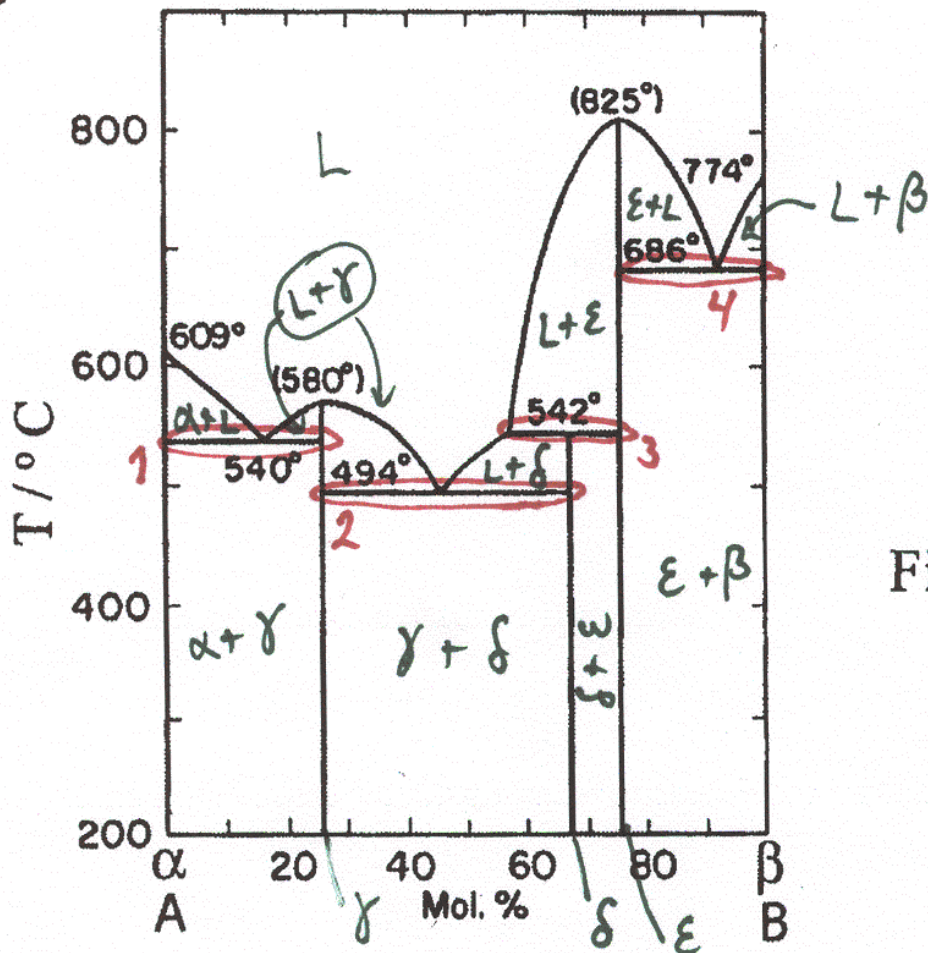


Solution to Phase diagrams

Task 1:

a)

The phases are named: α , β , γ , δ , ϵ and L and are noted by green colour.



Figur 1.

The points for invariant reactions are noted by red circles and can be interpreted as:

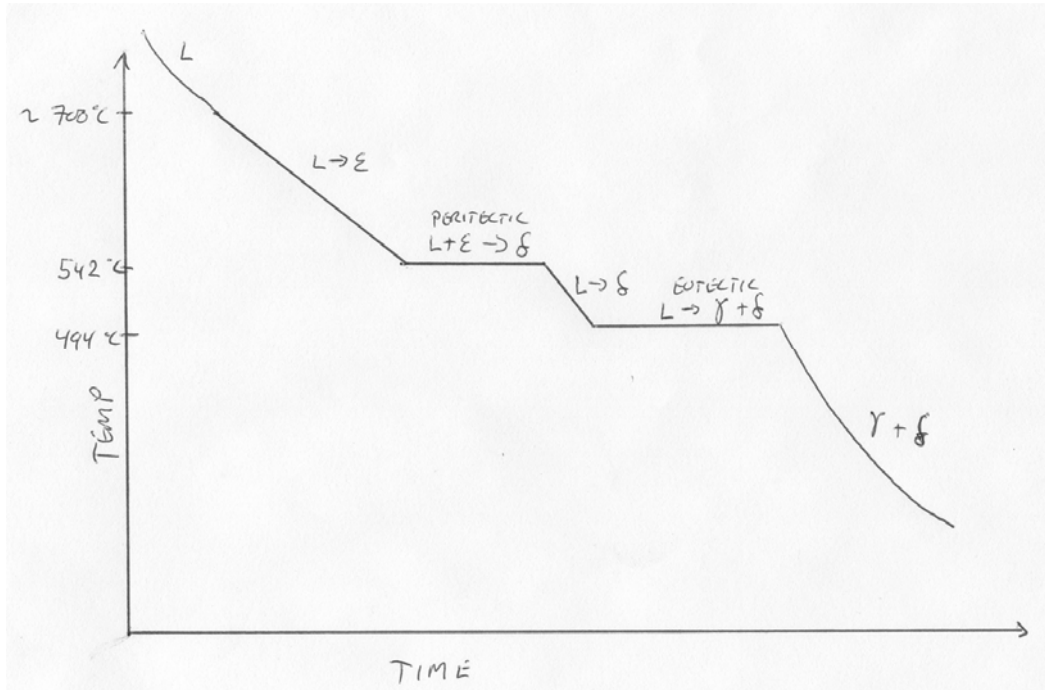
- 1: Eutectic reaction: $L \rightarrow \alpha + \gamma$
- 2: Eutectic reaction: $L \rightarrow \gamma + \delta$
- 3: Peritectic reaction: $L + \epsilon \rightarrow \delta$
- 4: Eutectic reaction: $L \rightarrow \epsilon + \beta$

In addition to this there are:

- Melting of pure A at 609 °C
- Melting of pure γ at 580 °C

- Melting of pure ϵ at 825 °C
- Melting of pure B at 774 °C

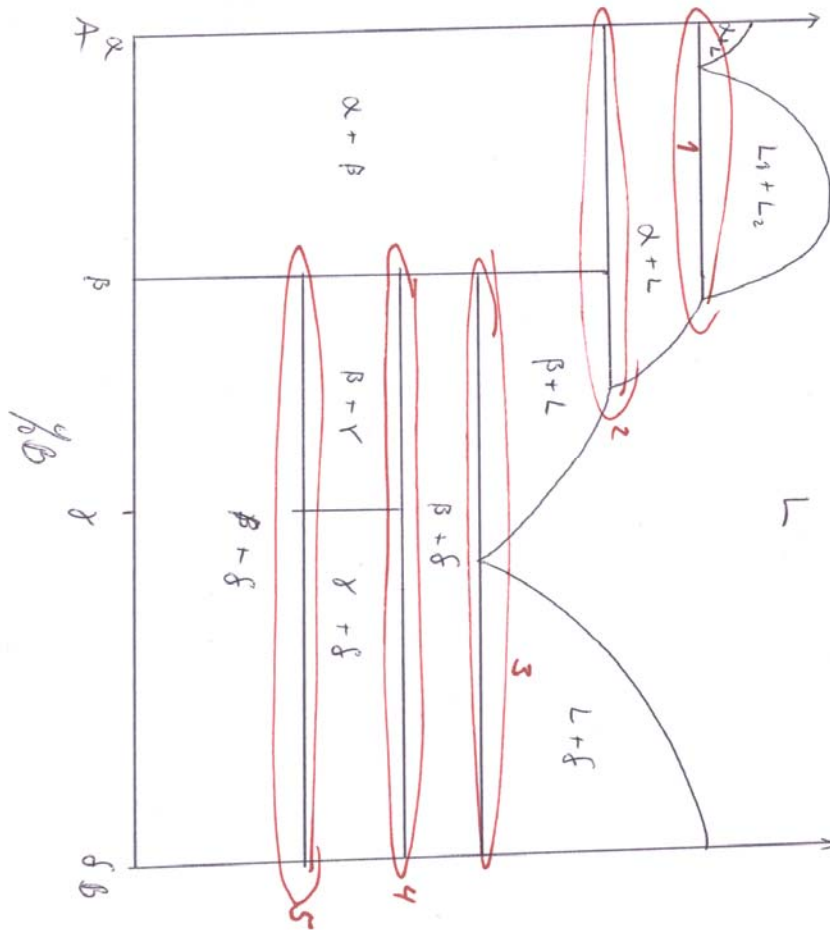
b)



c) The invariant reactions are given in a) and are Eutectic and Peritectic. They can be considered as invariant since three phases are in equilibrium. The condensed Gibbs phase rule ($P + F = C + 1$) for this 2-component system then gives $F = 0$, viz. zero degrees of freedom.

The melting of pure compounds can also be interpreted as invariant reactions if one reduces the number of components need in order to describe the system to 1 component. Then the number of degrees of freedoms becomes 1.

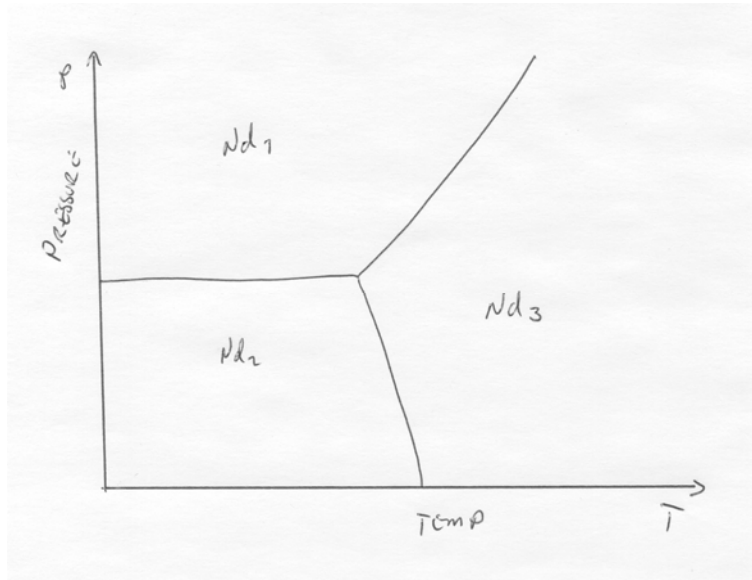
Task 2



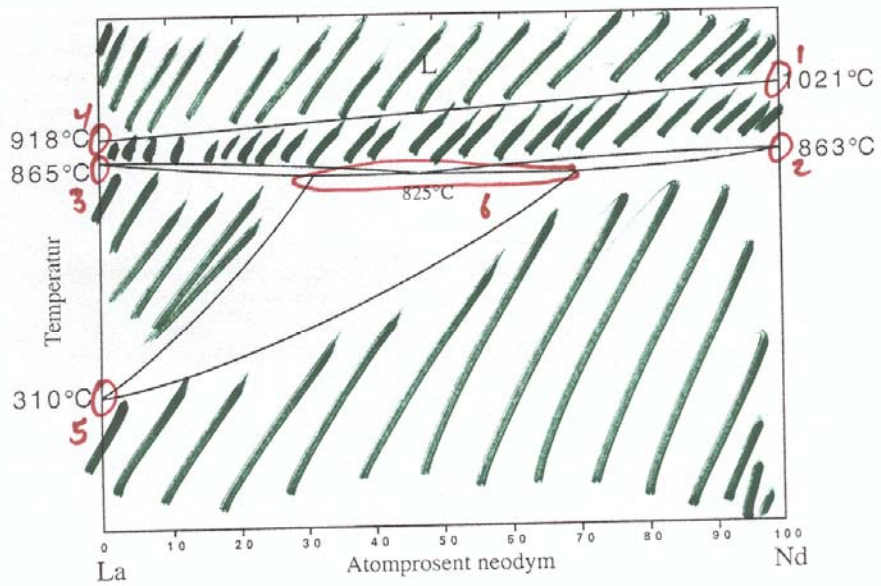
Task 3

a) Allotrope

b)



c)



Figur 2. Fasediagram for systemet La-Nd. (L angir stabilitetsområdet til smelten.)

The invariant reactions are:

- 1: Melting of pure Nd
- 2: Phase transition of pure Nd
- 3: Phase transition of pure La
- 4: Melting of pure La
- 5: Phase transition of pure La

All above reactions involve one component and two phases, hence zero degrees of freedom according to the condensed Gibbs phase rule.

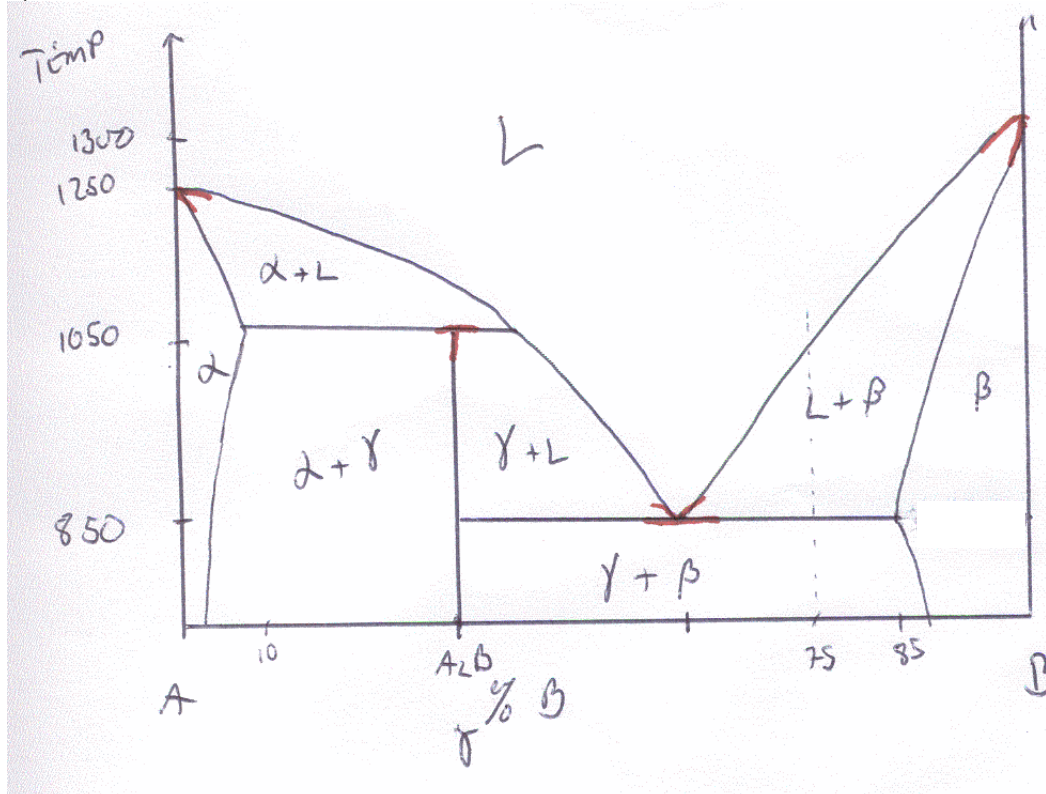
6: Eutectoid reaction

The eutectoid reaction involves three solid phases in equilibrium and needs two components in order to be describes. Hence zero degrees of freedom according to Gobbs phase rule.

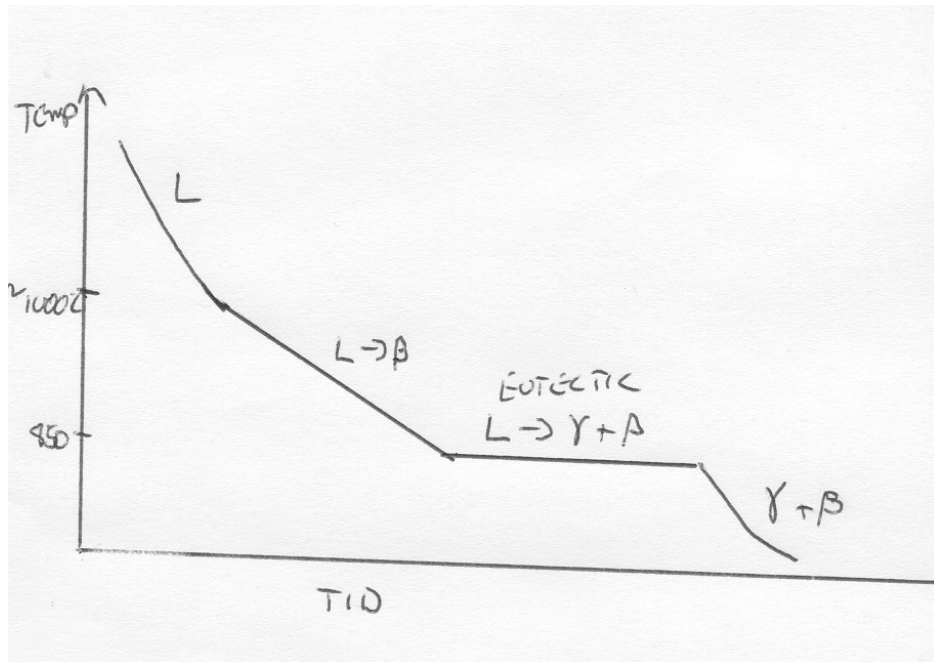
The liquidus/solidus curve appears as one line; however, this is not thermodynamically possible and is in fact an area, but so small so that it appears as one line.

Task 4:

a)



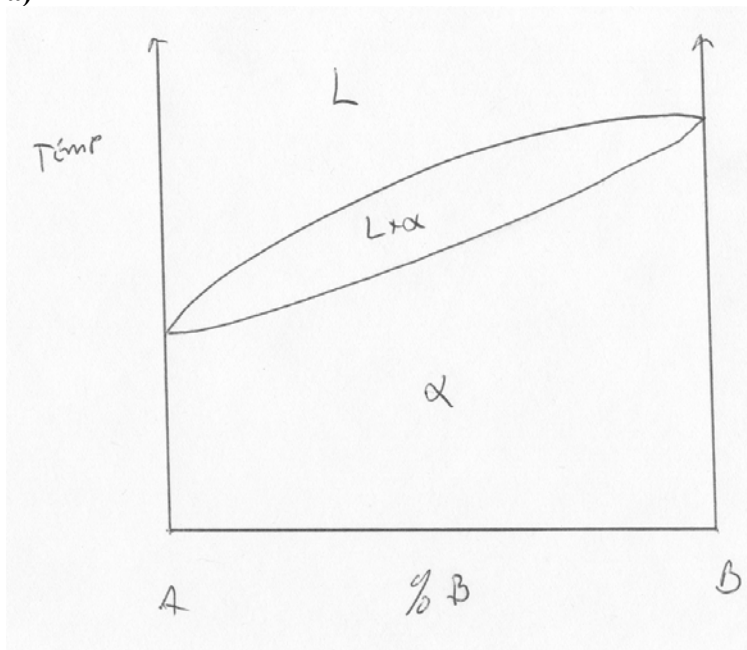
b)



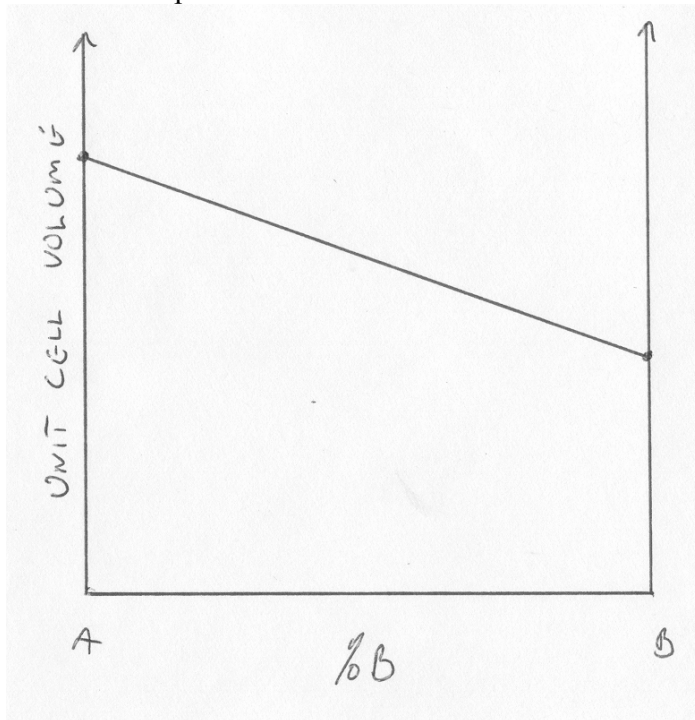
There will be an invariant reaction at 850 °C since there are three phases in equilibrium (L, γ , β). By applying the condensed Gibbs phase ($P + F = C + 1$) rule and that two components can describe the system (A, B) one obtains zero degrees of freedom (F) and hence a horizontal line in the temperature vs. time curve.

Task 5

a)



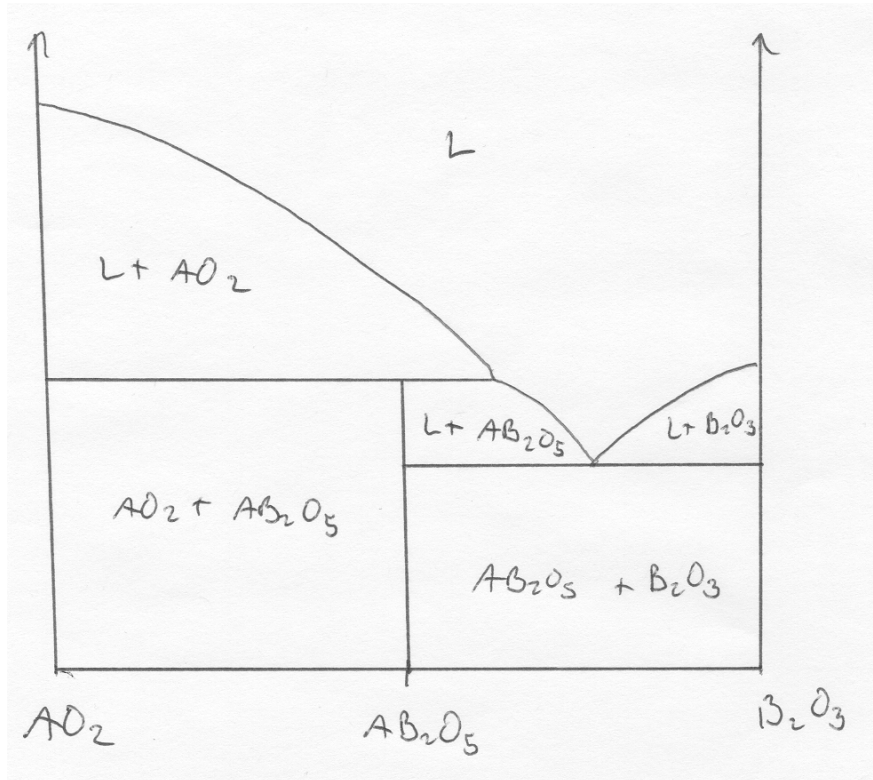
The unit cell volume changes according to the graph below if it follows Vegard's law. This means that the unit cell volume will be linearly dependent on the atomic ratio of the different components in the solid solution.



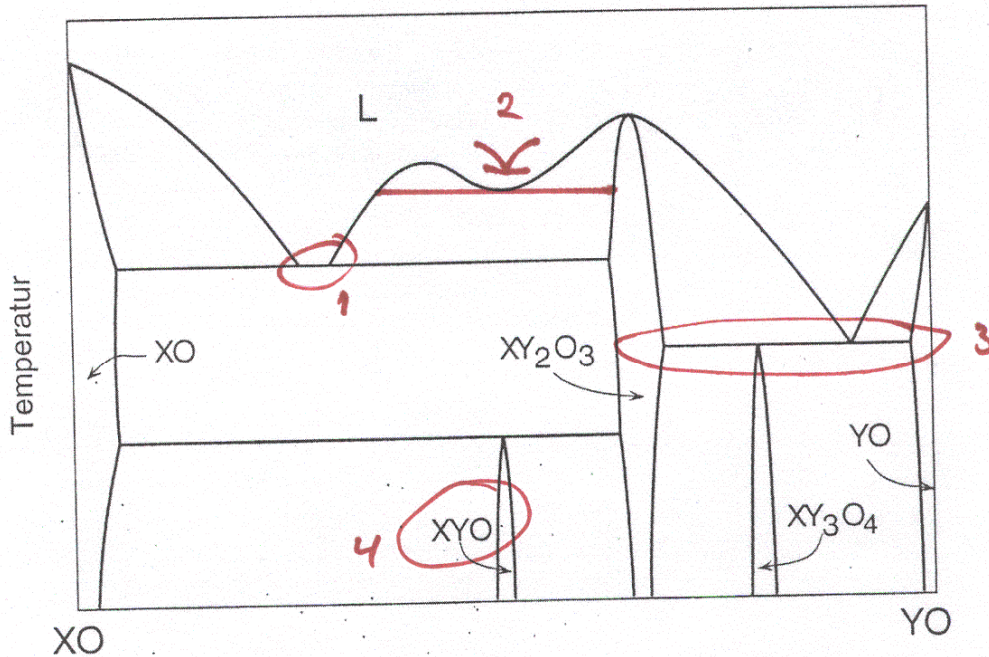
Factors that influence the extent of solid solubility are:

- The ions should be of same charge
- The ions should be of similar size (for metals < 15% difference)
- High temperature helps
- The crystal structures of the end members must be isostructural for complete solid solubility
- The ions should have preference for the same type of sites
- The components in metallic alloys should have similar electronegativity

b)



c)



Figur 3: Fasediagram med feil (eller usannsynlige faseforhold).

1: The liquid can not have a composition range since this is an invariant reaction according to the condensed Gibbs phase rule ($P + F = C + 1$). The number of components are 2 (XO, and YO), and the number of phases in equilibrium are 2 (XO, L, XY_2O_3).

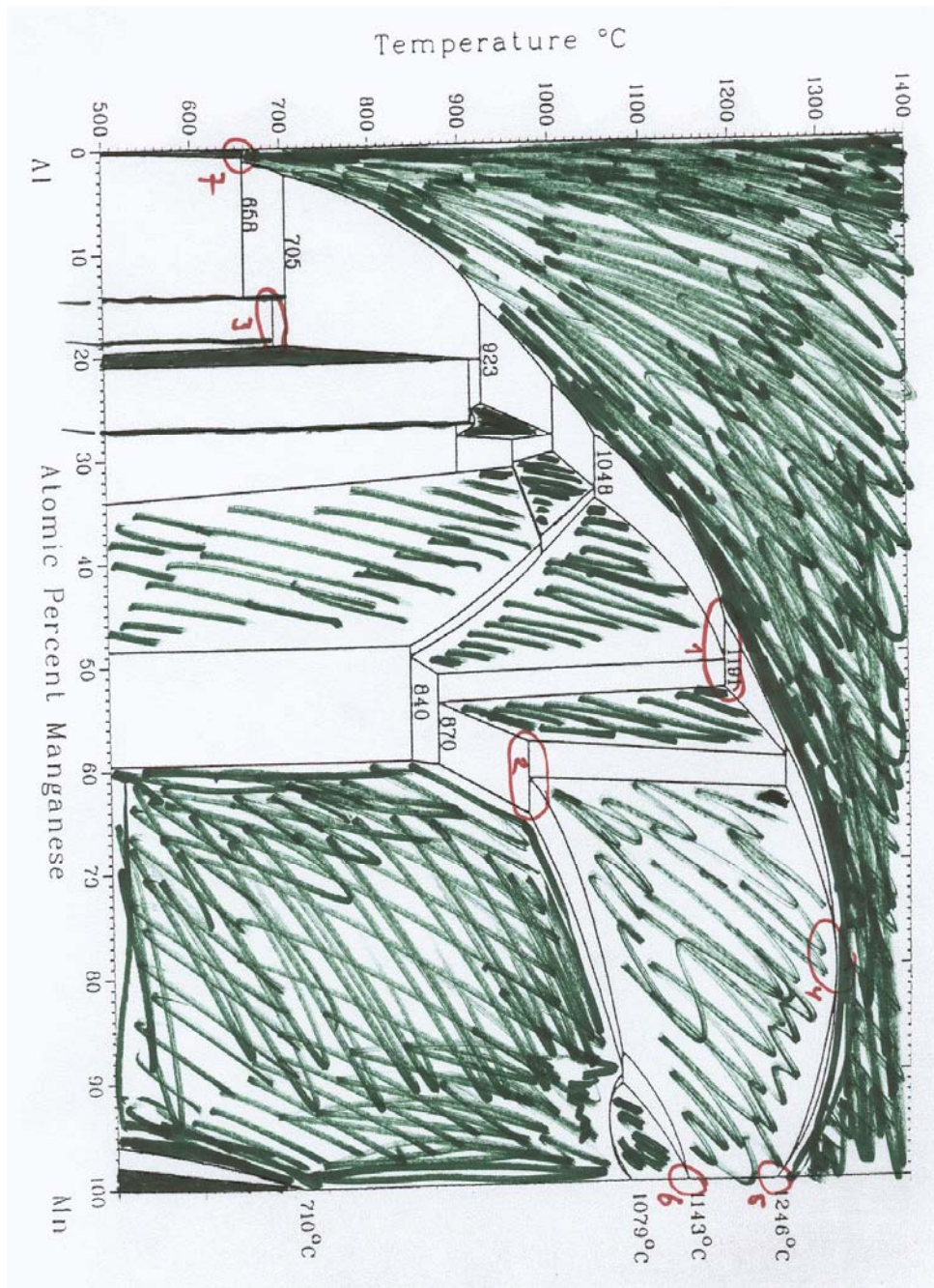
2: There should be a horizontal line here that indicates that there is a monotectic reaction, viz. an invariant reaction. The phases that are in equilibrium are XY_2O_3 , L1 and L2.

3: This situation indicates that there are four phases in equilibrium: XY_2O_3 , XY_3O_4 , L and YO. This apparently violates the condensed Gibbs phase rule. However, if one considers the complete Gibbs phase rule ($P + F = C + 2$) and inserts $P = 4$, $C = 2$ one obtains $F = 0$ and it is possible. This situation can be considered as a very special situation and can occur if the stability of the XY_3O_4 phase or the eutecticum temperature is pressure dependent. This binary phase diagram can then be taken at the magic pressure where these four phases are in equilibrium.

4: The composition XYO can not be described from the end members XO and YO and can thus not be part of this diagram.

Task 6

a)



The singular phases are marked in green.

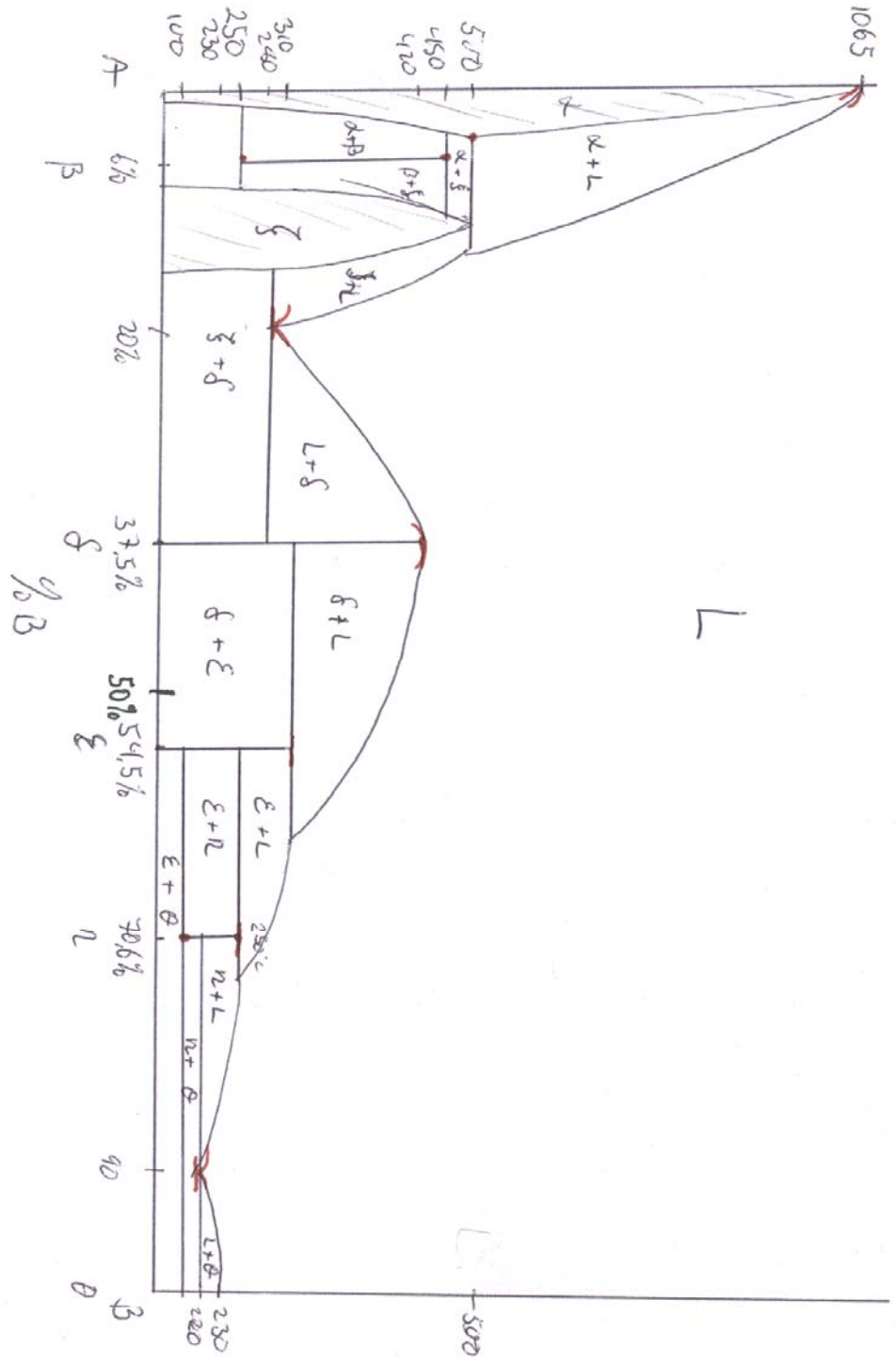
b)

Examples of invariant reactions are given in red circles:

- 1: Peritectic, two components, three phases, $L + \text{solid} \rightarrow \text{solid}$
- 2: Eutectoid, two components, three phases, $\text{solid} \rightarrow \text{solid} + \text{solid}$
- 3: Peritectoid, two components, three phases, $\text{solid} + \text{solid} \rightarrow \text{solid}$
- 4: Congruent melting, one magic component, two phases, $\text{solid} \rightarrow L$
- 5: Melting of pure compound, one component, two phases, $\text{solid} \rightarrow L$
- 6: Phase transition of pure compound, one component, two phases, $\text{solid} \rightarrow \text{solid}$
- 7: Eutectic, two components, three phases, $L + \text{solid} \rightarrow \text{solid} + \text{solid}$

The last example (7) is really hard to observe in the phase diagram, but really is there. It is however not a necessity since it also can be described by a peritectic reaction at this place as well.

c)



d)

A sample with overall composition of 50 wt% B contains δ and ϵ .

δ has composition 37.5 wt% B

ϵ has composition 54.5 wt% B

Difference in wt% is $54.5 - 37.5 \text{ wt\%} = 17 \text{ wt\%}$

Amount of δ is $100 \cdot (54.5 - 50) / 17 = 26.47 \text{ wt\%}$

Amount of ϵ is $100 \cdot (50 - 37.5) / 17 = 73.53 \text{ wt\%}$

e)

δ contains 37.5 wt% B

Assume 100 g of compound.

Number of moles of B is then $37.5 \text{ g} / 120 \text{ g/mol} = 0.3125 \text{ mol}$

Number of moles of A is then $(100 - 37.5) \text{ g} / 200 \text{ g/mol} = 0.3125 \text{ mol}$

Ratio of A/B = 1 thus the chemical formula is AB

ϵ contains 54.5 wt% B

Assume 100 g of compound.

Number of moles of B is then $54.5 \text{ g} / 120 \text{ g/mol} = 0.4541 \text{ mol}$

Number of moles of A is then $(100 - 54.5) \text{ g} / 200 \text{ g/mol} = 0.2275 \text{ mol}$

Ratio of A/B = 0.5 thus the chemical formula is AB₂

η contains 70.6 wt% B

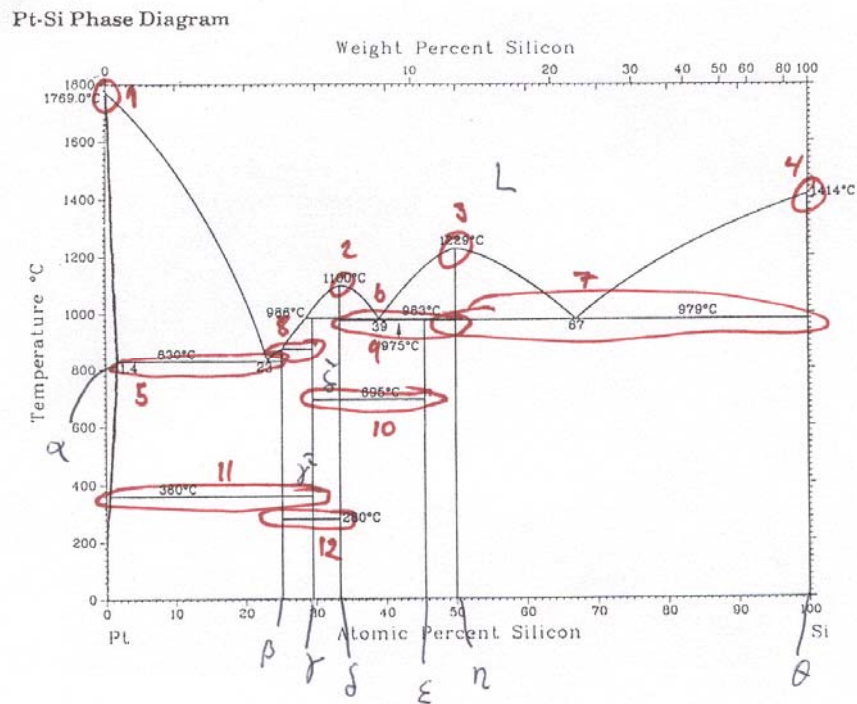
Assume 100 g of compound.

Number of moles of B is then $70.6 \text{ g} / 120 \text{ g/mol} = 0.5883 \text{ mol}$

Number of moles of A is then $(100 - 70.6) \text{ g} / 200 \text{ g/mol} = 0.147 \text{ mol}$

Ratio of A/B = 0.25 thus the chemical formula is AB₄

Task 7



The phases are named as: α , β , β' , γ , γ' , δ , δ' , ϵ , ϵ' , η , θ .

The invariant reactions are:

- 1: Melting of α .
- 2: Congruent melting of δ' .
- 3: Congruent melting of η .
- 4: Melting of θ .

The above reactions are invariant if one describes the system by one component and two phases in equilibrium.

- 5: Eutectic reaction: $L \rightarrow \alpha + \beta$.
- 6: Eutectic reaction: $L \rightarrow \delta' + \eta'$.
- 7: Eutectic reaction: $L \rightarrow \eta' + \theta$.
- 8: Peritectic reaction: $L + \gamma' \rightarrow \beta$.

The above reactions are invariant if one describes the system by two component and three phases in equilibrium.

9: Phase transition: $\varepsilon' \rightarrow \varepsilon$.

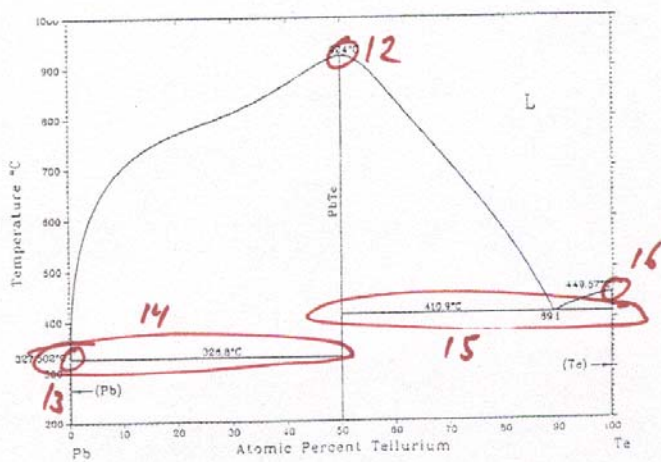
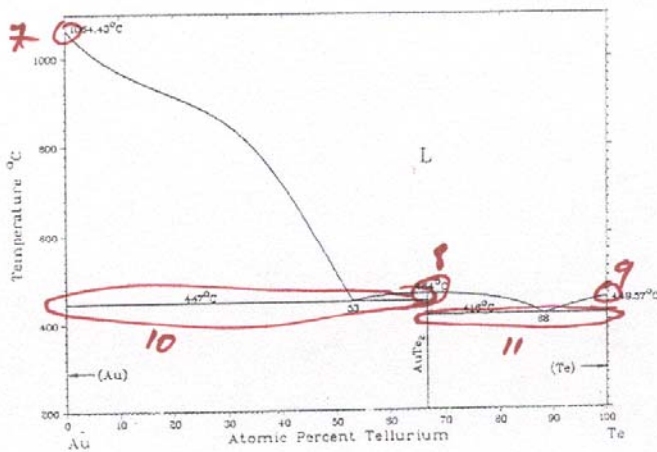
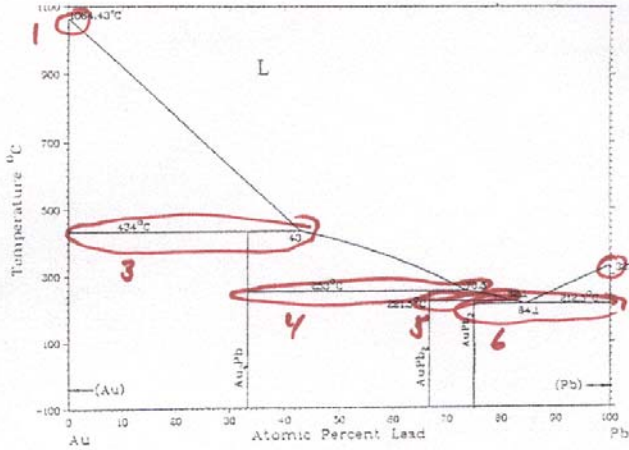
10: Phase transition: $\delta' \rightarrow \delta$.

11: Phase transition: $\beta' \rightarrow \beta$.

12: Phase transition: $\gamma' \rightarrow \gamma$.

The above reactions are invariant if one describes the system by one component and two phases in equilibrium.

Task 8:
a)



The invariant reactions are:

- 1+7: Melting of pure Au
- 2+13: Melting of pure Pb
- 9+16: Melting of pure Te
- 8: Congruent melting of AuTe₂
- 12: Congruent melting of PbTe

The above reactions are invariant if one describes the system by one component and two phases in equilibrium.

- 3: Peritectic reaction: $L + (Au) \rightarrow (Au_2Pb)$.
- 4: Peritectic reaction: $L + (Au_2Pb) \rightarrow (AuPb_2)$.
- 5: Peritectic reaction: $L + (AuPb_2) \rightarrow (AuPb_3)$.
- 6: Eutectic reaction: $L \rightarrow (AuPb_3) + (Pb)$.
- 10: Eutectic reaction: $L \rightarrow (Au) + (AuTe_2)$.
- 11: Eutectic reaction: $L \rightarrow (AuTe_2) + (Te)$.
- 14: Eutectic reaction: $L \rightarrow (Pb) + (PbTe)$.
- 15: Eutectic reaction: $L \rightarrow (PbTe) + (Te)$.

The above reactions are invariant if one describes the system by two component and three phases in equilibrium.

b)

Overall composition Au₆₀Te₄₀. The sample is then in a two phase area between the phases (Au) (with virtually no solid solution and (AuTe₂) (also this with virtually no solid solution) (Can also be expressed as Au_{33.33}Te_{66.67}).

The composition with respect to mol% can be calculated by assuming 100 moles of atoms.

The total length of the lever (conode) expressed in Te moles is then: 66.67 moles.

The amount of Au expressed in mole% is then $(66.67-40) \text{ moles Te} / 66.67 \text{ moles Te} * 100\% = \mathbf{40 \text{ mole\%}}$

The amount of AuTe₂ expressed in mole% is then $(40) \text{ moles Te} / 66.67 \text{ moles Te} * 100\% = \mathbf{60 \text{ mole\%}}$

The composition with respect to weight% can be calculated by recalculating the compositions into weight%. Assuming 100 moles of compound totally:

A sample that contains 40 mole% of Au can be converted to 40 moles of Au giving a weight of $40 \text{ moles} * 196.97 \text{ g mole}^{-1} = 7878.8 \text{ g}$

60 mole% of AuTe₂ gives 60 moles of AuTe₂ (Au_{0.33}Te_{0.67}) giving a weight of 60 moles
* (196.97 + 2* 127.60)*1/3 g mole⁻¹ = 9043.4 g.

Weight % of Au = 7878.8 g / (7878.8 + 9043.4)g * 100% = **46.55 wt%**

Weight % of AuTe₂ = 9043.4 g / (7878.8 + 9043.4)g * 100% = **53.44 wt%**