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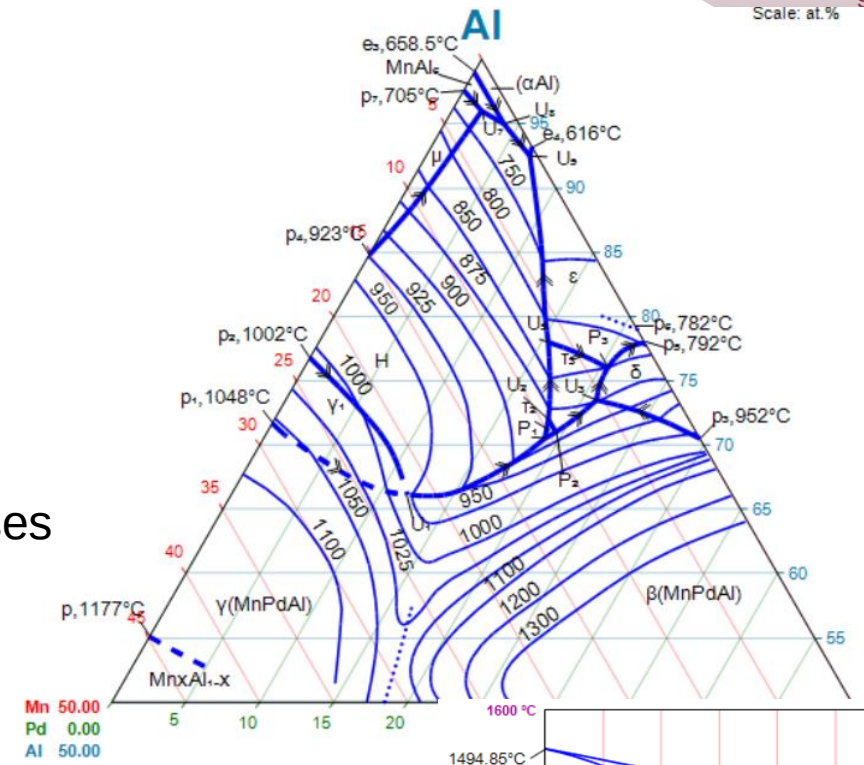
# Different types of data included in Evaluation Reports in MSI Eureka

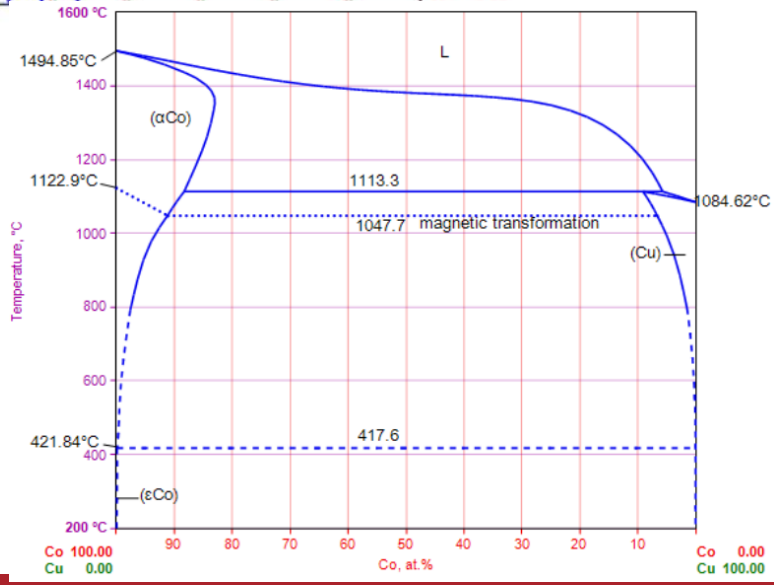
1) Phase Equilibria
2) Crystal Structures
3) Morphology, Reactions
4) Various physical properties, e.g. mechanical, magnetic, kinetics, electrical, amorphous, semi-/superconductivity, interface phenomena, etc.
5) Thermodynamic Properties
6) Electronic Structures
7) Appplications

others

# Phase Equilibria Data

- Literature Data Overview
- Binary Boundary Systems
- Crystallographic Data of Solid Phases
- Quasibinary Systems
- Invariant Equilibria
- Liquidus, Solidus and Solvus Surfaces
- Isothermal Sections
- Temperature - Composition Sections
- Thermodynamics



# Crystal Structure Data

**Table 2: Crystallographic Data of Solid Phases**

| Phase/ Temperature Range (°C) | Pearson Symbol/ Space Group/ Prototype | Lattice Parameters (pm) | Comments/References |
|---|---|---|---|
| (Al)<br>< 660.5 | cF4<br>Fm$\bar{3}$m<br>Cu | a = 404.96<br><br>a = 405.2 | pure Al at 25°C [Mas2]<br>Solubility limits:<br>at 0% Ti, 0.04 at.% Ta [1972Fer],<br>at 0% Ta, 0.8 at.% Ti [2007Wit] or<br>0.6 at.% Ti [1992Kat] |
| β, (βTi,Ta)<br>$Ti_{1-x-y}Ta_xAl_y$<br>< 3020 | cI2<br>Im$\bar{3}$m<br>W | | complete solid solution [Mas2], 0 < x < 1<br>at T = 1440°C, x = 0 to 1 and y = 0 to 0.5 [1993Das];<br>at T = 1350°C, x = 0 to 1 and y = 0 to 0.42 [1995Wea]; |
| (Ta)<br>< 3020<br>(βTi)<br>1670 - 882 | | a = 330.30<br><br>a = 330.65 | |
| $β_0$, $Ti_{1-x-y}Ta_xAl_y$<br>< 1427 | cP2<br>Pm$\bar{3}$m<br>CsCl | - | |
| α, (αTi)<br>$Ti_{1-x-y}Ta_xAl_y$<br>1491 - 1119 and | hP2<br>$P6_3/mmc$<br>Mg | | |

| | | | |
|---|---|---|---|
| σ, CrFe<br>830 - 440 | tP30<br>$P4_2/mnm$<br>CrFe | a = 879.95<br>c = 454.42 | 44.5 to 50.0 at.% Cr [V-C] |
| * ν | $P6_3/m$ | a = 4068.0 ± 0.07<br>c = 1254.6 ± 0.01<br>atoms/cell = 1184.56<br><br>a = 4000<br>c = 1240 | $Cr_{10.71}Fe_{8.68}Al_{80.61}$ single crystal, elicited from ingot after inductive melting followed cooling in sand bath [2000Mo2]. Sometimes called "H-CrFeAl".<br>$Cr_{11}Fe_8Al_{81}$ together with κ-CrFeAl in as-cast $CrFe_2Al_{12}$ alloy [1999Sui] |
| * "κ-CrFeAl" | hexagonal,<br>$κ\text{-}Cr_{18}Ni_6Al_{76}$ | - | In as-cast $CrFe_2Al_{12}$ alloy together with ν [1999Sui] |
| * "O-CrFeAl" | orthorhombic<br>body-centered | a = 1230<br>b = 1240<br>c = 3070 | In as-cast $Cr_{11}Fe_8Al_{81}$ alloy together with $O_1$-CrFeAl and |

**Fig. 1: Lattice parameters of gamma phase as function of composition**

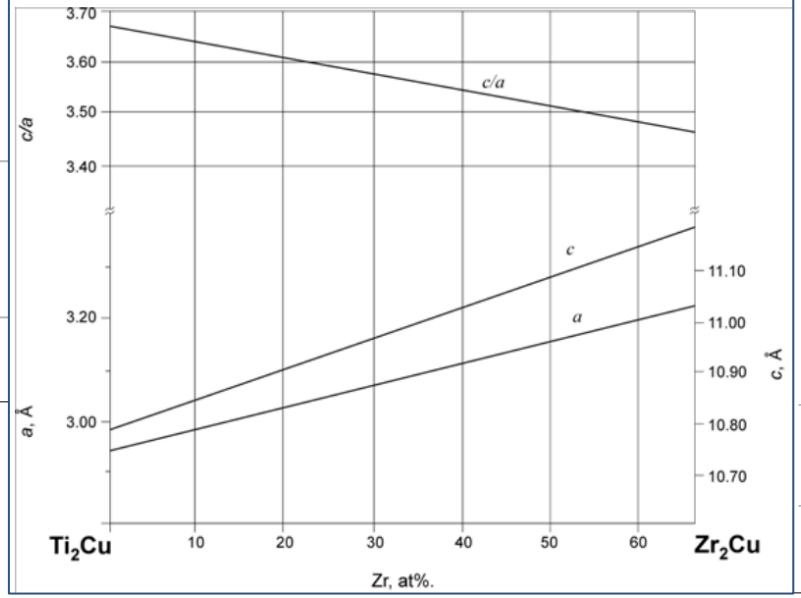



**Table 4: A Classification of Metastable Phases Based on the Crystal System**

| Phase Designation | Crystal System | Composition (mass%) Fe | Al | Si | Lattice Parameters (pm) | References |
|---|---|---|---|---|---|---|
| $μ_1$ | Cubic | 25.4 | 49.1 | 25.5 | - | [1937Ser] |
| | | 31.9 | 62.5 | 5.6 | a = 1254.83 | [1950Phr] |
| | | 27.3 | 65.7 | 7.0 | a = 1254.83 | [1952Arm] [1955Arm] |
| | | - | - | - | a = 1254.53 | [1954Spi] |
| | | 30.2-32.8 | 58.1-60.0 | 7.2-11.7 | a = 1254.8 | [1955Obi] |
| | | 31.9 | 61.7 | 6.4 | a = 1256 | [1967Coo] |
| | | - | - | - | a = 1250 to 1270 | [1967Mun] |
| | | 31.1 | 60.8 | 8.1 | a = 1250 ± 10 | [1967Sun] |
| | | - | - | - | a = 1260.0 | [1977Sim] |
| | | 29.2-30.7 | 61.0-64.2 | 5.1-9.8 | a = 1250 | [1985Don1] |
| | | 25.0 | 69.7 | 5.3 | a = 1256 | [1986Liu1] [1986Liu2] [1987Liu] |
| | | - | - | - | a = 1256 | [1987Tur] |
| | | - | - | - | a = 1250 | [1988Ben2] |
| | | | | | a = 1250 | [1996Mul] |
| | | | | | a = 1256 | [2004Kra] [2005Kra] [2006Kra] |
| $μ_2$ | Tetragonal | - | - | - | a = 495.0<br>c = 707.0 | [1951Now] |
| | | - | - | - | a = 1260.0<br>c = 3720.0 | [1982Wes] |
| $μ_3$ | Orthorhombic | - | - | - | a = 609.0<br>b = 996.0<br>c = 374.0 | [1936Jae] |
| | | 29.2 | 59.5 | 11.3 | a = 4360.0 | [1952Arm] |

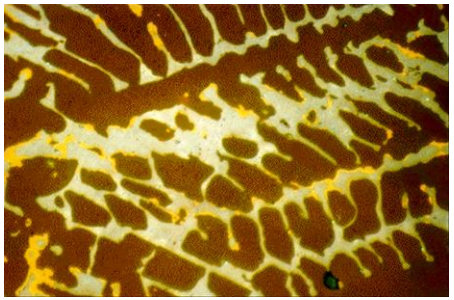
# Reactions, Morphology & Applications

**Table 3: Invariant Four-Phase Equilibria**

| Reaction | T (°C) | Type | Phase | Composition (at.%) | | |
|---|---|---|---|---|---|---|
| | | | | Cu | Zr | Ti |
| $L + TiCu \leftrightarrow Ti_3Cu_4 + Zr_{14}Cu_{51}$ | 882 | $U_1$ | L | 64.5 | 6.8 | 28.7 |
| | | | TiCu | 51.3 | 0 | 48.7 |
| | | | $Ti_3Cu_4$ | 57.1 | 0 | 42.9 |
| | | | $Zr_{14}Cu_{51}$ | 78.5 | 21.5 | 0 |
| $L + Ti_3Cu_4 + TiCu_2 \leftrightarrow Ti_2Cu_3$ | 874 | $D_1$(P) | L | 73.4 | 25.2 | 1.4 |
| | | | $Ti_3Cu_4$ | 57.1 | 0 | 42.9 |
| | | | $TiCu_2$ | 66.7 | 0 | 33.3 |
| | | | $Ti_2Cu_3$ | 60.0 | 0 | 40.0 |
| $L + TiCu_2 \leftrightarrow TiCu_4 + Ti_2Cu_3$ | 869 | $D_2$(U) | L | 73.7 | 2.0 | 24.3 |
| | | | $TiCu_2$ | 66.7 | 0 | 33.3 |
| | | | $TiCu_4$ | 78.7 | 0 | 21.3 |
| | | | $Ti_2Cu_3$ | | | |
| $L + (Cu) \leftrightarrow TiCu_4 + ZrCu_5$ | 863 | $U_2$ | L | | | |
| | | | (Cu) | | | |
| | | | $TiCu_4$ | | | |
| | | | $ZrCu_5$ | | | |
| $L + Zr_{14}Cu_{51} \leftrightarrow Zr_3Cu_8 + \tau_1$ | 861 | $U_3$ | L | | | |
| | | | $Zr_{14}Cu_5$ | | | |
| | | | $Zr_3Cu_8$ | | | |
| | | | $\tau_1$ | | | |
| $L + \gamma \leftrightarrow \tau_1 + TiCu$ | 856 | $U_4$ | L | | | |
| | | | γ | | | |

**Table 10: Key Phenomena that Control Fuel Performance**

| Phenomena | Experimental Observations | Consequences |
|---|---|---|
| Fuel swelling | irradiation growth and grain boundary tearing;<br>Xe/Kr bubble growth;<br>solid fission product accumulation;<br>alloy and burnup rate effects | reactivity loss;<br>rate of gas release;<br>fiel/clad interaction stresses;<br>thermal conductivity loss |
| Fuel constituent migration | U/Zr interdiffusion;<br>critical Pu threshold | lowered solidus;<br>complexities of properties modeling |
| Fuel/cladding chemical interaction | penetration into cladding by U, Pu, and lanthanide series fission products;<br>diffusion of cladding constituents into fuel;<br>extensive nickel loss in austenitics | cladding wall thinning;<br>ductility degradation of interaction layer in cladding;<br>eutectic composition approached in fuel |
| Cladding deformation | irradiation/thermal creep by fission gas pressure loading; | stress-rupture lifetime determines ultimate burnup achieved; |



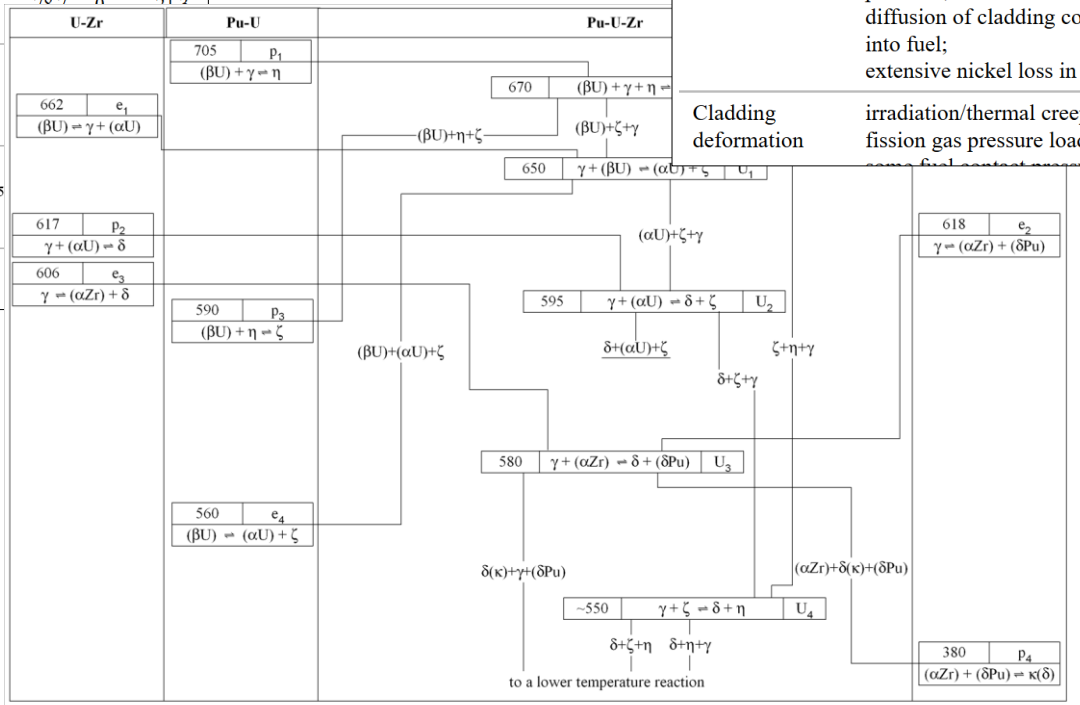
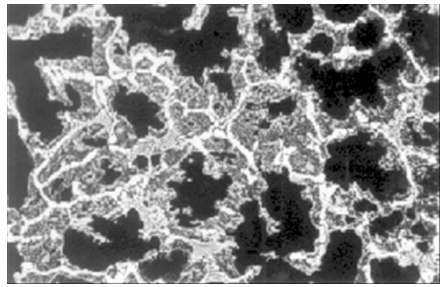



Fig. 1: **Pu-U-Zr.** Partial reaction scheme



# Physical Properties

**Fig. 9: Magnetic phase diagram of polycrystalline sample of NaFeO2**

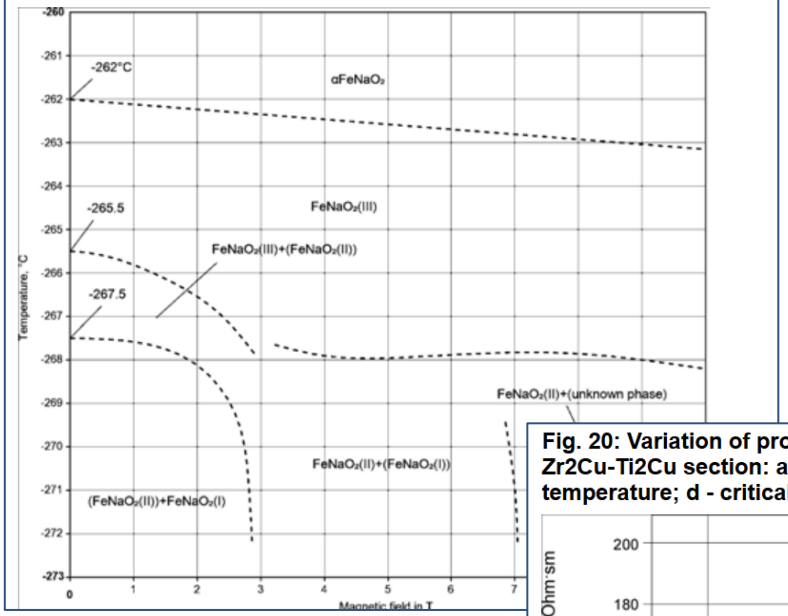



**Fig. 20: Variation of properties of amorphous alloys with compositio Zr2Cu-Ti2Cu section: a - electroresistance; b - microhardness; c - en temperature; d - critical thickness of amorphous alloys**

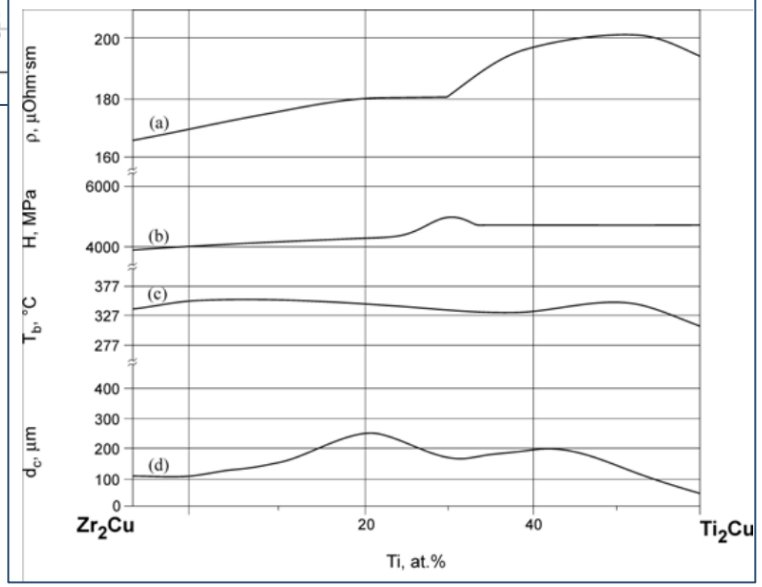
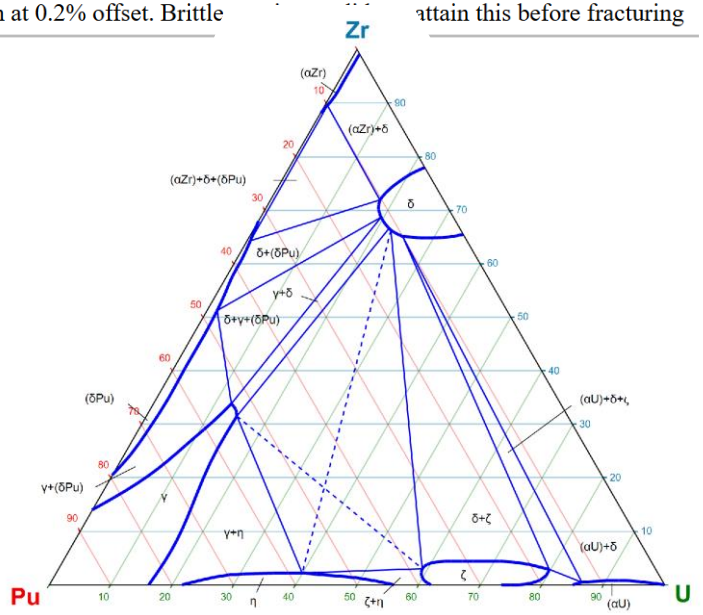



**Table 8: Variations of Tensile Properties with Temperature in Homogenized a Plutonium-Zirconium Alloys**

| Alloy, at.% | T (°C) | Tensile strength | | Yong's modulus (E) (GPa) | Type failure |
|---|---|---|---|---|---|
| | | Ultimate (MPa) | Yield** (MPa) | | |
| U-9.5Pu-14.4Zr | 25 | 177.56 | | 170.69 | Brittle |
| | 675 | 11.77 | 10.79 | 13.73 | Ductile |
| U-14.2Pu-14.5Zr | 25 | 39.24 | | 103.99 | Brittle |
| | 675 | 11.77 | 10.79 | 15.70 | Ductile |
| U-14.4Pu-29.5Zr | 25 | 75.54 | | 127.53 | Brittle |
| | 675 | 28.45 | 27.47 | 18.64 | Ductile |

* All specimens were tested in creep prior the tensile tests and therefore contain (<5%) hot work.

strength at 0.2% offset. Brittle attain this before fracturing



# Thermodynamic Data

**Table 4: Heat Treatment Schedule for Different Alloys by [1958Chu]**

| Alloys with > 50 mass% Fe | | Alloys with > 10 mass% Al | |
|---|---|---|---|
| Temperature (°C) | Time (h) | Temperature (°C) | Time (h) |
| 750 | 720 | 900 | 100 |
| 700 | 1000 | 750 | 200 |
| 650 | 720 | 700 | 500 |
| 600 | 720 | 650 | 250 |
| 500 | 2000 | 600 | 250 |
| 480 | 2200 | 500 | 1200 |

**Table 5: Partial Pressures of Cr, Fe and Al over the Alloy Cr-75.4Fe-4 Measurements &Dgr;T [1992Hil]. Errors of A and B Values are Stand Overall Errors**

| Gaseous species i | $p_i$ (Pa) at 1500 K | ΔT (K) | $\ln p_i = -A \cdot 10^4/T+B$ |
|---|---|---|---|
| Cr | $1.6 \cdot 10^{-2} \pm 14$ % | 1313 | |
| Fe | $7.5 \cdot 10^{-3} \pm 15$ % | 1313 | |
| Al | $4.5 \cdot 10^{-3} \pm 43$ % | 1313 | |

**Table 6: Chemical Activities $a_i$, I in the Alloy Cr-75.4Fe-4.8Al (ma**

| Alloy Component i | $a_i$ (at 1500 K |
|---|---|
| Cr | 0.28 ± 0.04 |
| Fe | 0.50 ± 0.07 |

**Table 4: Thermodynamic Data of Reaction or Transformation**

| Reaction or Transformation | T (°C) | Quantity, per mol of compound ($kJ \cdot mol^{-1}$) | Comments |
|---|---|---|---|
| L → InSb | 525.7 | $\Delta_{cr}H = 47.0 \pm 6.1$ | quantitative differential thermal analysis, [1988Evg] |
| L → xInSb + (1-x)InBi | $T_L$-$T_S$ | $\Delta_{cr}H = 56.4 \pm 7.3$ | x = 0.99 |
| | $T_L$-$T_S$ | $\Delta_{cr}H = 37.8 \pm 4.9$ | x = 0.95 |
| | $T_L$-$T_S$ | $\Delta_{cr}H = 38.8 \pm 5.0$ | x = 0.80 |
| | $T_L$-$T_S$ | $\Delta_{cr}H = 26.2 \pm 3.4$ | x = 0.60 |
| | $T_L$-$T_S$ | $\Delta_{cr}H = 22.5 \pm 2.9$ | x = 0.38 |
| | $T_L$-$T_S$ | $\Delta_{cr}H = 31.2 \pm 4.0$ | x = 0.20 |
| | $T_L$-$T_S$ | $\Delta_{cr}H = 31.4 \pm 4.1$ | x = 0.05 |
| | $T_e$ = 110 | $\Delta_{cr}H = 10.0 \pm 1.3$ | Eutectic |
| L → xInSb + (1-x)$In_2Bi$ | $T_L$-$T_S$ | $\Delta_{cr}H = 37.8 \pm 4.9$ | x = 0.95 |
| | $T_L$-$T_S$ | $\Delta_{cr}H = 38.8$ | |
| | $T_L$-$T_S$ | $\Delta_{cr}H = 26.2$ | |

**Fig. 29: Enthalpy of mixing in the Fe2O3-Al2O3 solid solution. The da miscibility gap**

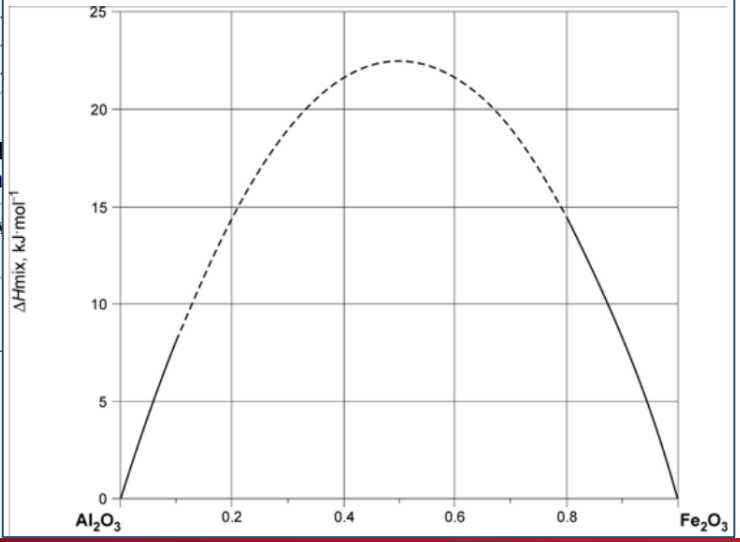
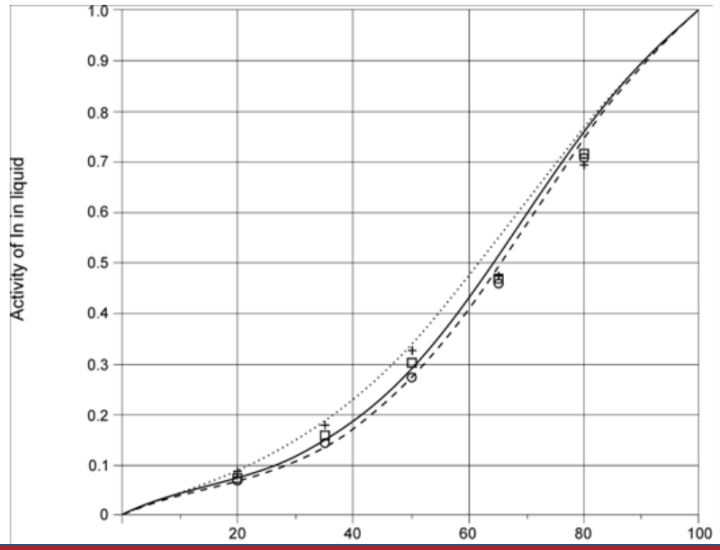



**Fig. 15: Activity of In in liquid alloys at 727°C along sections with results [1997Kam] (crosses - In-Bi0.8Sb0.2, squares - InBi0.5Sb0. [2002Cui] (dots - In-Bi0.8Sb0.2, solid - In-Bi0.5Sb0.5, dashed - In-B**



# Electronic Structure

**Fig. 19a: Composition dependence of the band gap EG at 0 (a), 77 (**

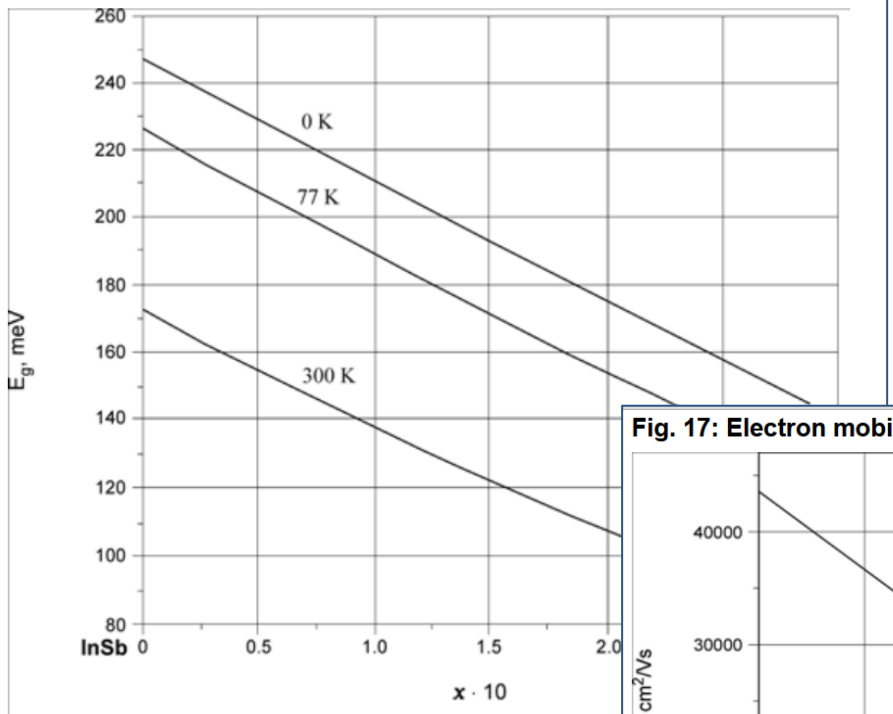



**Fig. 16: Electron concentration of InSb1-xBix vs Bi concentration**

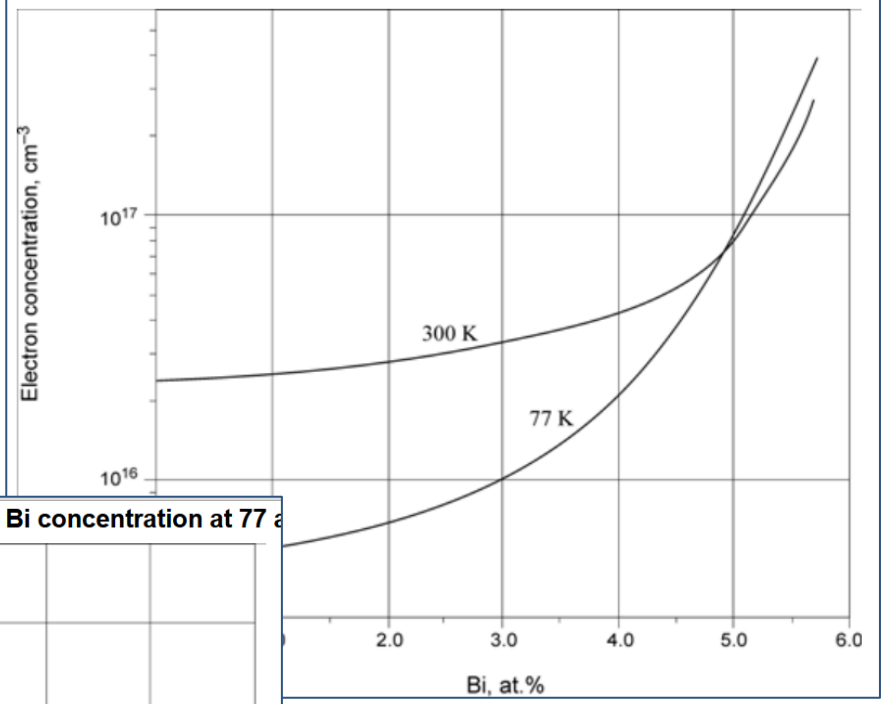
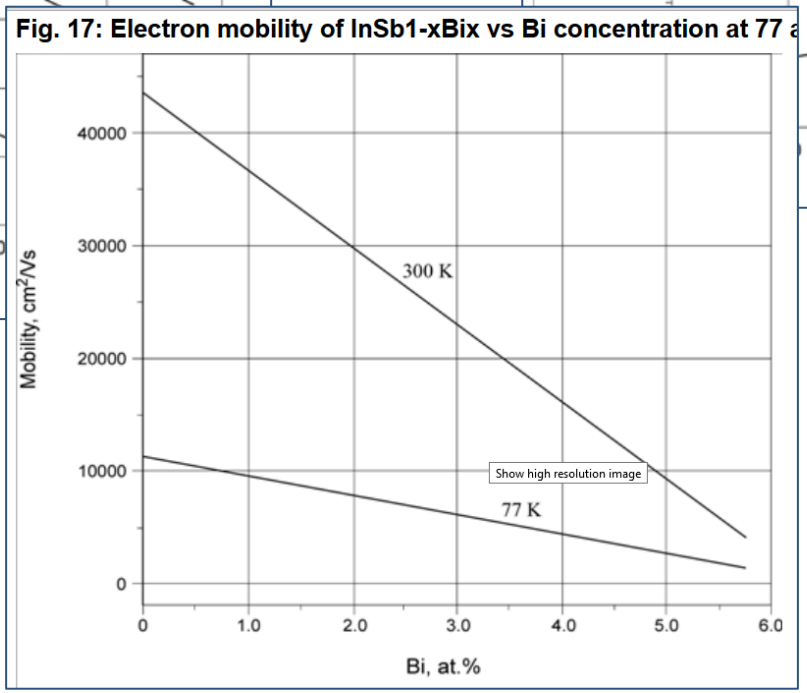
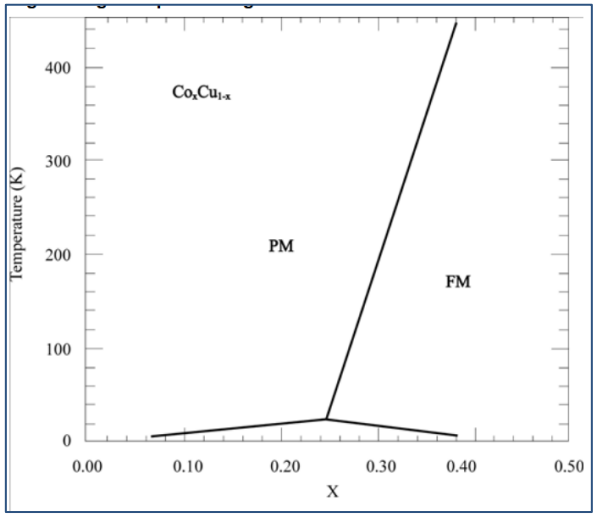



**Fig. 17: Electron mobility of InSb1-xBix vs Bi concentration at 77 a**

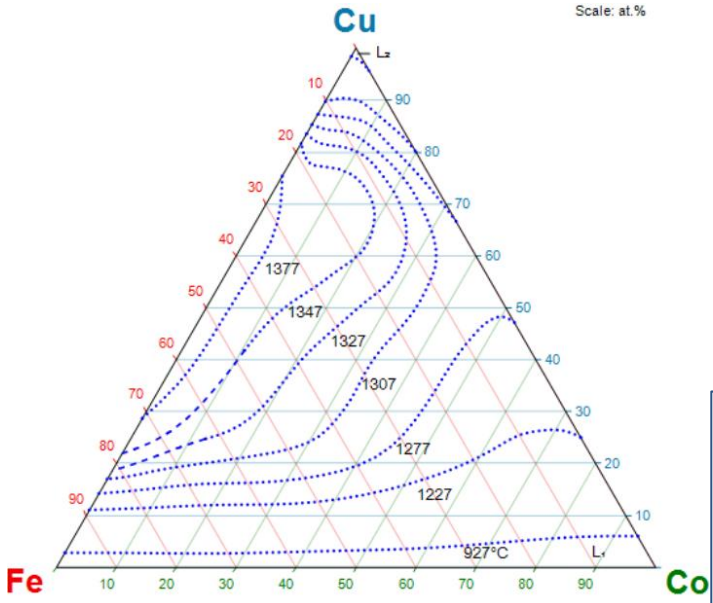


# Other types of phase diagrams

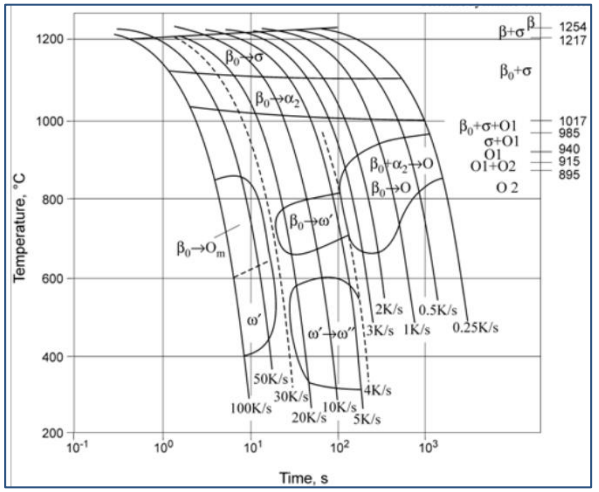
## Magnetic Phase Diagrams



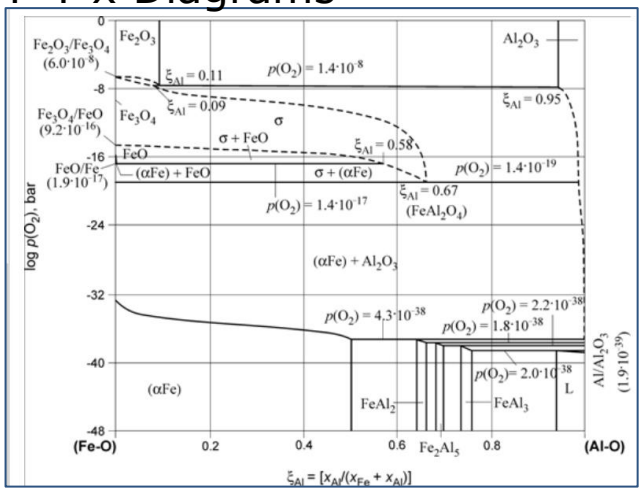

## Metastable Diagrams



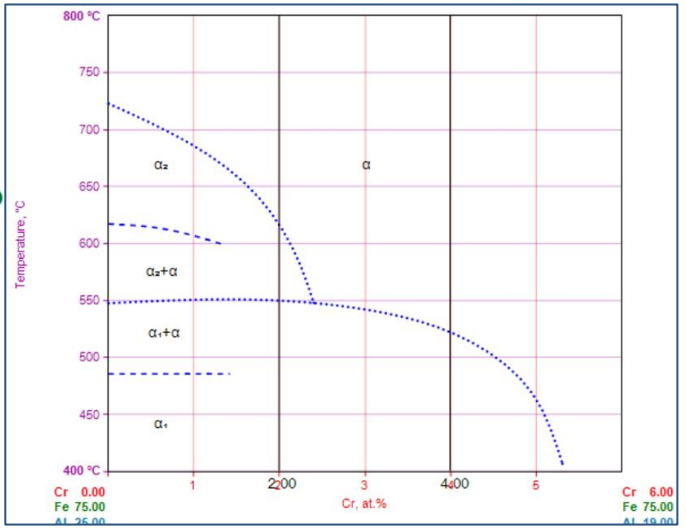

## CCT & TTT Diagrams




## P-T-x Diagrams




## Order-Disorder Diagrams



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# Direct Answers from the Phase Diagrams in MSI Eureka

Example case studies for the following areas of materials research

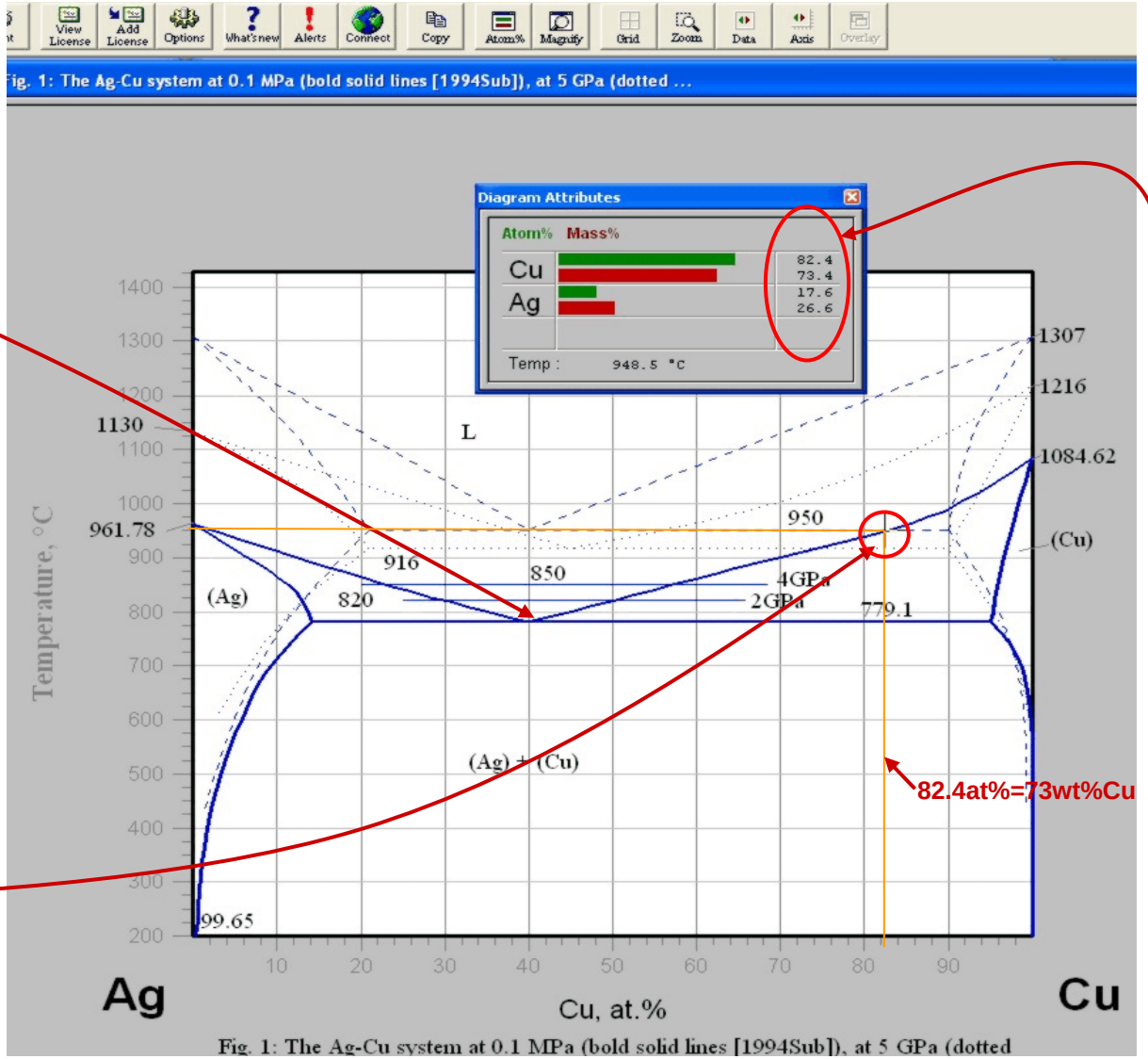
1) Brazing
2) Brazing & Solidification
3) Materials Compatibility
4) Solidification

# Area: Brazing

## CASE 1: Brazing Cu-parts with a eutectic braze alloy

QUESTION:
Brazing at 950°C; does the braze material change significantly its composition during brazing of Cu-parts with a eutectic Ag-28wt%Cu braze material. How much Cu can dissolve in the melt at 950°C ?

ANSWER:
FROM Ag-Cu, Fig. 1
The melt can pick up about 73 wt.% Cu at ambient pressure.



## Area: Brazing/Solidification

**CASE 2: 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

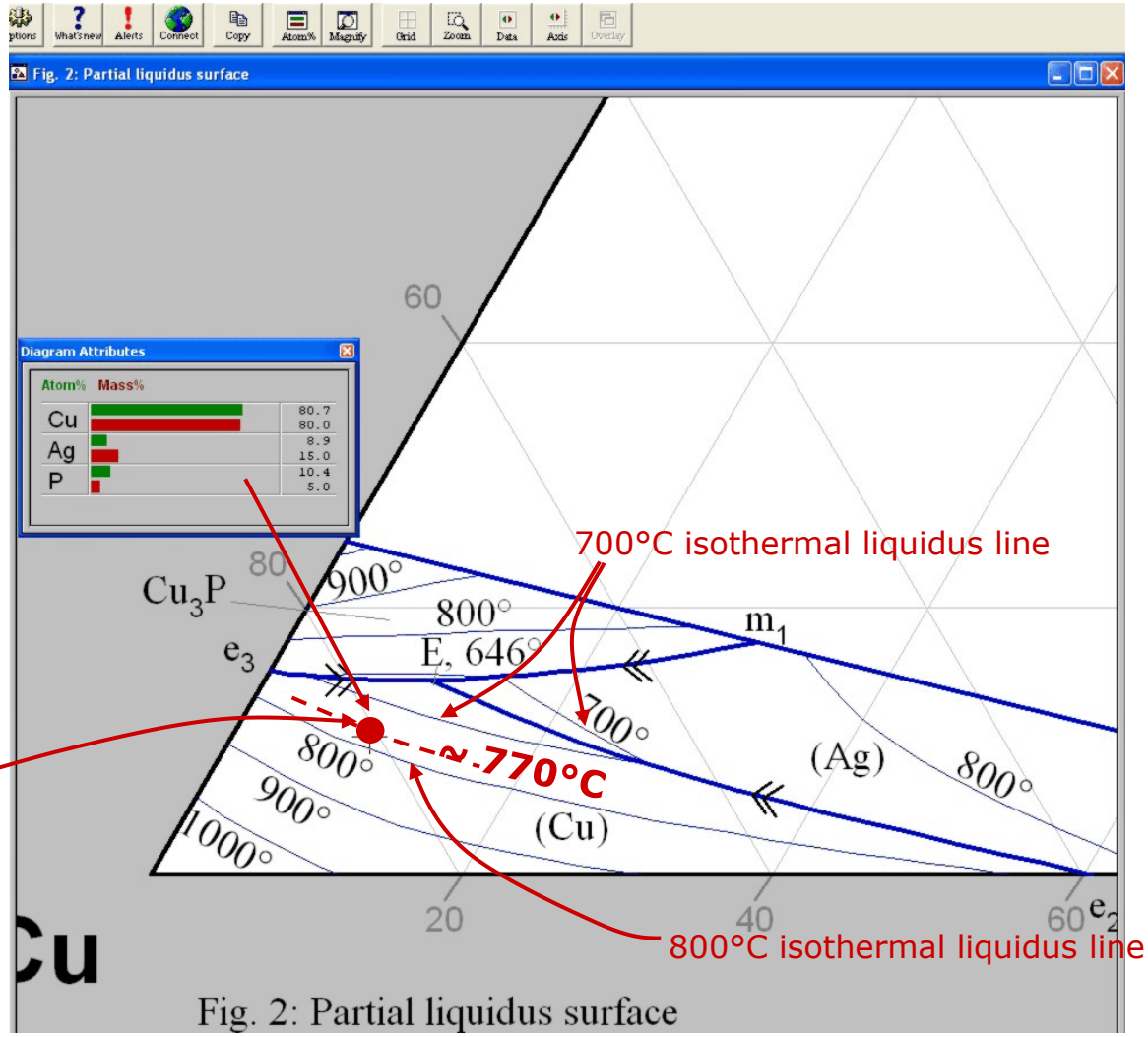



Fig. 2: Partial liquidus surface

# Area: Brazing/Solidification

## CASE 2: 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

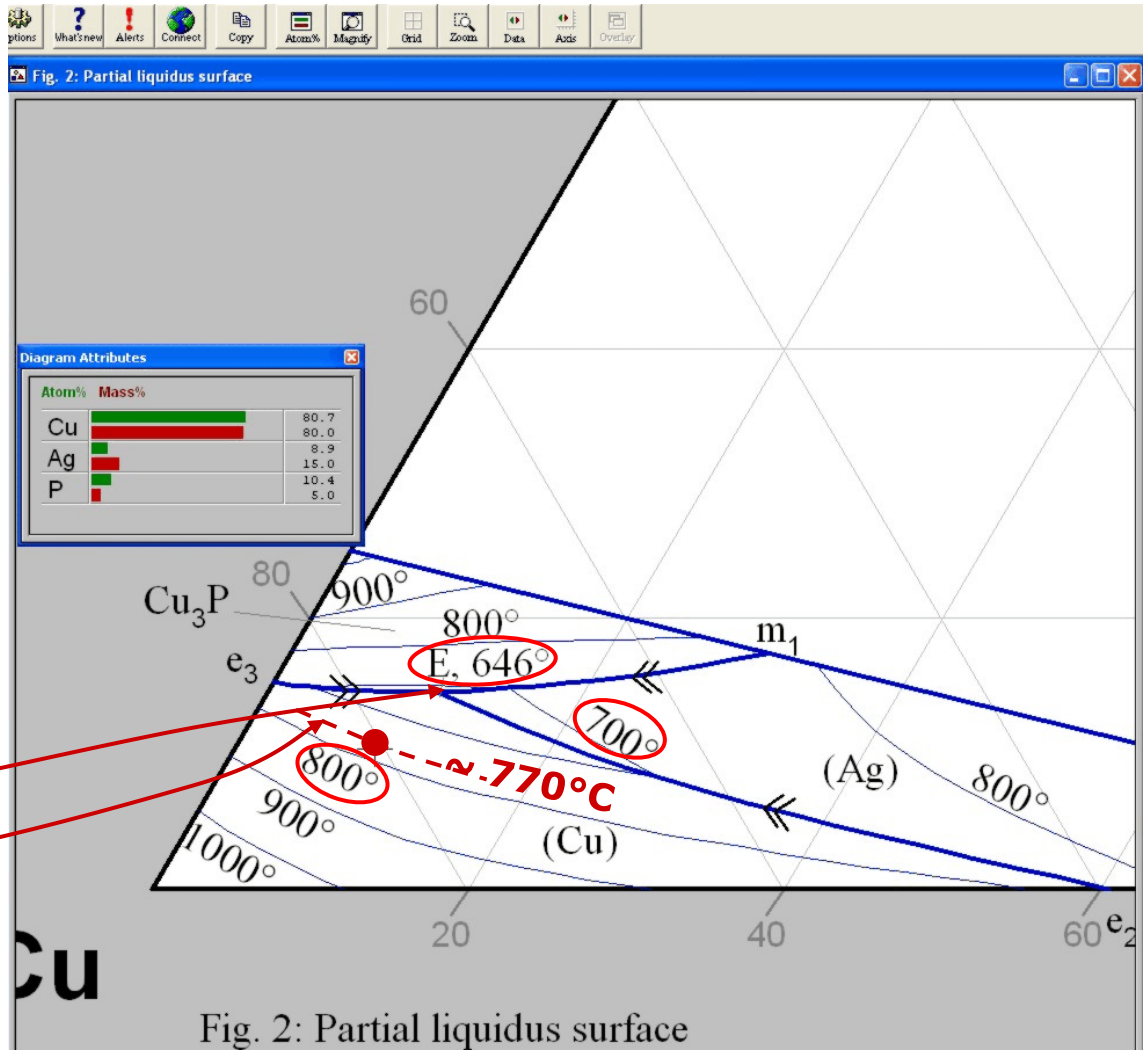



Fig. 2: Partial liquidus surface

# Area: Brazing/Solidification

## CASE 2: 2nd answer was favourable, case continued:

QUESTION (**3**)
Materials costs: Can silver be substituted by copper, still staying in favorable melting conditions? How much?

ANSWER (**3**):
FROM Ag-Cu-P, Fig. 2:
Yellow area: concentration area for alloys having the same melting interval, but lower Ag contents /costs

**Overall conclusion: promising material. Now check engineering properties, wettability, etc.**

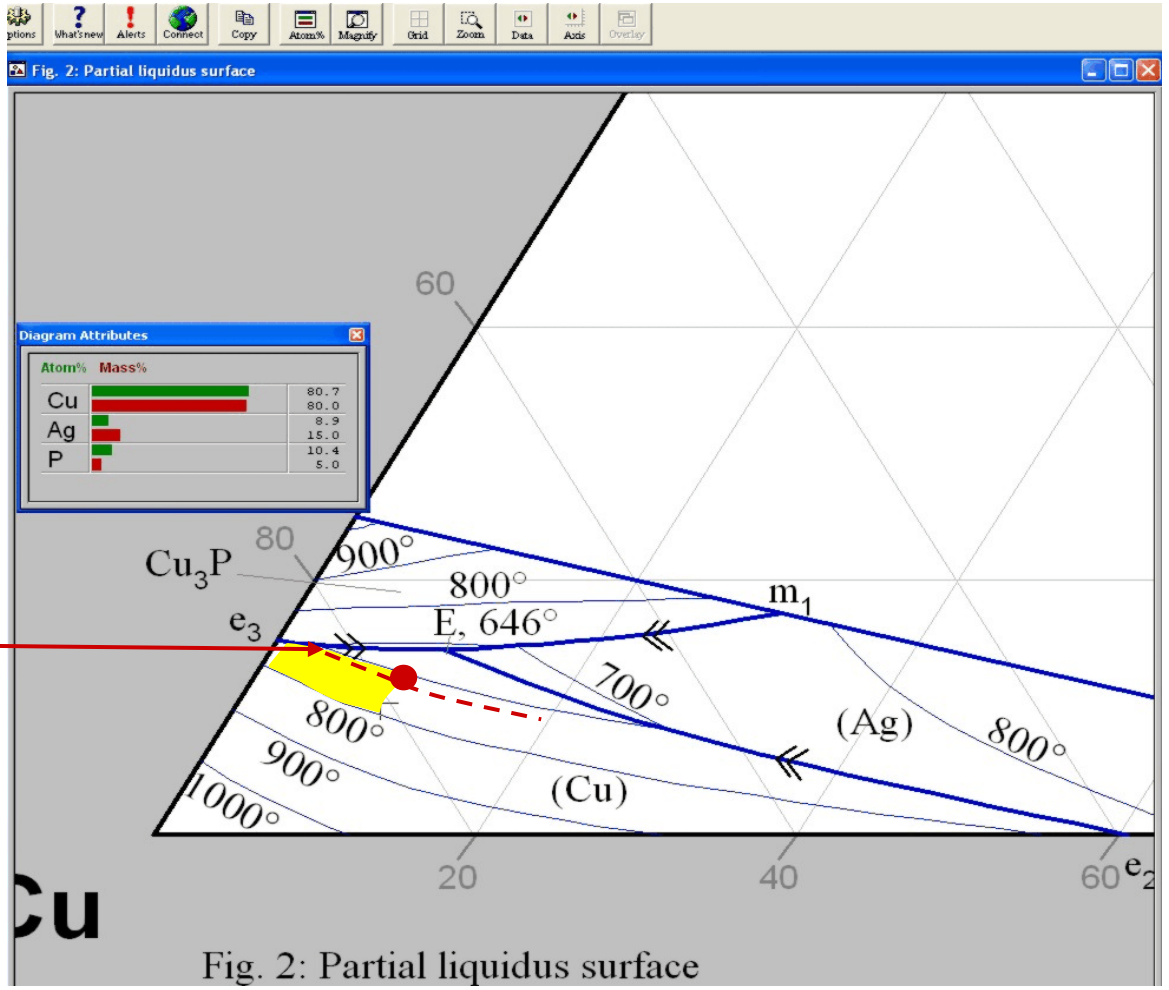


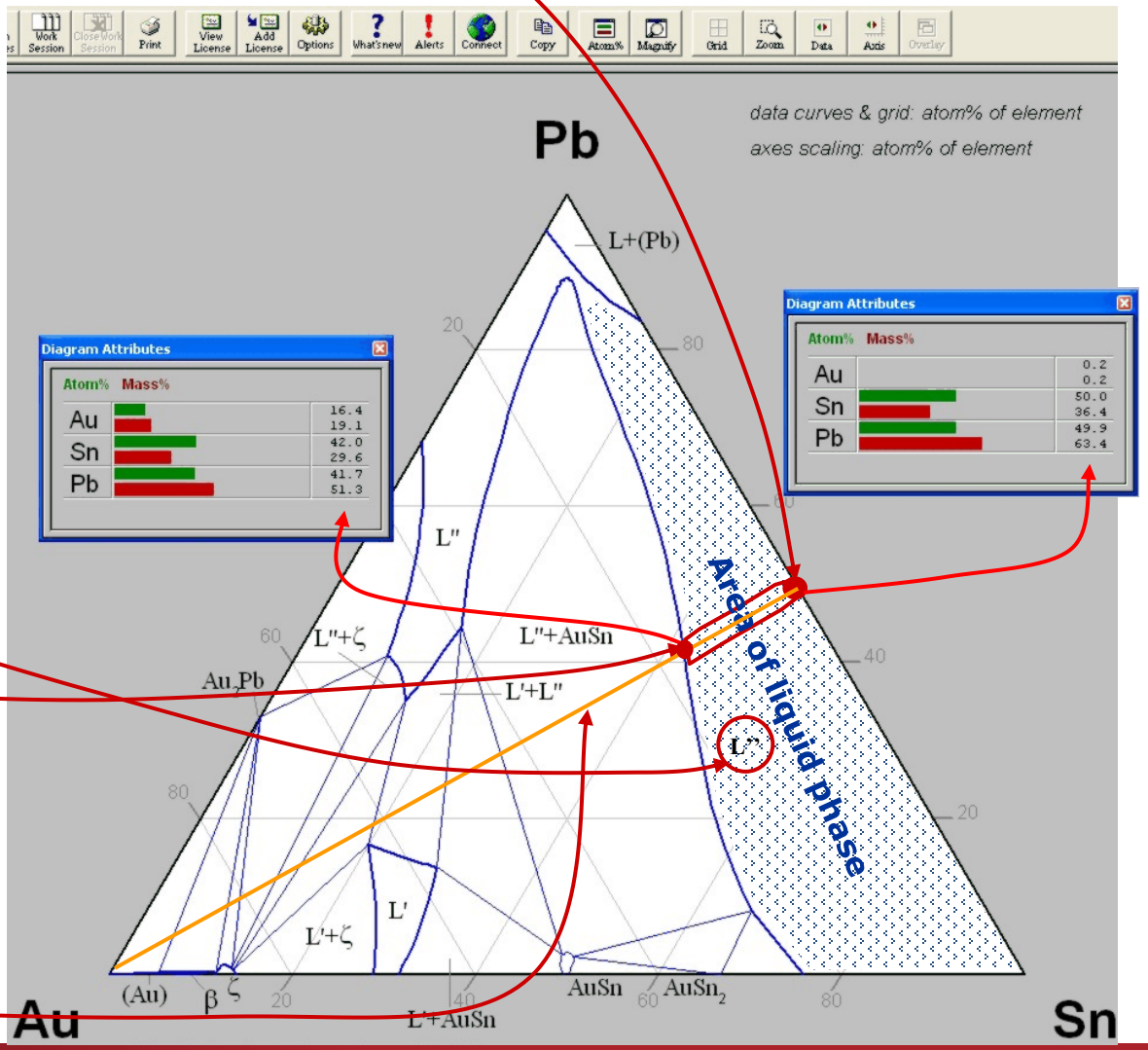
Fig. 2: Partial liquidus surface

# Area: Materials compatibility

**CASE 3: Gold coated contacts in electronic devices are to be soldered. Suggested solder material: Sn50-Pb50.**

QUESTION:
Is the gold barrier inert against the attack of a Sn50-Pb50 alloy at 300°C?

ANSWER:
From Au-Pb-Sn, Fig. 9:
No, the alloy is liquid and dissolves Au along the yellow line, up to 19 wt.% Au before an intermetallic layer of AuSn starts forming at the interface.



# Area: Materials compatibility

## CASE 4: Laboratory work, in the course of research Ni50Al50 alloys should be molten

QUESTION:
Could a graphite crucible be used to melt a NiAl alloy with 50 at.% Al ?

ANSWER:
From Al-C-Ni, Fig. 1:
Yes, it is possible to melt Ni50Al50 in graphite, but at least 3 wt.% C (10 at.% C) will dissolve in the melt.
Attention:
the further studies are not on an NiAl alloy anymore
but on a Ni-Al-C alloy.

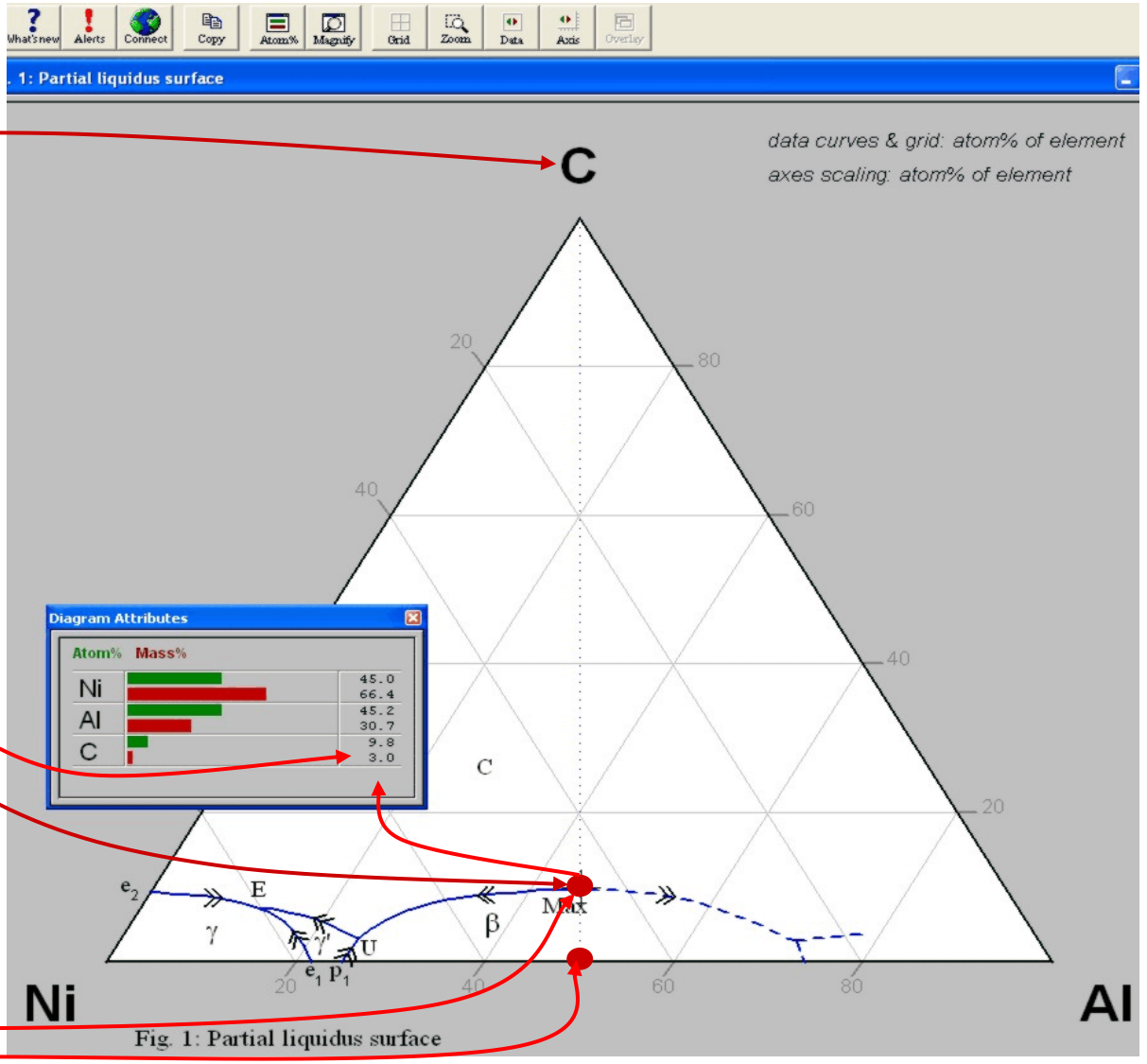


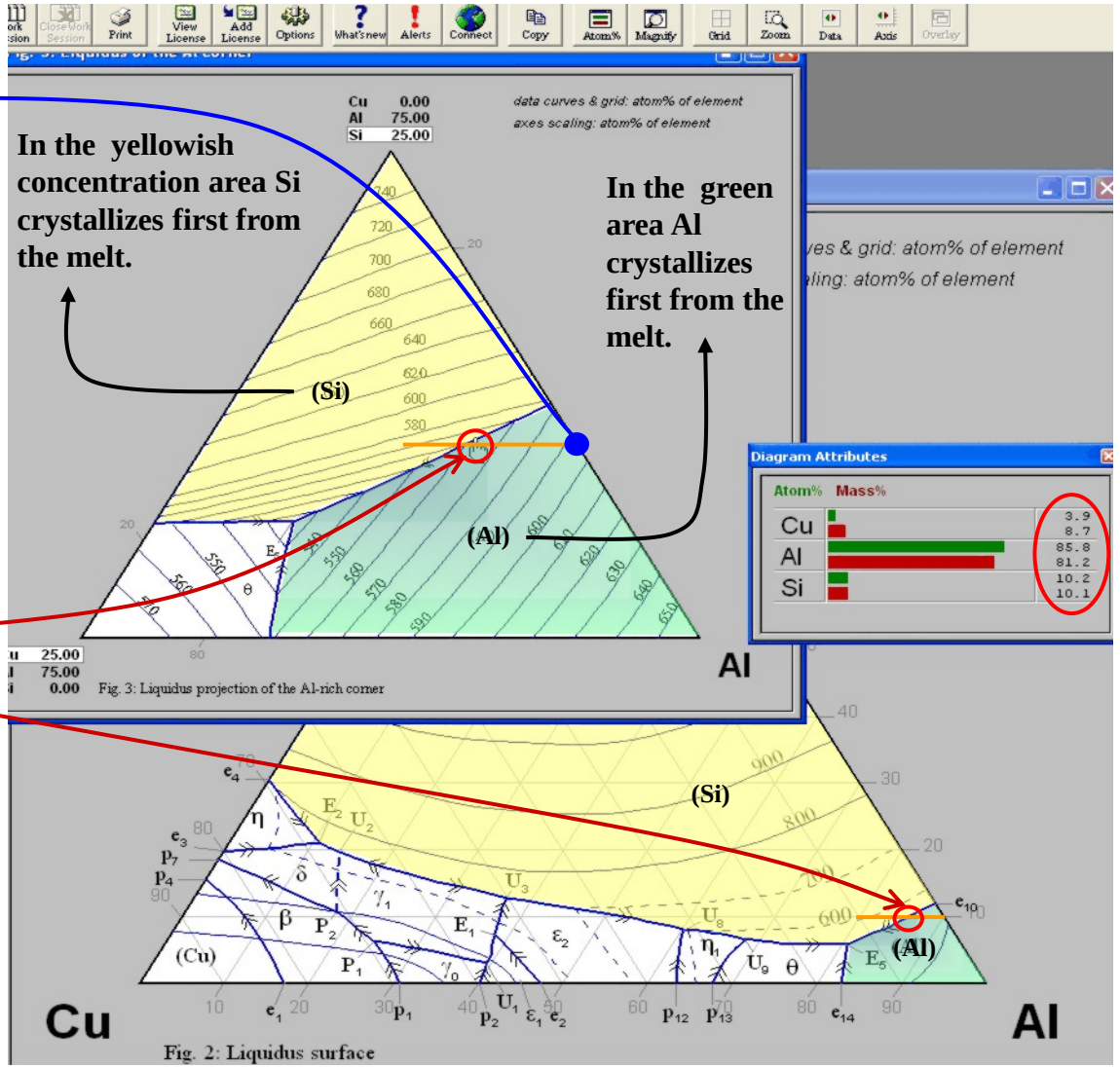
Fig. 1: Partial liquidus surface

# Area: Solidification

**CASE 5: In photolithographic processing our Al-Cu-Si alloys corrode.**
**To reduce the corrosion, we need Silicon to precipitate primarily.**

QUESTION:
In a Al90-10Si (wt.%) alloy, how much Al can be substituted by Cu before the primary solidification switches from Al to Si crystals ?

ANSWER:
From Al-Cu-Si, Figs. 2&3:
Al81-Cu9-Si10
is the critical alloy; at that composition, having a liquidus temperature of 560°C, Silicon will crystallize from the melt



# What information can one get from a phase diagram?

Phase diagrams are usually representations of a system A–B(– C…) which show the equilibrium phases and the phase equilibria among them in dependence of the two state variables T and $x_B$ at p = 1 bar.

<u>A phase diagram shows:</u>

- Which phases exist
- Homogeneity ranges of the phases
- Phase equilibria at given T or $x_B$
- Melting (solidus) temperature at $x_B$
- Melting behaviour of phases
- Compositions of coexisting phases
- Phase fractions (volume fractions)
- Type and T of invariant reactions
- Cooling/Heating path

<u>More information from phase diagrams:</u>

- Many properties scale with the melting temperature $T_m$
- Hints for the synthesis of specific phases or alloys
- Alloy development strategies (compositions, cooling rates, microstructures)
- Processing of the alloys (thermomechanical, heat treatment)

Source: MSIT Winter School, Dr. Martin Palm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