



Materials Science International (MSI) Phase Diagrams

High-Quality Evaluated Phase Diagrams in MedeA

MSI EUREKA¹ is the world's leading and most comprehensive database for critically evaluated phase diagrams and related materials property data for metals, alloys, non-metals, and composites. Integration with *MedeA*^{®2} makes *MSI Phase Diagrams* an indispensable resource for materials science and engineering.

At-a-Glance

MSI Phase Diagrams offers phase diagrams, thermodynamic properties, and crystallographic data, critically evaluated and reviewed by experts of the **Materials Science International Team (MSIT)**[®]. The *MSI Phase Diagrams* module greatly enhances *MedeA*'s modeling capabilities for materials discovery, design, and optimization projects.

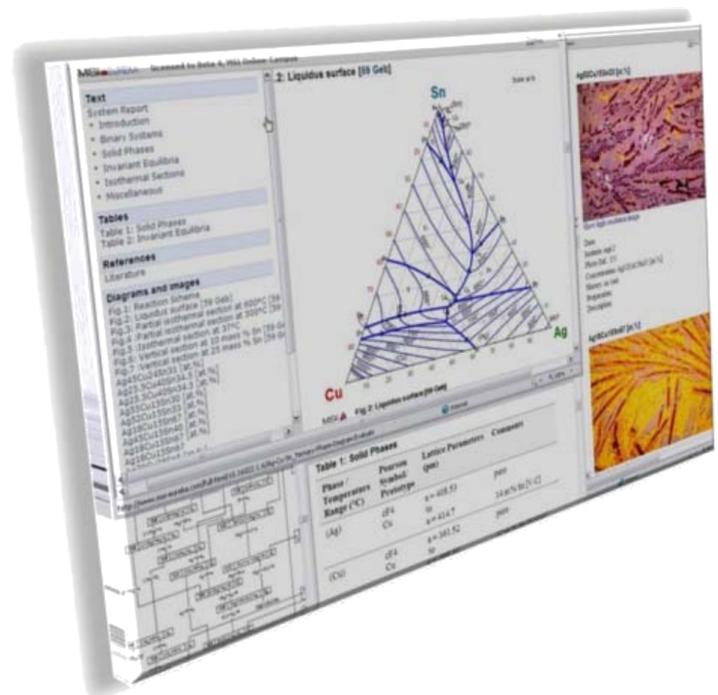
Key Benefits

- Build modeling strategies on expertly validated thermodynamic data
- Swift access to full-text documents and critical evaluation reports
- Seamless integration with *MedeA*

MSI Phase Diagrams provides critical intellectual evaluations of all data on constitutional properties, phase equilibria, thermodynamic and crystallographic data. Critical evaluation includes the resolution of contradictory published results, comparing and analyzing conclusions, and interpreting results based on assessing all available knowledge. (MSIT)[®] evaluation reports discuss and remedy conflicting data and rationalize the choice of the most appropriate data sets. The evaluation reports

¹ *MSI Phase Diagrams* is curated and maintained by the **Materials Science International Team (MSIT)**[®], a network of materials scientists and laboratories with considerable experience in materials constitutional science, experimental methods, and computational thermodynamics.

² *MedeA* and *Materials Design* are registered trademarks of *Materials Design, Inc.*



are authentic publications, peer reviewed under the auspices of the (MSIT)[®] editorial board. Reliable phase diagrams provide scientists and engineers with basic information of crucial importance for fundamental research and for the development and optimization of materials. The evaluation reports are an ideal source for computer-aided modeling and simulations, and are a repository of reliable validated data.

Specifications

- Provides over 4,380 critically evaluated reports for ternary and binary inorganic systems
- Altogether, more than 12,600 phase diagrams, graphs, charts, and schemes
- Approximately 8,600 tables with crystallographic data, invariant reactions, materials properties, experimental details, thermodynamic properties, etc.

- Data are obtained from 70,000 and more peer-reviewed original publications
- Around 2,000 additional phase diagrams in the category “Diagrams as published”, which are not evaluated by the MSIT[®].

Key Features

- Full integration with *MedeA* provides efficient and flexible database search capabilities
- Quick, efficient retrieval of full-text documents and phase diagrams using an intuitive, menu-based query language
- Complements *MedeA* builders, compute engines, and analysis tools

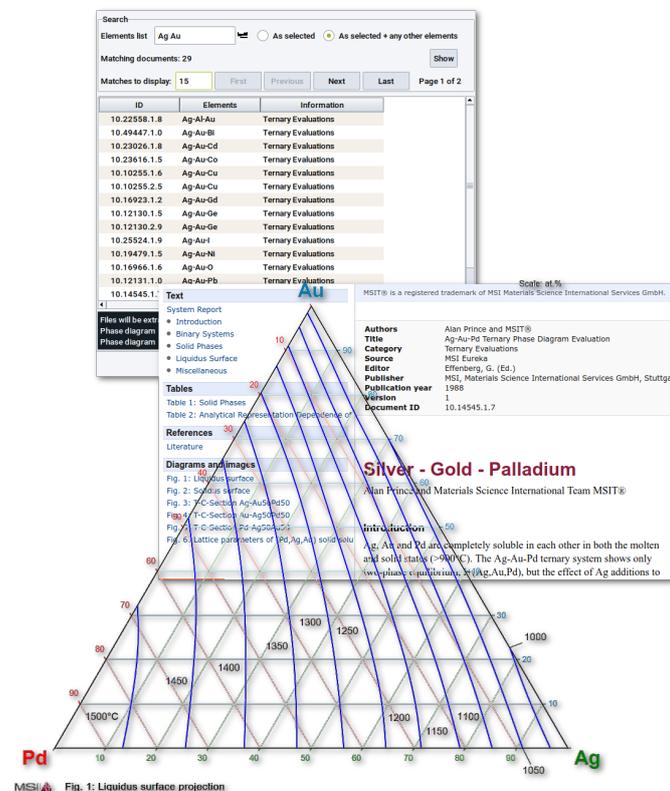


Figure 1: The MSI Phase Diagrams module provides intuitive search capabilities with rapid access to full-text materials properties information in the MedeA environment.

Properties

- Constitutional properties of inorganic materials

- Liquidus / solidus / solvus projections
- Isothermal and vertical sections
- Reaction schemes
- Invariant equilibria
- Crystallographic data, lattice parameters, space group, Pearson symbol, prototype lattice

- Temperature- and composition-ranges of phases
- Materials properties and applications
- Accompanied by descriptive texts
- Bibliographic references

Required Modules

- *MedeA Environment*

Recommended Modules

- *MedeA Pearson*
- *MedeA COD*
- *MedeA ICSD*
- *MedeA NCD*
- *MedeA VASP 5*
- *MedeA HT-Launchpad*

‘Phase diagrams are the beginning of wisdom - not the end of it.’

Sir William Hume-Rothery

Find Out More

Learn how *MSI Phase Diagrams* can inform your work and about *MedeA* capabilities including Databases, Builders, Compute Engines, Property Modules, and Analysis Tools.