Simple Phase Diagram and Free Energy vs. Composition Curves
UG Course : Phase Transformations

- To construct free energy vs. composition curves given a simple phase diagram and vice versa.

Learning Objectives :

After going through this learning aid ,user will be able to:

- Construct a phase diagram given free energy vs. composition curves at different temperatures.
- Draw the schematic free energy vs. composition curves at different temperatures given the phase diagrams.
- State and interpret the Gibbs Phase Rule.

Author:

Kartikay Agarwal
10D110030
UG sophomore year
Dept. of ME & MS

Shrey Singh
10D110010
UG sophomore year
Dept. of ME & MS

Mentor:
Prof. M. P. Gururajan
Dept. of ME & MS

Definition and Keywords

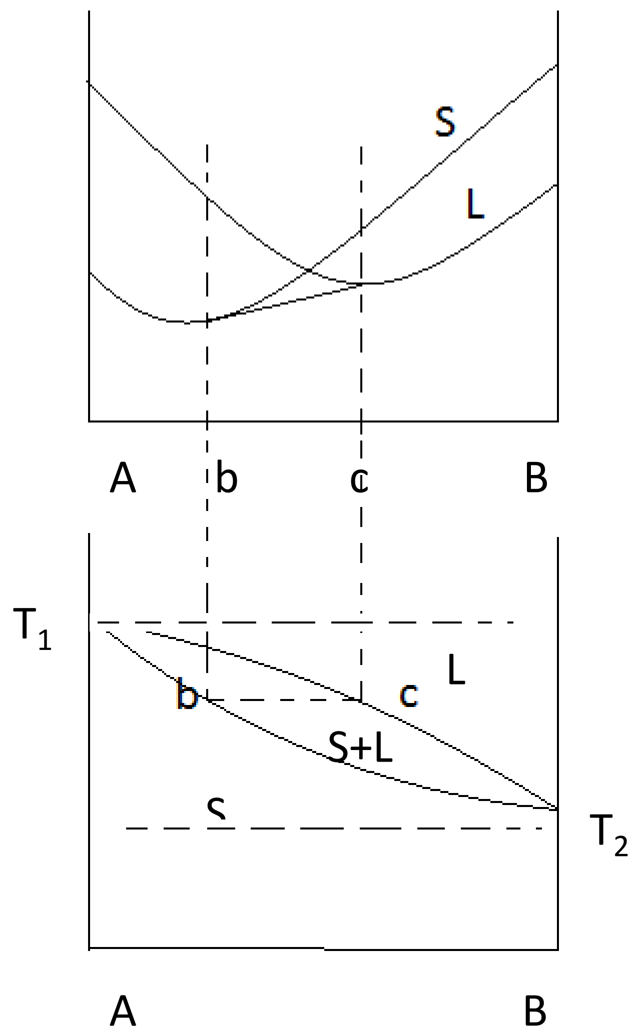
Phase Diagram - Phase Diagrams are charts which give the information regarding the equilibrium phases in a system under the given thermodynamic constraints.

Binary alloy – A system with two components.

Gibbs Phase Rule – At constant pressure $\underline{P+F-C=1}$
where C=no. of components,
F=no. of Degrees of freedom, P=no of phases.

Solidus and Liquidus – The lines on a phase diagram which separate the solid and liquid regions respectively from the two phase Solid + liquid region.

Master Layout 1



Slide 1

Slide 2

Introduction | Glossary | Explanation | Tab 04 | Tab 05 | Tab 06 | Tab 07

Binary Phase Diagrams

Instructions/ Working area

Credits

Step 1.1 Explanation

No Figure

Action/Description	Audio narration	Text to be displayed
Display the text without any figure	Same as the text alongside	Phase Diagrams are a way of cataloguing the information regarding the equilibrium phases in a system under the given thermodynamic constraints. In this learning object, we will consider a system of a binary alloy at constant pressure and different temperatures . So the phase diagram is a plot of composition vs. temperature with the equilibrium phases marked at different combinations of these two parameters. Specifically in this animation we consider a system that shows only the existence of a single phase or two phases at any temperature and composition. We will show that the equilibrium phases are a result of the minimization of the free energy of the system.

Step 1.2 Explanation

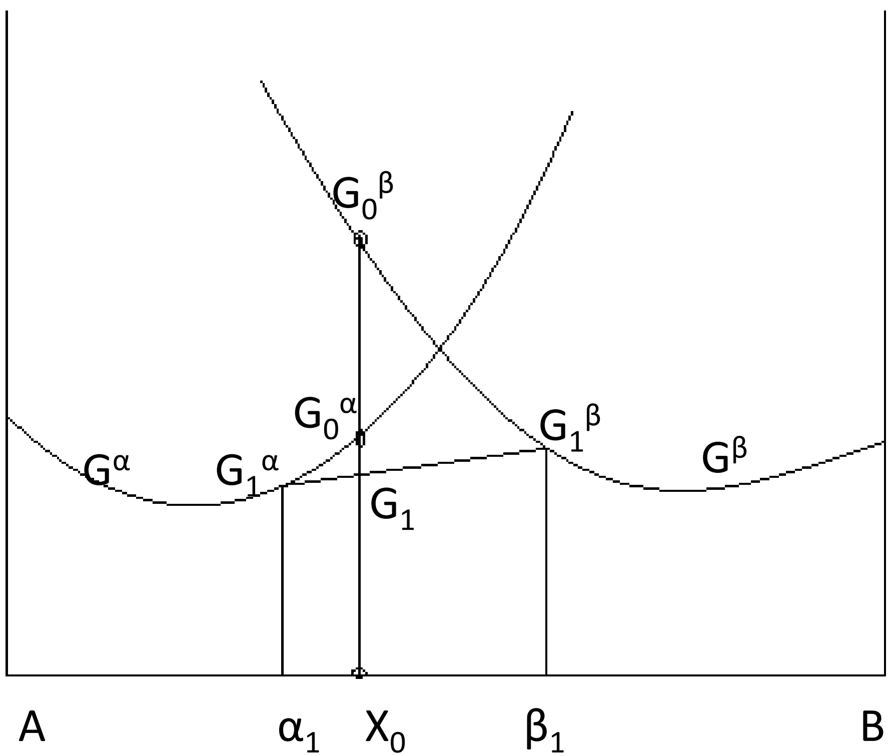


Figure 1

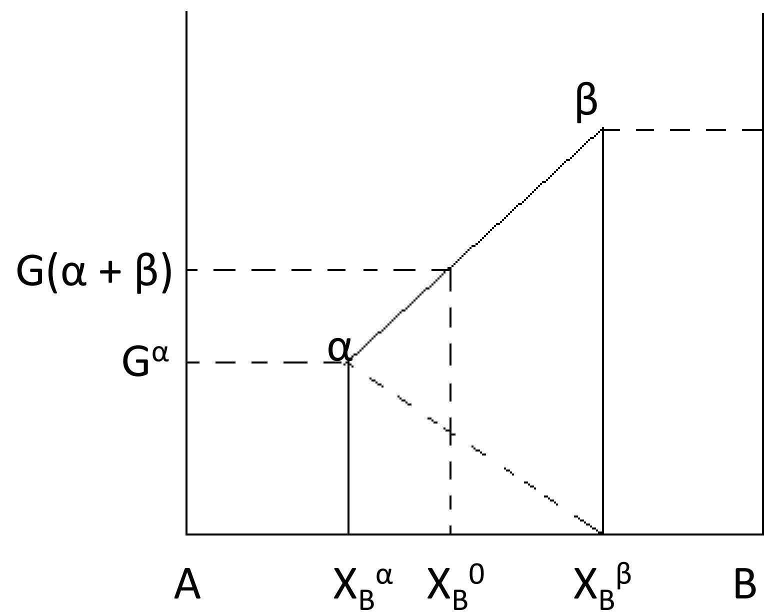
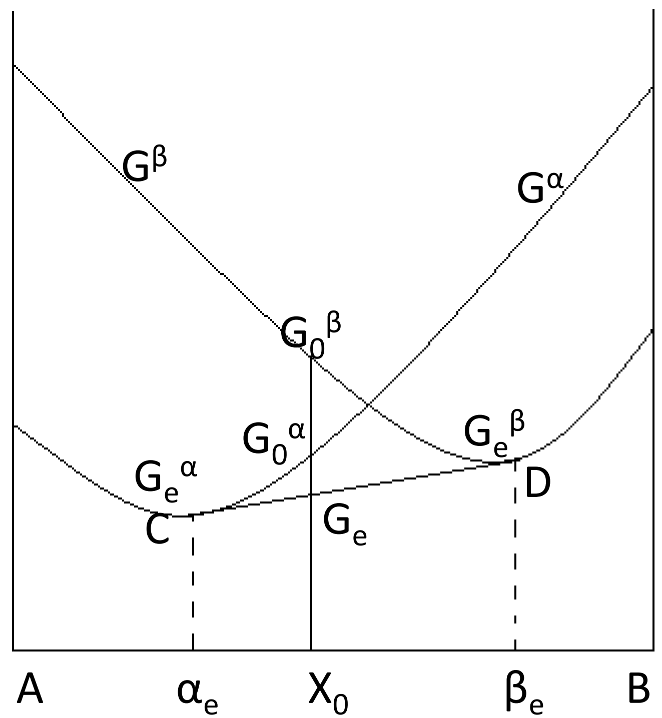


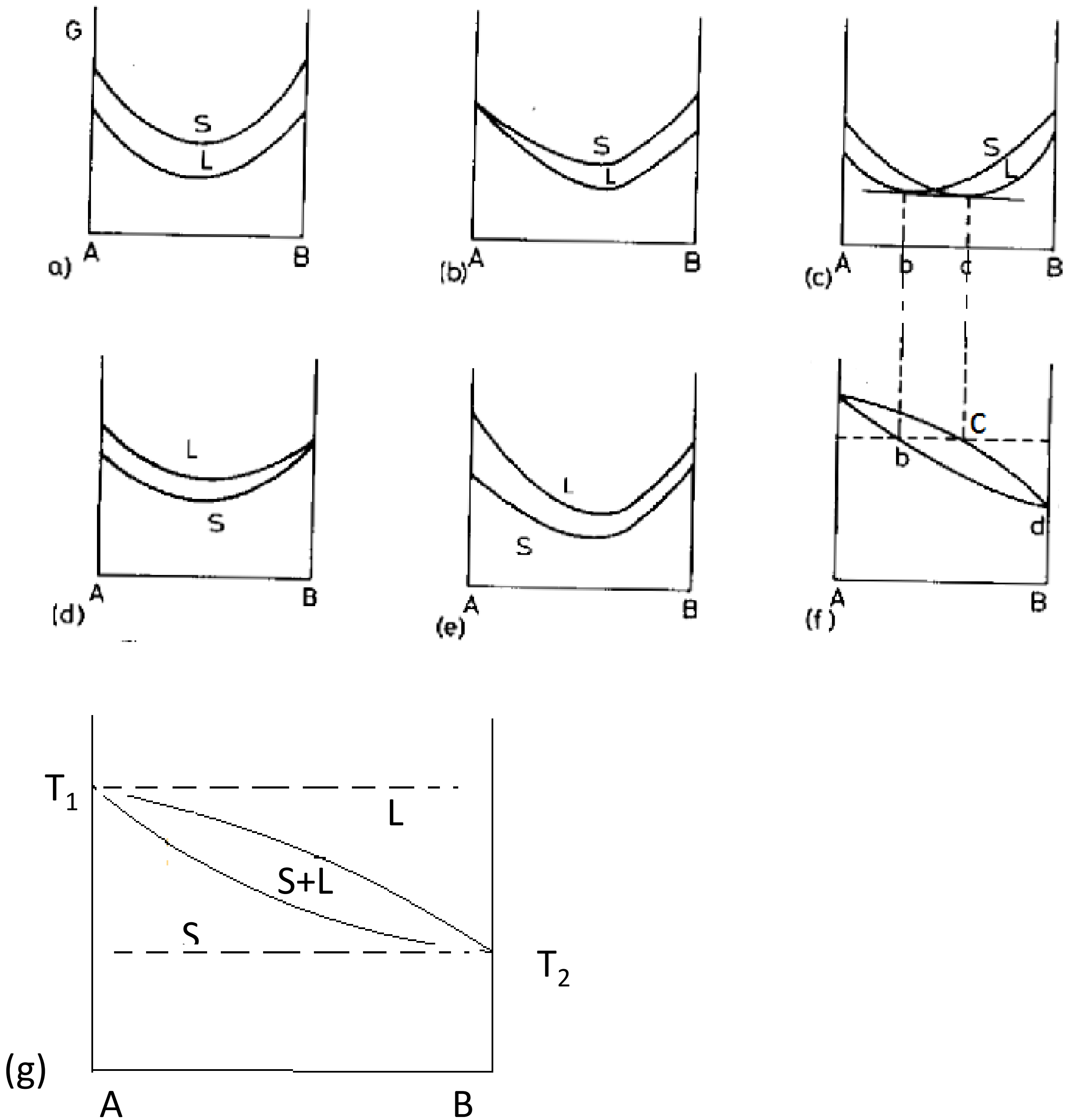
Figure 2

Action/Description	Audio narration	Text to be displayed
Display the figures followed by the text	Same as text alongside	In figure 1, we show the free energies of two different phases called alpha and beta. If G^{α} is the free energy of the alpha phase (per mole) and G^{β} is the free energy of the beta phase (per mole) then a mechanical mixture of X_B^{α} moles of alpha and X_B^{β} moles of beta will have a free energy of (X_B^{α} G^{α} + X_B^{β} G^{β}). That is as shown in figure 2 , for any composition between X_B^{α} and X_B^{β} the total free energy of the mechanical mixture lies on the straight line that connects G^{α} and G^{β}. Hence from figure 1, it is clear that an alpha phase or a beta phase of uniform composition x0 will have higher free energy as compared to a mechanical mixture of compositions alpha1 and beta1 for the alpha and beta phases respectively.

Step 1.3 Explanation



Action/Description	Audio narration	Text to be displayed
Display the figure followed by the text	Same as text alongside	Taking the argument further it is clear that for any composition between α_e and β_e a mechanical mixture of alpha and beta phases of equilibrium compositions α_e and β_e will have the lowest free energy. Pictorially the equilibrium compositions of the phases that form the mechanical mixture are given by the common tangent constructed to the free energies where they are concave. Conversely any region of a phase diagram where a mechanical mixture is seen the free energy vs. composition curve will have a concave curvature.



The Animator has to make diagrams by himself of all the figures(a to g in this slide so the figures made by the animator will be used for all the animation that is described ahead)

Next slide

Introduction | Glossary | Explanation | Animation | Tab 05 | Tab 06 | Tab 07

Binary Phase Diagrams

Instructions/ Working area

Credits

Step

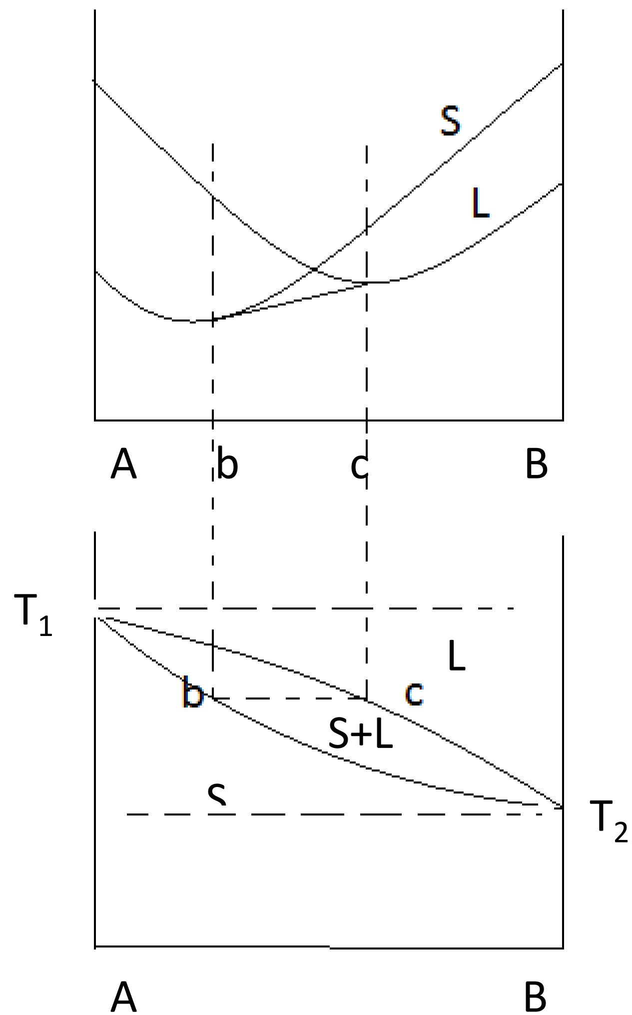


Figure A

Figure B

Action/Description	Audio narration	Text to be displayed
The Complete figure will appear on the screen in this tab but the figure A in the layout will be figure (a) and figure **B** will be figure (g) as shown in the previous slide instead what is shown in the master layout slide	Until the melting temperature of component A is reached ,the free energy curve of solid phase will lie above to that of liquid so the system will exist in liquid phase.	Same as Audio Narration
The Figure **A** will change from figure (a) to (b)(figure (a) and (b) are to be made by the animator as been described in the previous slide) the Figure **B** will remain same as (g)	As the melting temperature of component A is reached Free energy of pure A in both the phases will be same	Same as Audio Narration
Now figure A will change from b to c with corresponding change in B from g to f A sample of the demo can be seen by observing the figure c and f given in previous slide. Also a snapshot of demo's state is given in the slide of animation area	The mechanical mixture of phases will exist in the region between the points where common tangent touches the two curves in figure A and the region where horizontal line corresponding to existing temperature cuts the solidus and liquidus line in Figure B	Same as Audio Narration

Action/Description	Audio narration	Text to be displayed
	The volume fraction of both the components in both the phases remains the same throughout this region but the volume fraction of the mixture changes in both the phases.	Same as Audio Narration
Similarly, figure A will change from c to d with corresponding change in B from f to g.	As the melting point of component B is reached ,free energy of pure B in both the phases will be same.	
The Figure A change figure d to e, the Figure B will remain constant as (g). During transition curve s will move downward and l will move upward gradually relative to each other. Next Button Appears on the Right Bottom	On decreasing the temperature further from the melting temperature of component B, the free energy curve of solid lies below to that of liquid so the system will exist in solid phase. Click on Next for next animation	Same as Audio Narration

Step

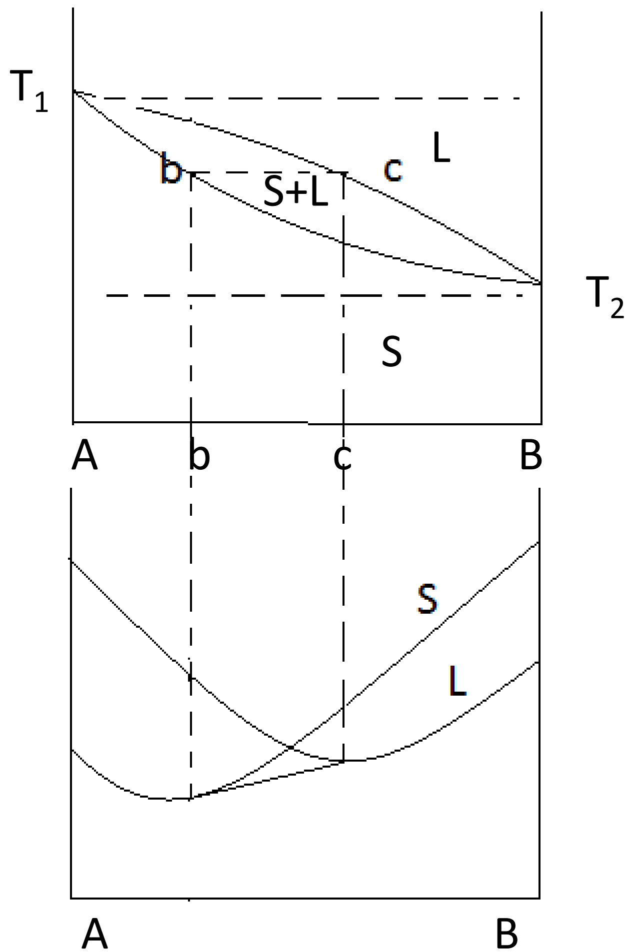


Figure A

Figure B

Complete Figure will appear on the screen in this tab but the figure A in the layout will be figure g and figure B will be figure a as shown in the previous slide instead what is shown in the master layout slide . The Figure B will change from figure a to b(figure a and b are to be made by the animator as been described in the previous slide) the Figure B will remain same as (g)	For region above temperature T1,No of Phases is just 1 i.e., solid and components are 2 so by Gibbs Phase Rule degrees of freedom will be 1 which means that we can obtain a particular composition of liquid phase by varying temperature and composition simultaneously.	Same as Audio Narration
Now figure B will change from b to c with corresponding change in A from g to f A sample of the demo can be seen by observing the figure c and f given in previous slide. Also a snapshot of demo's state is given in the slide of animation area	On moving from T1 to T2, the region where exists a mechanical mixture of two phases, F comes out to be 1 which means that in order to obtain a particular composition of a phase we can chose either one of temperature or composition independently but the other one needs to be fixed.	Same as Audio Narration

Action/Description	Audio narration	Text to be displayed
A sample of the demo can be seen by observing the figure c and f given in previous slide. Also a snapshot of demo's state is given in the slide of animation area		Same as Audio Narration
Similarly, figure A will change from c to d with corresponding change in B from f to g.		
The Figure A change transit change figure d to e, the Figure B will remain constant as (g).	For region below T2 ,degrees of freedom will be two as per Gibbs Phase Rule which means that we can vary temperature and composition independently.	Same as Audio Narration
During transition curve s will move downward and l will move upward gradually relative to each other.		

Next Slide

Binary Phase Diagrams

Instructions/ Working area

Credits

Questionnaire

Q.1 If the free energy curve have a concave down curvature at some temperatures and composition, will the system exist in a mechanical mixture at that temperature or composition

Ans. No

Q.2 What will be the degrees of freedom for the region XYZ

Ans. 2

{By Gibbs Phase Rule

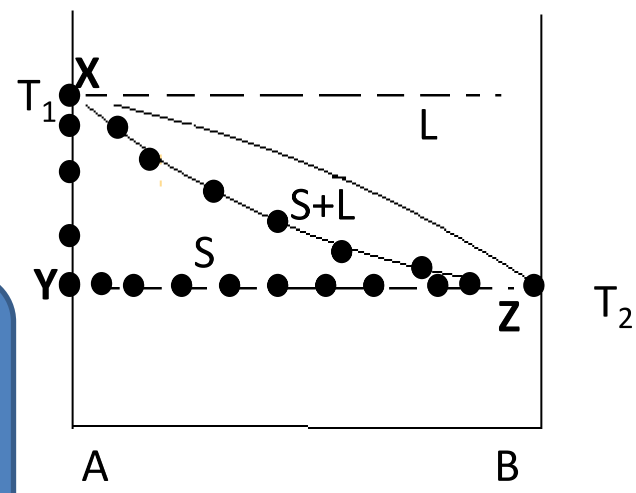
P+C-F=1

Here P=1(Only Solid),

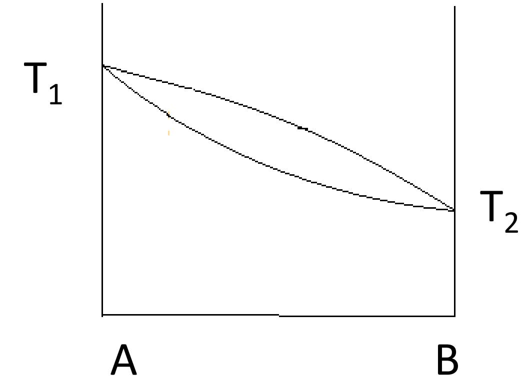
C=2(A and B)

=> F=1}

The region outlined with dots needs to be outlined with a bold line.

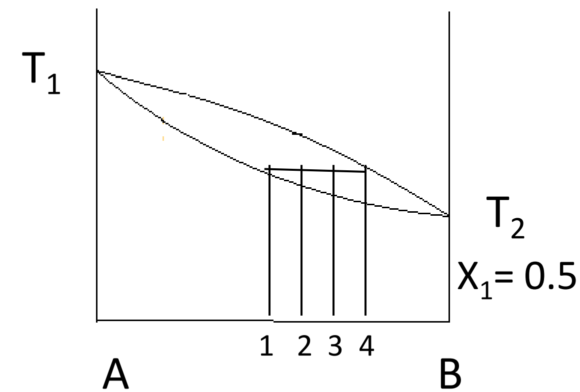


Q.3 If the phase diagram of an isomorphous binary system is as shown and then the system is heated from temperature T(T< T_2) with X_B= 0.5.



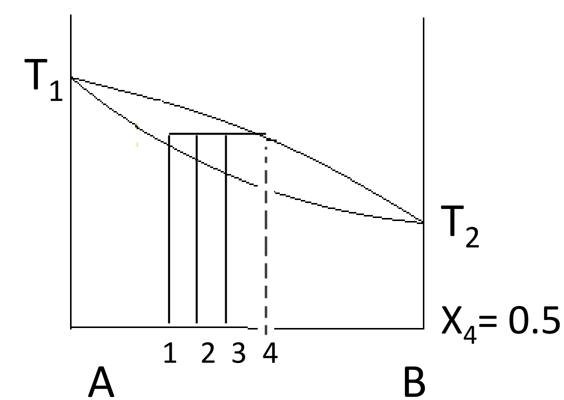
(1) What will be the composition of the first melt?

Ans. 4



(2) What will be the composition of last formed solid?

Ans. 1



Binary Phase Diagrams

Instructions/ Working area

Summary

By the interpretation of free energy vs. composition curves ,we can estimate the phase diagram and also the free energy vs. composition curves can be estimated on the basis of phase diagrams. Free energy vs. composition curves explain the reason behind the existence of multiple phases at different temperatures and compositions.

The phase or a mixture of phases with the lowest free energy will exist at all combination of temperatures and compositions in order to attain equilibrium.

Further Reading

Books

- *Phase Transformations in Metals and Alloys* by **David A Porter K.E. Easterling** Published by Chapman & Hall, *2-6* Bormdary Row, London

  SEl 8HN, UK

Links

- http://www.sv.vt.edu/classes/MSE2094_NoteBook/96ClassProj/analytic/anmeth.html
- http://www.matter.org.uk/matscicdrom/manual/td.html
- http://en.wikipedia.org/wiki/Phase_diagram