

---

# MSI Phase Diagrams and NOMAD Database

---

## Contents

- *Materials Science International (MSI) Phase Diagrams*
  - *The Novel Materials Discovery (NOMAD) Repository*
- 

## 1 Materials Science International (MSI) Phase Diagrams


### 1.1 Overview

With a license for *MedeA MSI Phase Diagrams* you have access to the world's leading and most comprehensive database for phase diagrams and related materials property data for metals, alloys, non-metals, and composites.

### 1.2 Starting *MSI Phase Diagrams*

If your license key enables this database then you can start the search mask and dialogue, respectively, for this database with **Tools** >> **MSI Phase Diagrams** .

Search

Elements list    As selected  As selected + any other elements

Matching documents: Show

Matches to display:  First Previous Next Last Page 1 of 1


ID	Elements	Information

MSI Phase Diagrams database connected: /apps/MedeA/3.2/Databases/msipd.db version: 8.4  
 Files will be extracted in: /home/ /MedeA/tmp/PhaseDiagrams

Close

### 1.3 Searching Data

To search for available phase diagrams enter relevant element symbols in the empty field for the option **Elements list** . One way to enter the element symbols is by typing them in the empty field, e.g. Au Ag, and click **Show** .

**Note:** Enter single element symbols or a list of element symbols. In the latter case separate the elements with spaces (blanks). Alternatively, click on the icon  and select relevant elements in the period table of the elements.

By default the option **As selected** is enabled which implies that only records are listed in the below table which exactly match with the entered list of elements.

**Search**

Elements list   As selected  As selected + any other elements

Matching documents: 1 Show

Matches to display:  First Previous Next Last Page 1 of 1

ID	Elements	Information
20.10705.1.7	Ag-Au	Binary Evaluations

MSI Phase Diagrams database connected: /apps/MedeA/3.2/Databases/msipd.db version: 8.4

Files will be extracted in: /home/ /MedeA/tmp/PhaseDiagrams

Close

To extend the search to find more phase diagrams that are relevant for the defined elements and also for other elements mark the check box of the option **As selected + any other elements** and confirm with **Show**.

Search

Elements list   As selected  As selected + any other elements

Matching documents: 29 Show

Matches to display:      Page 1 of 1

ID	Elements	Information
10.22558.1.8	Ag-Al-Au	Ternary Evaluations
10.49447.1.0	Ag-Au-Bi	Ternary Evaluations
10.23026.1.8	Ag-Au-Cd	Ternary Evaluations
10.23616.1.5	Ag-Au-Co	Ternary Evaluations
10.10255.1.6	Ag-Au-Cu	Ternary Evaluations
10.10255.2.5	Ag-Au-Cu	Ternary Evaluations
10.16923.1.2	Ag-Au-Gd	Ternary Evaluations
10.12130.1.5	Ag-Au-Ge	Ternary Evaluations
10.12130.2.9	Ag-Au-Ge	Ternary Evaluations
10.25524.1.9	Ag-Au-I	Ternary Evaluations
10.19479.1.5	Ag-Au-Ni	Ternary Evaluations
10.16966.1.6	Ag-Au-O	Ternary Evaluations
10.12131.1.0	Ag-Au-Pb	Ternary Evaluations
10.14545.1.7	Ag-Au-Pd	Ternary Evaluations
10.14545.2.6	Ag-Au-Pd	Ternary Evaluations

MSI Phase Diagrams database connected: /apps/MedeA/3.2/Databases/msipd.db version: 8.4  
 Files will be extracted in: /home/ /MedeA/tmp/PhaseDiagrams

**Note:** It is also possible to enter element symbols by clicking on the icon and select relevant elements in the periodic system of the elements.

Search

Elements list   As selected  As selected + any other elements

Matching documents: 29 Show

Matches to display Read scheme Write scheme MedeaA default

ID																																																																																																							
10.22558.1.8	1	1																	2																																																																																				
10.49447.1.0																			He																																																																																				
10.23026.1.8																			4.00																																																																																				
10.23616.1.5	2	3	4															5	6	7	8	9	10																																																																																
10.10255.1.6		Li	Be															B	C	N	O	F	Ne																																																																																
10.10255.2.5		6.94	9.01															10.81	12.01	14.01	16.00	19.00	20.18																																																																																
10.16923.1.2	3	11	12															13	14	15	16	17	18																																																																																
10.12130.1.5		Na	Mg															Al	Si	P	S	Cl	Ar																																																																																
10.12130.2.9		22.99	24.30															26.98	28.09	30.97	32.07	35.45	39.95																																																																																
10.25524.1.9	4	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36																																																																																				
10.19479.1.5		K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr																																																																																				
10.16966.1.6		39.10	40.08	44.96	47.88	50.94	52.00	54.93	55.85	58.93	58.69	63.55	65.39	69.72	72.61	74.92	78.96	79.90	83.80																																																																																				
10.14545.1.7	5	37	38	39	40	41	42	43	44	45	46	Ag	48	49	50	51	52	53	54																																																																																				
10.14545.2.6		Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd		Cd	In	Sn	Sb	Te	I	Xe																																																																																				
		85.47	87.62	88.91	91.22	92.91	95.94	98.91	101.07	102.91	106.42		112.41	114.82	118.71	121.75	127.60	126.90	131.29																																																																																				
	6	55	56	57	72	73	74	75	76	77	78	Au	80	81	82	83	84	85	86																																																																																				
		Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt		Hg	Tl	Pb	Bi	Po	At	Rn																																																																																				
		132.91	137.33	138.91	178.49	180.95	183.85	186.21	190.20	192.22	195.08		200.59	204.38	207.20	208.98	209.98	209.99	(222)																																																																																				
	7	87	88	89	104	105	106	107	108	109																																																																																													
		Fr	Ra	Ac	Rf	Ha	Sg	Bh	Hs	Mt																																																																																													
		223.02	226.03	227.03	261.11	262.11	263.11	262.12	(270)	(268)																																																																																													
		<table border="1" style="width: 100%; border-collapse: collapse; text-align: center;"> <tr> <td>58</td><td>59</td><td>60</td><td>61</td><td>62</td><td>63</td><td>64</td><td>65</td><td>66</td><td>67</td><td>68</td><td>69</td><td>70</td><td>71</td> </tr> <tr> <td>Ce</td><td>Pr</td><td>Nd</td><td>Pm</td><td>Sm</td><td>Eu</td><td>Gd</td><td>Tb</td><td>Dy</td><td>Ho</td><td>Er</td><td>Tm</td><td>Yb</td><td>Lu</td> </tr> <tr> <td>140.12</td><td>140.91</td><td>144.24</td><td>146.92</td><td>150.36</td><td>151.97</td><td>157.25</td><td>158.93</td><td>162.50</td><td>164.93</td><td>167.26</td><td>168.93</td><td>173.04</td><td>174.97</td> </tr> <tr> <td>90</td><td>91</td><td>92</td><td>93</td><td>94</td><td>95</td><td>96</td><td>97</td><td>98</td><td>99</td><td>100</td><td>101</td><td>102</td><td>103</td> </tr> <tr> <td>Th</td><td>Pa</td><td>U</td><td>Np</td><td>Pu</td><td>Am</td><td>Cm</td><td>Bk</td><td>Cf</td><td>Es</td><td>Fm</td><td>Md</td><td>No</td><td>Lr</td> </tr> <tr> <td>232.04</td><td>231.04</td><td>238.03</td><td>237.05</td><td>244.06</td><td>243.06</td><td>247.07</td><td>(247)</td><td>(251)</td><td>(252)</td><td>257.10</td><td>(258)</td><td>(259)</td><td>(266)</td> </tr> </table>																		58	59	60	61	62	63	64	65	66	67	68	69	70	71	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	140.12	140.91	144.24	146.92	150.36	151.97	157.25	158.93	162.50	164.93	167.26	168.93	173.04	174.97	90	91	92	93	94	95	96	97	98	99	100	101	102	103	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	232.04	231.04	238.03	237.05	244.06	243.06	247.07	(247)	(251)	(252)	257.10	(258)	(259)	(266)
58	59	60	61	62	63	64	65	66	67	68	69	70	71																																																																																										
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu																																																																																										
140.12	140.91	144.24	146.92	150.36	151.97	157.25	158.93	162.50	164.93	167.26	168.93	173.04	174.97																																																																																										
90	91	92	93	94	95	96	97	98	99	100	101	102	103																																																																																										
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr																																																																																										
232.04	231.04	238.03	237.05	244.06	243.06	247.07	(247)	(251)	(252)	257.10	(258)	(259)	(266)																																																																																										

OK
Cancel

To limit the amount of records that are displayed in the table, e.g. to 10 rows only, modify the number for the option **Matches to display** accordingly. The table will adapt automatically within a few seconds.

**Search**

Elements list   As selected  As selected + any other elements

Matching documents: 29

Matches to display:      Page 1 of 3

ID	Elements	Information
10.22558.1.8	Ag-Al-Au	Ternary Evaluations
10.49447.1.0	Ag-Au-Bi	Ternary Evaluations
10.23026.1.8	Ag-Au-Cd	Ternary Evaluations
10.23616.1.5	Ag-Au-Co	Ternary Evaluations
10.10255.1.6	Ag-Au-Cu	Ternary Evaluations
10.10255.2.5	Ag-Au-Cu	Ternary Evaluations
10.16923.1.2	Ag-Au-Gd	Ternary Evaluations
10.12130.1.5	Ag-Au-Ge	Ternary Evaluations
10.12130.2.9	Ag-Au-Ge	Ternary Evaluations
10.25524.1.9	Ag-Au-I	Ternary Evaluations

MSI Phase Diagrams database connected: /apps/MedeA/3.2/Databases/msipd.db version: 8.4  
 Files will be extracted in: /home/ /MedeA/tmp/PhaseDiagrams

With limiting the amount of displayed records to a small number the entire table is distributed among several pages. To open the next page click on

**Search**

Elements list   As selected  As selected + any other elements

Matching documents: 29

Matches to display:      Page 2 of 3

ID	Elements	Information
10.19479.1.5	Ag-Au-Ni	Ternary Evaluations
10.16966.1.6	Ag-Au-O	Ternary Evaluations
10.12131.1.0	Ag-Au-Pb	Ternary Evaluations
10.14545.1.7	Ag-Au-Pd	Ternary Evaluations
10.14545.2.6	Ag-Au-Pd	Ternary Evaluations
10.23054.1.6	Ag-Au-Pt	Ternary Evaluations
10.23054.2.5	Ag-Au-Pt	Ternary Evaluations
10.16377.1.7	Ag-Au-S	Ternary Evaluations
10.19045.1.1	Ag-Au-Sb	Ternary Evaluations
10.16378.1.4	Ag-Au-Se	Ternary Evaluations

MSI Phase Diagrams database connected: /apps/MedeA/3.2/Databases/msipd.db version: 8.4  
 Files will be extracted in: /home/ /MedeA/tmp/PhaseDiagrams

To display the next and last page click on  and , respectively.

Search

Elements list   As selected  As selected + any other elements

Matching documents: 29 Show

Matches to display:  First Previous Next Last Page 3 of 3

ID	Elements	Information
10.14844.1.8	Ag-Au-Si	Ternary Evaluations
10.14844.2.7	Ag-Au-Si	Ternary Evaluations
10.19046.2.3	Ag-Au-Sn	Ternary Evaluations
10.12159.1.8	Ag-Au-Te	Ternary Evaluations
10.55396.1.4	Ag-Au-Y	Ternary Evaluations
10.14551.1.3	Ag-Au-Zn	Ternary Evaluations
10.14551.2.2	Ag-Au-Zn	Ternary Evaluations
10.52603.1.1	Ag-Au-Zr	Ternary Evaluations
20.10705.1.7	Ag-Au	Binary Evaluations

MSI Phase Diagrams database connected: /apps/MedeA/3.2/Databases/msipd.db version: 8.4  
 Files will be extracted in: /home/ /MedeA/tmp/PhaseDiagrams

Close

To display again previous pages or the first page click on Previous and First , respectively.

## 1.4 Retrieving Data

To retrieve a phase diagram and related data from the database, right-click on the relevant table row to open a context menu. In the context menu click on View document ... .



**Search**

Elements list   As selected  As selected + any other elements

Matching documents: 29 [Show](#)

Matches to display:  [First](#) [Previous](#) [Next](#) [Last](#) Page 3 of 3

ID	Elements	Information
10.14844.1.8	Ag-Au-Si	Ternary Evaluations
10.14844.2.7	Ag-Au-Si	Ternary Evaluations
10.19046.2.3	Ag-Au-Sn	Ternary Evaluations
10.12159.1.8	Ag-Au-Te	Ternary Evaluations
10.55396.1.4	Ag-Au-Y	Ternary Evaluations
10.14551.1.3	Ag-Au-Zn	Ternary Evaluations
10.14551.2.2	Ag-Au-Zn	Ternary Evaluations
10.52603.1.1	Ag-Au-Zr	Ternary Evaluations
20.10705.1.7	Ag-Au	Bina

- Sort Ascending
- Sort Descending
- Format...
- Copy full column
- Copy column selected content
- View document 20.10705.1.7

MSI Phase Diagrams database connected: /apps/MedeA/3.2/Databases/msipd.db version: 8.4

Files will be extracted in: /home/ /MedeA/tmp/PhaseDiagrams

[Close](#)

The retrieved data is displayed in your preferred web browser. Use the browser features to browse through the displayed document.

MSI EUREKA World's leading database for evaluated materials constitution data
Print

<p><b>Text</b></p> <p>System Report</p> <ul style="list-style-type: none"> <li>• Literature Data</li> <li>• Solid Phases</li> <li>• Phase Equilibria</li> <li>• Thermodynamics</li> <li>• Notes on Materials Properties and Applications</li> </ul> <p><b>Tables</b></p> <p>Table 1: Investigation of the Ag-Au Phase Equilibria</p> <p>Table 2: Solid Phases</p> <p>Table 3: Thermodynamic Data of Reaction or Transformation</p> <p><b>References</b></p> <p>Literature</p> <p><b>Diagrams and images</b></p> <p>Fig. 1: Assessed phase diagram of the Ag-Au system</p>	<p><b>Cite as</b> Pierre Perrot, "Ag-Au Binary Phase Diagram Evaluation", in <i>MSI Eureka</i>, Effenberg, G. (Ed.), MSI, Materials Science International Services GmbH, Stuttgart (2003), Document ID: 20.10705.1.7</p> <p><b>Authors</b> Pierre Perrot</p> <p><b>Title</b> Ag-Au Binary Phase Diagram Evaluation</p> <p><b>Category</b> MSIT® Binary Evaluations</p> <p><b>Source</b> MSI Eureka</p> <p><b>Editor</b> Effenberg, G. (Ed.)</p> <p><b>Publisher</b> MSI, Materials Science International Services GmbH, Stuttgart</p> <p><b>Publication year</b> 2003</p> <p><b>Version</b> 1</p> <p><b>Document ID</b> 20.10705.1.7</p>
---	--

## Ag - Au (Silver - Gold)

Pierre Perrot

**Literature Data**

The Ag-Au system was assessed by [1983Oka] with an intensive literature survey up to 1982. Many experimental investigations have been carried out on this system since the work of [1909Jae]. Recent experimental works are reported in Table 1. The system was also theoretically investigated using potential energies of surrounded atoms [1942Hir], activity calculations from Miedema's model [1994Din, 1999Din], the three-dimensional fcc Ising model [1987Wei], the cluster variation method [1991Moh], the valence electronic structure theory [1991Zhe], the Debye-Gruneisen model taking into account the lattice vibration effects [1993Moh] and quantum-mechanical calculations [1995Lu]. Gibbs energy of solid solutions was estimated based on the relationship between the number of binding electrons and the ratio volume/bulk modulus [1995Bar]. Thermodynamic relationships were derived between enthalpy of mixing and excess entropy in binary alloys [1996Tan]. The excess entropy of mixing has been evaluated by [2001Som] as the sum of configurational, vibrational, electronic and magnetic contributions.

**Solid Phases**

Solid phases are given in Table 2. The lattice parameter of the solid solution shows a significantly

**Note:** Feel free to open several documents with phase diagrams and related data side-by-side. Simply show the context menu of other table rows and open the associated document via [View document ...](#)

## 2 The Novel Materials Discovery (NOMAD) Repository

The NoMaD repository [1] is a free and unrestricted service for publishing and storing the results of materials simulations. To use the service you must sign up for a NoMaD account using their website. The supported file formats and types that can be uploaded are summarized on the NoMaD page [How to upload input and output files](#) [2]. Once signed up your NoMaD account page contains a token which is a text string of 64 alpha-numeric characters. This token, associates file uploads with your NoMaD account.

Within *MedeA* you can either select input and output files in a directory from disk or a previously completed job. During the upload process you will see a progress dialog and, once the upload has completed, a message from the NoMaD servers. The NoMaD parsers inspect every file in the upload to locate any output files produced by any of the supported compute engines (calculation codes) and file formats, respectively. If supported file formats are detected, the output files are added to the NoMaD repository. Any output files which are not supported by NoMaD are omitted and not added to the repository and database, respectively.

[1] <http://repository.nomad-coe.eu/>

[2] <http://www.nomad-coe.eu/the-project/nomad-repository/nomad-repository-howtoupload>

## 2.1 Define your NoMaD upload token

The NoMaD upload token can be entered at two places in the *Medea GUI*:

- File >> Preferences , Directories tab, NoMaD upload token
- File >> Upload files to NoMaD

Please enter your NoMaD upload token:

UXthu3PxNnfhMUxGYPHggNLXhMnbX3yuBQBUvf3Tt925EqpvPVnGzYftnuuV7Ceyl

Directory from Disk Previous Calculation Cancel Help

Copy your token from your NoMaD account page and paste it into the relevant field.

Then select whether files should be uploaded from a **Directory from Disk** of your computer or from a **Previous Calculation** stored on a *Medea* JobServer.

---

**Hint:** For the option **Previous Calculation** it is important to select the proper JobServer via **Jobs >> Select Server >> ...**

---

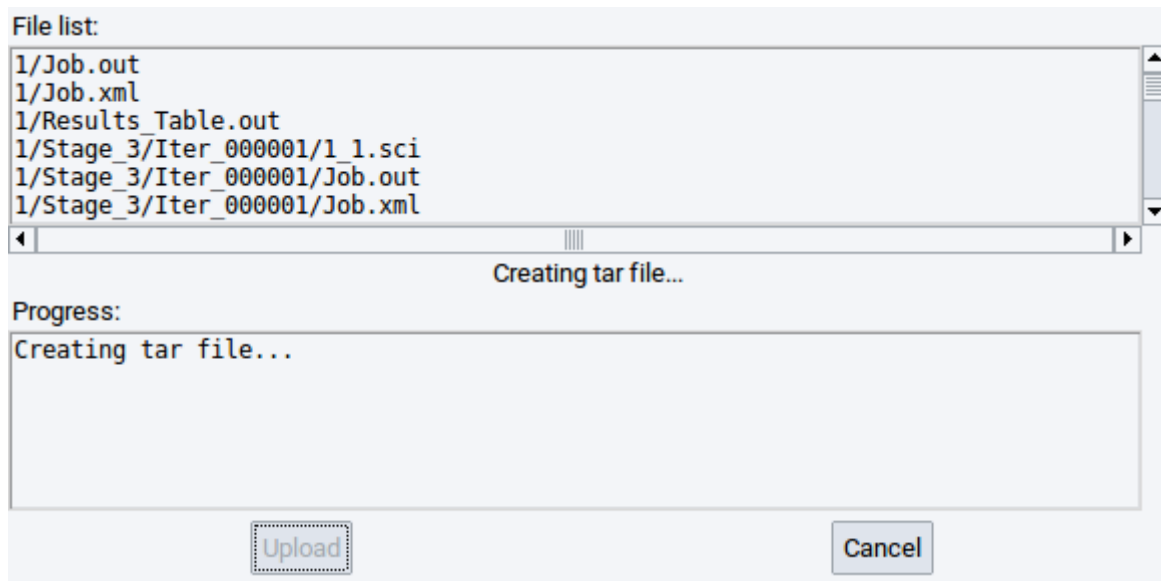
## 2.2 Upload files from disk

Upon selecting the option **Directory from Disk** a folder browser pops up to navigate to the relevant directory and to select files that should be uploaded. Start the actual upload with the **Upload** option.

Directory: /home/medea/MD/2.0/Jobs

Selection: /home/medea/MD/2.0/Jobs

OK Cancel



## 2.3 Upload files from previous jobs

Upon selecting the option **Previous Calculation** a dialog pops up to select files of relevant jobs. Files are selected if tagged with a checkmark. Confirm the selection with **Open**.

**Filtering options** ↑

User: is anyone ▾

Job name: is anything ▾

Submitted: any time ▾

Started: any time ▾

Finished: any time ▾

Status: is anything ▾

Job Numbers: <= ▾

Hide intermediate files

Number of jobs to display:  Refresh

Expand All Collapse All Collapse unselected

Job/File	File size	User
▷ 1394 (5 files) -- PAGs add relevant QSPR descriptors to revised structure list		
▷ 1393 (5 files) -- PAGs add relevant QSPR descriptors to revised structure list		
▷ 1390 (78 files) -- PAGs revised structure list		
▷ 1383 (5 files) -- PEGs add descriptors to revised structure list		
▷ 1382 (42 files) -- PEGs revised structure list		
▷ 1381 (5 files) -- PPGs add descriptors to revised structure list		
▷ 1380 (37 files) -- PPGs revised structure list		
▽ 1377 (19 files) -- (Li I)4 (Fm-3m) ~ Lithium iodide - alpha (ICSD #414244)_1 SP (VASP)		
CONTCAR	523 B	
EIGENVAL	4.1 kB	
IBZKPT	657 B	
INCAR	590 B	
Job.out	3.8 kB	
Job.xml	1.5 kB	
KPOINTS	46 B	
OSZICAR.out	1.2 kB	
OUTCAR.out	52.1 kB	
POSCAR	310 B	
POTCAR	353.0 kB	
PROCAR	18.6 kB	
VASP.out	1.0 kB	

3991 files in 50 jobs over 542 matching jobs    1 selected files (1.3 kB) More

Open Cancel

## 2.4 Monitor file upload

Once the upload was successfully started the progress is monitored. The upload is complete once the message Upload finished appears in the dialog. To continue working with the *MedeA* GUI click on Close.

File list:

1377/initial.sci

Upload finished.

Progress:

% Total	% Received	% Xferd	Average Speed	Time	Time	Time	Current
			Dload	Upload	Total	Spent	Left
							Speed
1 10588	100	114	0	0	1527	0	1540

Upload      Close