REFERENCES

Science and Design of Engineering Materials
James P. Schaffer, Ashok Saxena,
Thomas H. Sanders, Stephen D. Antolovich,
Steven B. Warner

Materials Science and Engineering: An Introduction
by William D. Jr. Callister
Phases in Metallic Alloys and Use of Phase Diagrams
Processing

Properties

Microstructure

Performance
OUTLINE

• What is a phase?
  • Basis of phase diagrams
  • What do phase diagrams tell us?
    - how do you use them?
    - equilibrium versus non-equilibrium
  • Complete Solid Solubility Systems
  • Systems with no complete solid solubility
  • Invariant transformations
    - eutectic; peritectic; eutectoid
  • Examples - uses of phase diagrams
    - Pb-Sn system
    - Fe-C system
• Modern navigation tools
Pb-Sn system
When we combine two elements...

- In particular, if we specify...
  --a composition (e.g., wt%Cu - wt%Ni), and
  --a temperature (T)

then...

How many phases do we get?
What is the composition of each phase?
How much of each phase do we get?

Phase A
- Nickel atom
  - Copper atom

Phase B
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**THE SOLUBILITY LIMIT**

- **Solubility Limit:**
  Max concentration for which only a solution occurs.

- **Ex: Phase Diagram:**
  Water-Sugar System

  Question: What is the solubility limit at 20°C?
  Answer: 65wt% sugar.
  If $C_0 < 65$wt% sugar: sugar
  If $C_0 > 65$wt% sugar: syrup + sugar.

- **Solubility limit increases with $T$:**
  e.g., if $T = 100°C$, solubility limit = 80wt% sugar.
COMPONENTS AND PHASES

- **Components:**
  The elements or compounds which are mixed initially (e.g., Al and Cu)

- **Phases:**
  The physically and chemically distinct material regions that result (e.g., \( \alpha \) and \( \beta \)).

Aluminum-Copper Alloy

Adapted from Fig. 9.0, Callister 3e.
**EFFECT OF T & COMPOSITION (C₀)**

- Changing T can change # of phases: path A to B.
- Changing C₀ can change # of phases: path B to D.

**Water-sugar system**

![Graph showing the effect of temperature and composition on phase changes in a water-sugar system.](image)

- **A(70,20)**: 2 phases
- **B(100,70)**: 1 phase
- **D(100,90)**: 2 phases

**L** (liquid solution, i.e., syrup) + **S** (solid sugar)
• Tell us about phases as function of T, C₀, P.
• For practical considerations, P=1atm
  --binary systems: just 2 components.
  --independent variables: T and C₀ (P = 1atm is always used).

 PHASE DIAGRAMS

• Phase Diagram for Cu-Ni system

  2 phases:
  L (liquid)
  α (FCC solid solution)

  3 phase fields:
  L
  L + α

T(°C)

0 1000 1100 1200 1300 1400 1500 1600

wt% Ni

0 20 40 60 80 100
**PHASE DIAGRAMS: # and types of phases**

- **Rule 1**: If we know T and Co, then we know:
  -- the # and types of phases present.

- **Examples:**
  
  A(1100, 60):
  1 phase: $\alpha$

  B(1250, 35):
  2 phases: L + $\alpha$
• Rule 2: If we know \( T \) and \( C_0 \), then we know:
  --the composition of each phase.

• Examples:
  \( C_0 = 35\text{wt\% Ni} \)
  
  At \( T_A \):
  Only Liquid (L)
  \( C_L = C_0 \ ( = 35\text{wt\% Ni}) \)
  
  At \( T_D \):
  Only Solid (\( \alpha \))
  \( C_\alpha = C_0 \ ( = 35\text{wt\% Ni}) \)
  
  At \( T_B \):
  Both \( \alpha \) and L
  \( C_L = C_{\text{liquidus}} \ ( = 32\text{wt\% Ni here}) \)
  \( C_\alpha = C_{\text{solidus}} \ ( = 43\text{wt\% Ni here}) \)
**PHASE DIAGRAMS:** weight fractions of phases

- **Rule 3:** If we know T and C₀, then we know:
  - the amount of each phase (given in wt%).

- **Examples:**
  
  \[ C₀ = 35\text{wt\%Ni} \]

  - **At \( TA \): Only Liquid (L)**
    
    \[ W_L = 100\text{wt\%}, \ W_\alpha = 0 \]

  - **At \( TD \): Only Solid (\( \alpha \))**
    
    \[ W_L = 0, \ W_\alpha = 100\text{wt\%} \]

  - **At \( TB \): Both \( \alpha \) and L**

  \[
  W_L = \frac{S}{R + S} = \frac{43 - 35}{43 - 32} = 73\text{wt\%}
  
  W_\alpha = \frac{R}{R + S} = 27\text{wt\%}
  \]
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EX: COOLING IN A Cu-Ni BINARY

- Phase diagram: Cu-Ni system.
- System is:
  - **binary** i.e., 2 components: Cu and Ni.
  - **isomorphous** i.e., complete solubility of one component in another; α phase field extends from 0 to 100wt% Ni.
- Consider \( C_0 = 35\text{wt\%Ni} \).
• $C_\alpha$ changes as we solidify.
• Cu-Ni case: First $\alpha$ to solidify has $C_\alpha = 46\text{wt}\%\text{Ni}$.
  Last $\alpha$ to solidify has $C_\alpha = 35\text{wt}\%\text{Ni}$.
• Fast rate of cooling: Cored structure
• Slow rate of cooling: Equilibrium structure
Partitioning & Conservation of Mass

\[ k = \text{partition coefficient} = \frac{C_S}{C_L} \]

\[
\begin{align*}
&f_S' \cdot C_{S1} + f_L' \cdot C_{L1} = C_0 \\
&f_S^2 \cdot C_{S2} + f_L^2 \cdot C_{L2} = C_0 \\
&f_S^3 \cdot C_{S3} + f_L^3 \cdot C_{L3} = C_0 \\
&f_S^4 \cdot C_{S4} + f_L^4 \cdot C_{L4} = C_0
\end{align*}
\]
Mushy (Multi-Phase) Region

FIGURE 5-13
Schematic diagram of dendrite structure in Al–4.5% Cu alloy at (a) 50 percent solid and (b) 90 percent solid. (From Singh et al.)

20
region of interest
FIGURE 3-10
Solute distribution in low-alloy steel along path A-n as determined by electron microprobe. (Magnification x 55.) (From Kattamis and Flemings.7)
PRIMARY ARMS : $DAS = a t_f^{0.38}$

SECONDARY ARMS : $DAS = a t_f^{0.33}$

$DAS = a t_f^{1/2}$ to $1/3$

$DAS = a(G.R)^{-1/3}$ to $-1/2$
MECHANICAL PROPERTIES: Cu-Ni System

- Effect of solid solution strengthening on:
  - Tensile strength (TS)
  - Ductility (%EL, %AR)

---

**Tensile Strength (MPa)**

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<thead>
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<th>Composition, wt%Ni</th>
<th>TS for pure Cu</th>
<th>TS for pure Ni</th>
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<td>Cu</td>
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<tr>
<td>Ni</td>
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**Elongation (%EL)**

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<th>Composition, wt%Ni</th>
<th>%EL for pure Cu</th>
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<td></td>
</tr>
<tr>
<td>Ni</td>
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• What is a phase?
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  - how do you use them?
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• Complete Solid Solubility Systems
• **Systems without complete solid solubility**
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  - eutectic; peritectic; eutectoid
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  - Pb-Sn system
  - Fe-C system
• Modern navigation tools
2 components

has a special composition with a min. melting T.

Ex.: Cu-Ag system
• 3 single phase regions (L, $\alpha$, $\beta$)
• Limited solubility:
  $\alpha$: mostly Cu
  $\beta$: mostly Ag
• $T_E$: No liquid below $T_E$
• $C_E$: Min. melting T composition

Cu-Ag system

T(°C)

L (liquid)

L + $\alpha$

$\alpha + \beta$

$T_E$

8.0

779°C

71.9 91.2

$C_E$

80 100

$C_O$, wt% Ag

Co, wt% Ag
**EX: Pb-Sn EUTECTIC SYSTEM (1)**

- For a 40wt%Sn-60wt%Pb alloy at 150°C, find...
  - the phases present:
    - $\alpha + \beta$
  - the compositions of the phases:
EX: Pb-Sn EUTECTIC SYSTEM (2)

• For a 40wt%Sn-60wt%Pb alloy at 150°C, find...
  --the phases present: $\alpha + \beta$
  --the compositions of the phases:
    \[ C_\alpha = 11\text{wt}\%\text{Sn} \]
    \[ C_\beta = 99\text{wt}\%\text{Sn} \]
  --the relative amounts of each phase:
    \[ W_\alpha = \frac{59}{88} = 67\text{wt}\% \]
    \[ W_\beta = \frac{29}{88} = 33\text{wt}\% \]
MICROSTRUCTURES IN EUTECTIC SYSTEMS-I

- $C_0 < 2\text{wt}\%\text{Sn}$
- Result:
  -- polycrystal of $\alpha$ grains.
• 2wt%Sn < C₀ < 18.3wt%Sn
• Result:
  --α polycrystal with fine β crystals.
MICROSTRUCTURES IN EUTECTIC SYSTEMS-III

- $C_0 = C_E$
- Result: Eutectic microstructure
  --alternating layers of $\alpha$ and $\beta$ crystals.

Micrograph of Pb-Sn eutectic microstructure
• 18.3wt%Sn < $C_0$ < 61.9wt%Sn
• Result: $\alpha$ crystals and a eutectic microstructure

• Just above $T_E$:
  $C_\alpha = 18.3\text{wt}\%\text{Sn}$
  $C_L = 61.9\text{wt}\%\text{Sn}$
  $W_\alpha = \frac{S}{R + S} = 50\text{wt}\%$
  $W_L = (1-W_\alpha) = 50\text{wt}\%$

• Just below $T_E$:
  $C_\alpha = 18.3\text{wt}\%\text{Sn}$
  $C_\beta = 97.8\text{wt}\%\text{Sn}$
  $W_\alpha = \frac{S}{R + S} = 73\text{wt}\%$
  $W_\beta = 27\text{wt}\%$
HYPOEUTECTIC & HYPREUTECTIC

Adapted from Fig. 9.7, Callister 6e. (Fig. 9.7 adapted from Binary Phase Diagrams, 2nd ed., Vol. 3, T.B. Massalski (Editor-in-Chief), ASM International, Materials Park, OH, 1990.)

(Pb-Sn System)

<table>
<thead>
<tr>
<th>T(°C)</th>
</tr>
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<tbody>
<tr>
<td>300</td>
</tr>
<tr>
<td>200</td>
</tr>
<tr>
<td>100</td>
</tr>
<tr>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Co, wt% Sn</th>
</tr>
</thead>
<tbody>
<tr>
<td>18.3</td>
</tr>
<tr>
<td>61.9</td>
</tr>
<tr>
<td>97.8</td>
</tr>
</tbody>
</table>

- hypoeutectic: Co=50wt%Sn
- eutectic: Co=61.9wt%Sn
- hypereutectic: (illustration only)

Eutectic micro-constituent

175µm

160µm
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Result: Pearlite = alternating layers of α and Fe₃C phases.

• 2 important points
  - Eutectic (A): 
    \[ L \Rightarrow \gamma + Fe_3C \]
  - Eutectoid (B): 
    \[ \gamma \Rightarrow \alpha + Fe_3C \]

IRON-CARBON (Fe-C) PHASE DIAGRAM
Figure 9.25 Photomicrograph of a eutectoid steel showing the pearlite microstructure consisting of alternating layers of $\alpha$ ferrite (the light phase) and $\text{Fe}_3\text{C}$ (thin layers most of which appear dark). 500×. (Reproduced with permission from Metals Handbook, Vol. 9, 9th edition, Metallography and Microstructures, American Society for Metals, Materials Park, OH, 1985.)
HYPOEUTECTOID STEEL

The diagram illustrates the Fe-C system, focusing on hypoeutectoid steel. The phase transformations and compositions are represented by various lines and symbols.

- **γ (austenite)**
- **γ + L**
- **γ + Fe3C**
- **α + Fe3C**
- **L**
- **Fe3C (cementite)**

Key points and equations:

- \( w_\alpha = \frac{S}{R+S} \)
- \( w_\gamma = (1-w_\alpha) \)
- \( w_{\text{pearlite}} = w_\gamma \)
- \( w_{\text{Fe3C}} = (1-w_\alpha) \)

Where:
- \( S \) is the size of the austenite
- \( R \) is the size of the pearlite
- \( L \) is the liquid
- \( Fe3C \) is the cementite
- \( \gamma \) is the austenite
- \( \alpha \) is the ferrite

The diagram also includes temperature and composition axes, with specific temperatures and compositions marked:

- \( T(°C) \): 1600°C, 1400°C, 1200°C, 1000°C, 800°C, 600°C, 400°C
- \( C_0, \text{wt}\% \text{ C} \): 0, 0.7, 1, 6.7

The diagram provides a visual representation of the phase transformations and compositions for hypoeutectoid steel.
Figure 9.31  Photomicrograph of a 1.4 wt% C steel having a microstructure consisting of a white proeutectoid cementite network surrounding the pearlite colonies. 1000×. (Copyright 1971 by United States Steel Corporation.)
ALLOYING STEEL WITH MORE ELEMENTS

• $T_{\text{eutectoid}}$ changes:

• $C_{\text{eutectoid}}$ changes:

![Teutectoid Diagram](image)

![Ceutectoid Diagram](image)
Fig. 8. The triangle of concentrations of a mechanical mixture with eutectic.
Fig. 13.
Isothermal section at the temperature of the point O (Fig. 9).

Fig. 9.
The space diagram of a mechanical mixture shown in perspective.
Fig. 18. Position of the vertical section diagrams \( mB \) and \( Aq \).

Fig. 19. Section \( mB \) (Fig. 18).
SUMMARY

• Phase diagrams are useful tools to determine:
  --the number and types of phases,
  --the wt% of each phase,
  --and the composition of each phase
for a given T and composition of the system.

• Alloying to produce a solid solution usually
  --increases the tensile strength (TS)
  --decreases the ductility.

• Binary eutectics and binary eutectoid allow for
  a range of microstructures.
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• Examples - uses of phase diagrams
  - Pb-Sn system
  - Fe-C system

• Modern navigation tools
Features

1) **Point (0-D) Calculation** Calculate the stable phase equilibrium at a given point.

2) **Line (1-D) Calculation** Calculate the stable phase equilibrium at several points along a line. For example, as the temperature changes or as the composition changes.

3) **Section (2-D) Phase Diagram Calculation** Calculate stable two-dimensional phase diagrams in multi-component alloy systems. Mouse-click on phase regions to automatically label phase regions.

4) **Solidification Simulation** Simulate the solidification of a multi-component alloy using either the lever rule or Scheil model.

5) **Liquidus Projection** Project the liquidus surface of a multi-component alloy. Label the primary phase regions for a ternary liquidus projection.

6) **Output of Results** Calculated results are displayed in graphical form and exported to a text file.

7) **Database** A thermodynamic database of parameters is required to perform calculations.

8) **Pandat Batch File** Pandat can run a series of calculations predefined in a batch file.
Phase Diagrams
Phase Diagrams
Phase Diagrams

Al-Mg Phase Diagram

- **T[°C]**
- **W[Mg]**

- **fcc**
- **fcc+AlMg_Beta**
- **AlMg_Gamma**
- **hcp**
- **Liquid**
Point Calculations

![Image of point calculations interface]
Point Calculations

### Equilibrium found

**Calculated Point**

- **Temperature**: 500 [°C]
- **Pressure**: 1 [atm]

**System composition and chemical potential**:

- **Al** : $x = 0.782757$, $wt = 0.8$, $\mu = -29465.9$
- **Mg** : $x = 0.217243$, $wt = 0.2$, $\mu = -40489.9$

There are 2 stable phases:

- **Phase Liquid**: fraction = 0.547067
  - $G = -32742.3$
  - $H = 20823$
  - $S = 69.282$
  - $C_p = 30.0121$
  - $T = 773.15$ K
- **Phase FCC_AL**: fraction = 0.452933
  - $G = -30796$
  - $H = 13974$
  - $S = 57.906$
  - $C_p = 30.3318$
  - $T = 773.15$ K
Solidification Simulation
# Solidification Simulation

![Simulation Software Interface]

## Calculated Results

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<th>Stable Phases</th>
<th>fs</th>
<th>fraction(Liquid)</th>
<th>fraction(fcc_A1)</th>
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Ternary Diagrams
Complex Systems

PD: Al-4.5Mg-0.22Fe and Al-4.5Mg-0.22Fe-20Si

- L + Si
- L + Si + pi
- L + Si + pi + Al
- L + Al + pi
- L + Al
- LIQUID
- Si + Al + pi + Mg2Si

**Diagram:**
- Temperature (T°C) on the y-axis
- Weight percentage of Si (W[Si]) on the x-axis

The phase diagram illustrates the various phases and their stability regions based on temperature and composition.
Calculations Options