, according to reaction scheme, three-phase fields L+(Si)+τ4, L+τ4+τ6, and L+(Al)+τ6 were added."

Black lines – 1000°C 1990Kuz
Red lines – evaluation report 2018Kor



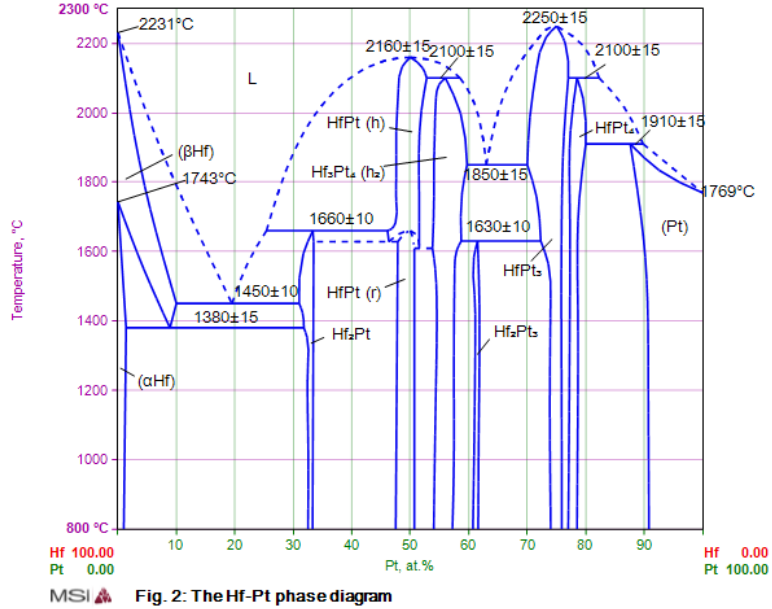
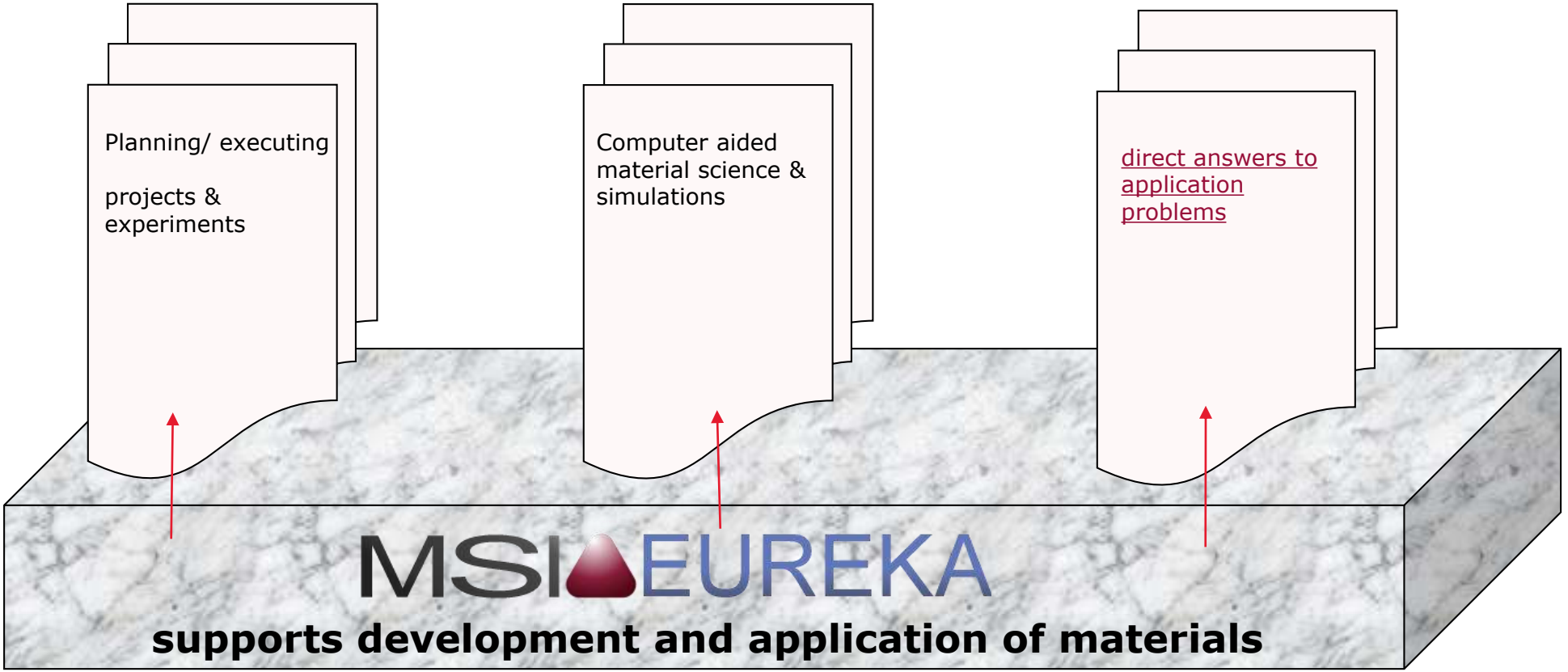




Fig. 2: The Hf-Pt phase diagram

A continuous series of solid solutions between the HfPd and HfPt compounds reported by [1990Kuz, 1990Sok] for 1000°C was not accepted in the present critical evaluation. According to the binary Hf-Pt system accepted in the present work, the low-temperature modification of HfPt(h) with orthorhombic CrB-type is stable at 1000°C. Therefore, this modification cannot form continuous solid solution with the HfPd compound (cubic CsCl-type) at this temperature. Moreover, authors of [1990Kuz, 1990Sok] did not present primary experimental data to support their conclusions. In Fig. 3 comparing to the original figure three-phase fields Hf2Pt+HfPd(h)+HfPt (r) and HfPd (h)+HfPt (r)+HfPd2 are added and shown with dashed lines. Extent of the Hf2Pd and Hf2Pt phases homogeneity ranges in depth of the ternary system is shown according to the data about solubility of third component which are represented in the texts of [1990Kuz, 1990Sok] articles. In Fig. 3 also the homogeneity ranges of the phases, which were not reported in [1990Kuz, 1990Sok], namely on the basis of Hf2Pd3, Hf3Pt5 and HfPt4, as well as three-phase fields corresponding to equilibria with participation of these phases are assigned schematically.

# MSI Eureka,
## what does it serve

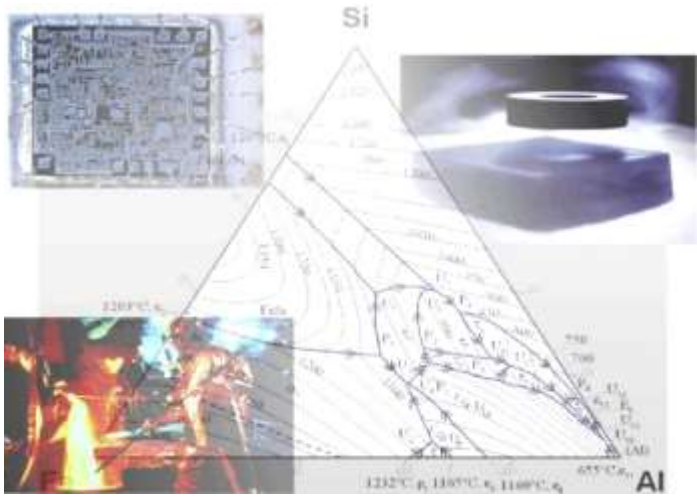


# Benefits for Engineers

## Developing / applying new materials & processes

### Problem

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




**road maps to solutions**

### 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

MSI
Science Simplified

# 2nd part: How to Access

# Alternative Access Options

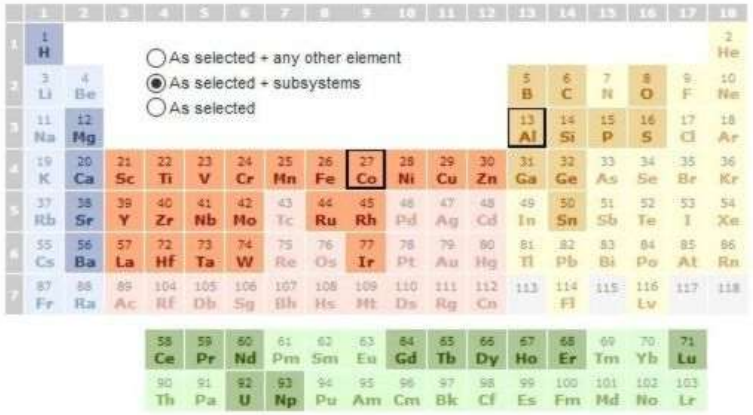
## MSI EUREKA.COM

- No download, direct access
- Licensee: read document online
- Non-licensee: read document preview

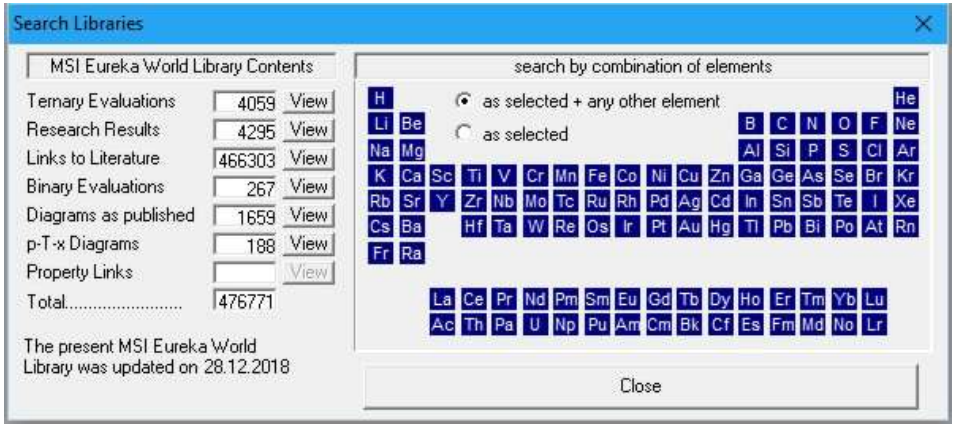
## MSI EUREKA VIEWER

- Search in text, tables & diagrams
- Work with interactive documents
  Read & convert concentrations, overlay diagrams, etc.

Goto: http://www.msi-eureka.com/search



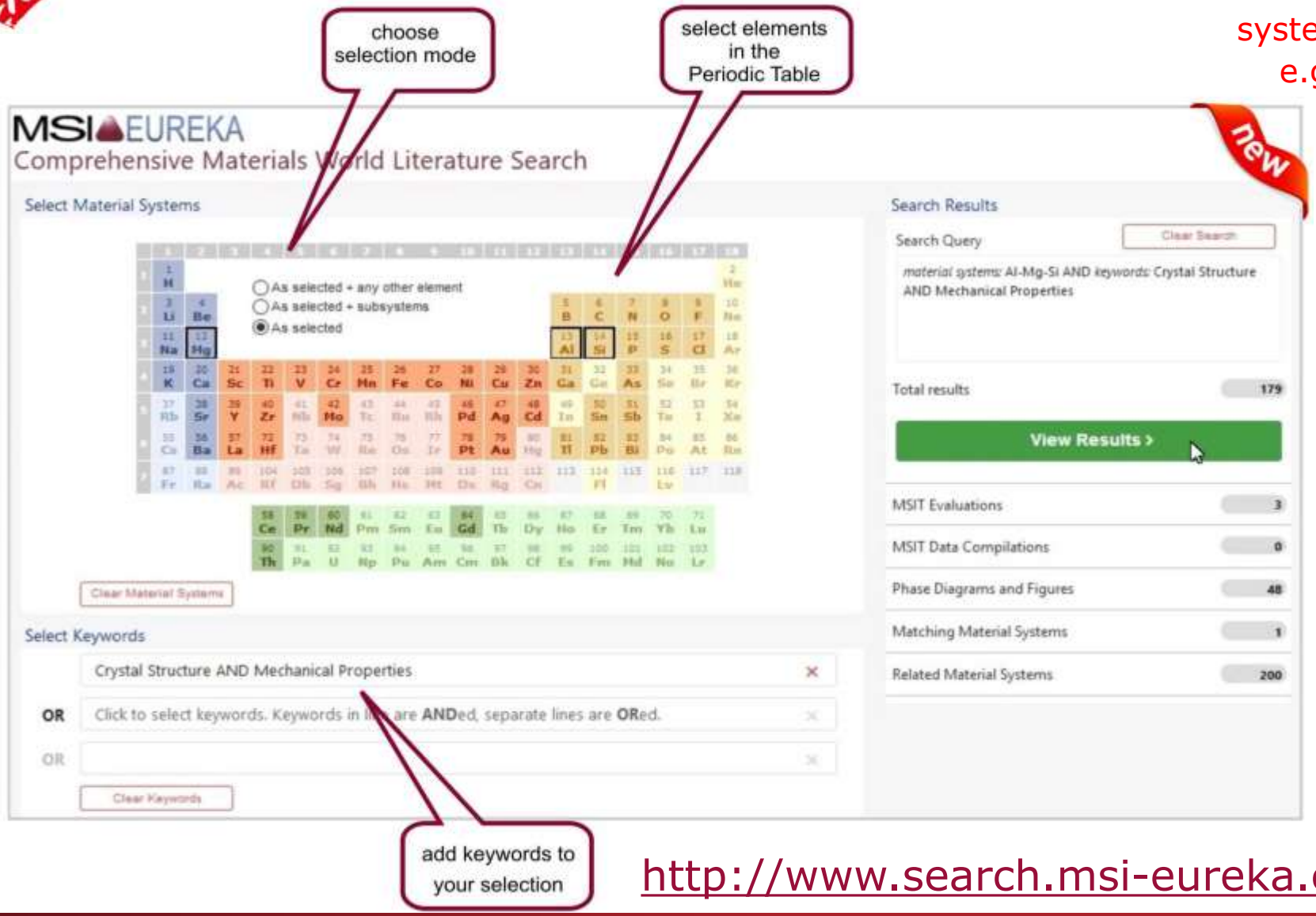

Install: MSI Eureka Viewer




In both options - access is through IP authentication

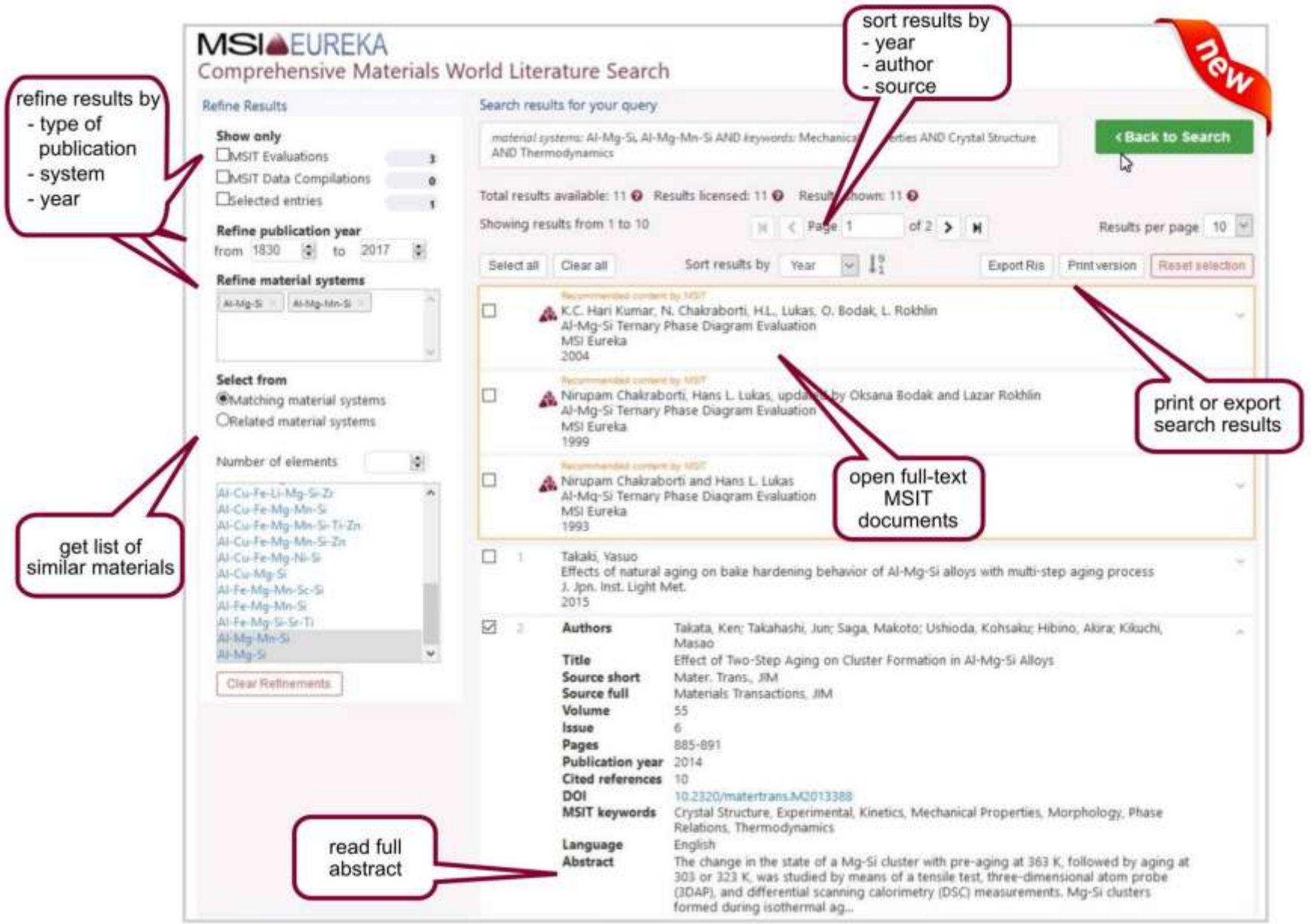
# New Search Functions

combined search : systems+keywords, e.g. properties




http://www.search.msi-eureka.com/search

# Materials Constitution: the Need for Critical Evaluation of Data



# Unique Features of MSI Eureka

- covers virtually all inorganic material systems ever studied- above 73,816 element combinations (as of June 2019).
- Modern search interface allowing to search for targeted properties and other keywords
- Largest bibliographic data base on materials constitution, 468,900 entries, (June 2019), continuous updating.
- Unary, binary, ternary and …more-component material systems.
- MSI Eureka evaluates entire material systems, not only phase diagrams
- Largest number of evaluated material systems, 4520 systems (June 2019).
- Largest phase diagram program ever, ongoing for over 34 years.

**MSI Eureka is made by scientists for scientists,**
**unique by content, coverage and quality & continuously updated**

# 4th MSIT Winter School

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 4-5 '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 OPENS IN SEPTEMBER

**The Programme includes:**

Principles of Chemical Thermodynamics
Phase Diagrams and Phase Equilibria (basic & advanced level) (incl. hands-on)
Experimental Determination of Phase Diagrams (incl. hands-on)
Crystallography (incl. hands-on)
Experimental Methods in Thermodynamics (incl. hands-on)
Ab-initio Techniques
Computational Thermodynamics
Calphad Method (incl. extended hands-on)

MORE...

**16 - 21 February 2020**
**Ringberg Castle**
**Kreuth, Germany**

**Organised by**

Dr. Günter Effenberg / **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 34th MSIT Annual International Seminar on Heterogeneous Multicomponent Equilibria.

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