

MSE-204 Thermodynamics for Materials Science

L6. INTRODUCTION TO PHASES OF NON-REACTING SYSTEMS

DEFINITION OF PHASE | FUNDAMENTAL RELATIONS OF MULTIPHASE SYSTEMS | CONDITIONS OF EQUILIBRIUM |
ROLE OF CHEMICAL POTENTIAL | PHASE RULE

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DEFINITION OF PHASE

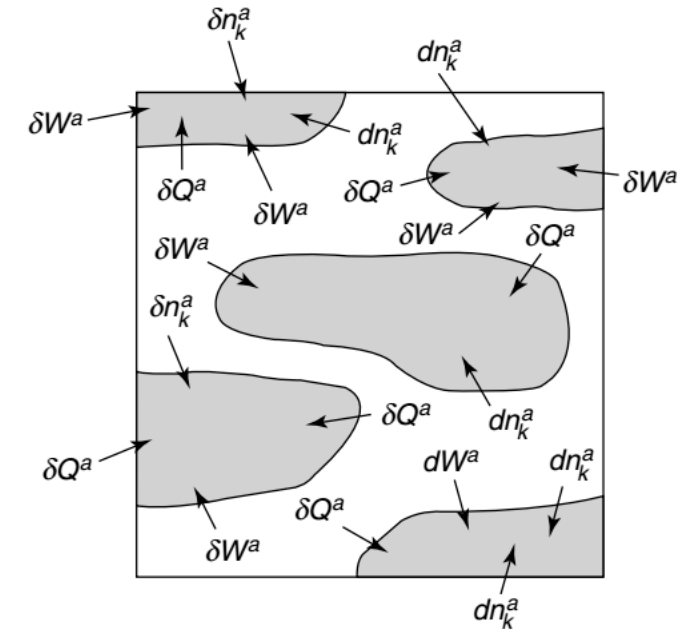
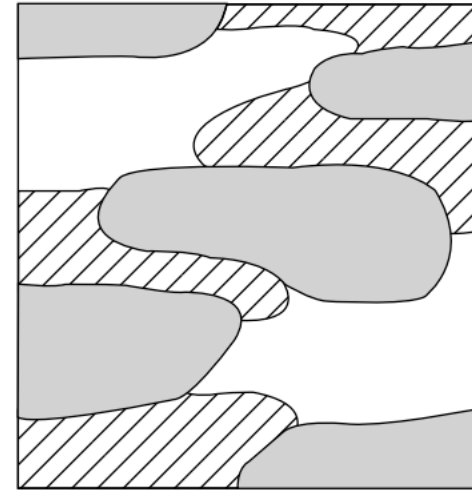
In real systems, we often find different materials and within these materials we can find different parts of the same materials coexisting. For example, a glass of water with ice cubes. In materials, this kind of coexistence is quite common.

A phase is a part of a system that on a macroscopic scale can be considered as homogeneous.

FUNDAMENTAL RELATIONS OF MULTIPHASE, CLOSED, NON-REACTING SYSTEMS

What we now need to study is what are the conditions of the multiple phases to coexist and to be at equilibrium.

Let us consider a heterogeneous closed system consisting of the homogeneous phases α, β, \dots . Each phase contains n_i^θ mole of component i .



TEMPERATURE CONDITIONS FOR EQUILIBRIUM

A possible process can be characterized by the following variations in entropy, volume and composition of the phases:

PRESSURE CONDITIONS FOR EQUILIBRIUM

CONDITIONS ON THE CHEMICAL POTENTIALS FOR EQUILIBRIUM

SPONTANEOUS TRANSFER OF A SPECIE FROM ONE PHASE TO ANOTHER

We will now consider a system that can only exchange volume work with its environment. It comprises of two phases and the various species can freely exchange from one phase to another. They do so at constant pressure and temperature.

GIBBS PHASE RULE (FOR NON-REACTING SYSTEMS)

We need to establish a rule, which will allow us to determine the number of intensive variables that can be independently modified. This modification will induce a change in all the other intensive variables in such a way that a new state of equilibrium will be reached.

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L7.1 SINGLE COMPONENT PHASE DIAGRAMS

PHASE EQUILIBRIA BETWEEN GASES, LIQUIDS, AND SOLIDS | ENTROPY ACCORDING TO BOLTZMANN

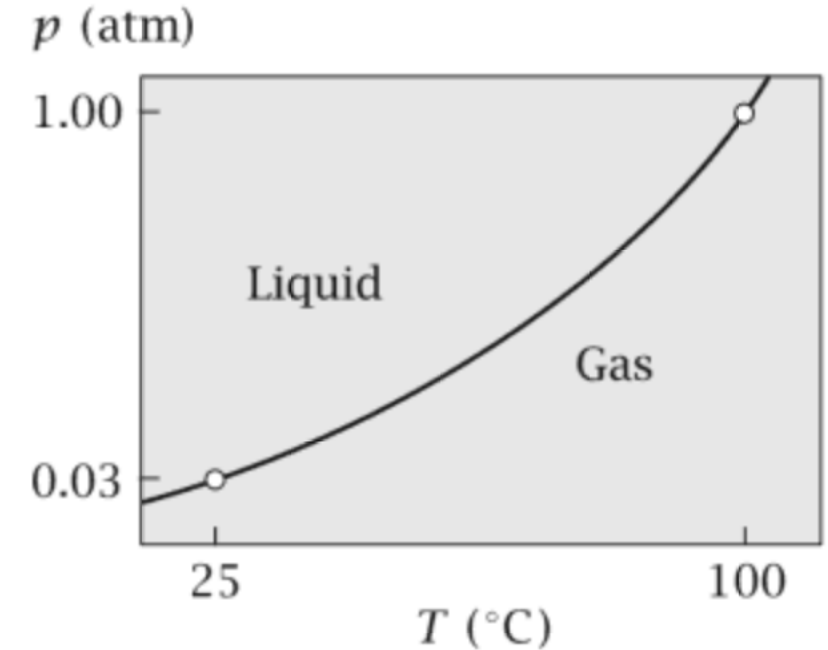
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PHASE EQUILIBRIA OF A PURE SUBSTANCE

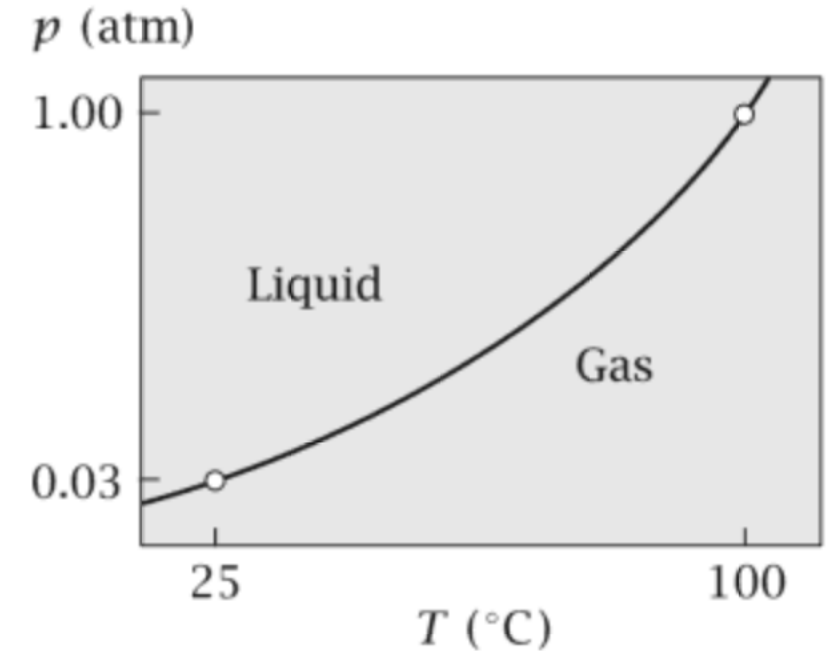
Let's apply the Gibbs phase rule to single component coexistence of phases.

EQUILIBRIUM OF TWO PHASES OF A PURE SUBSTANCE

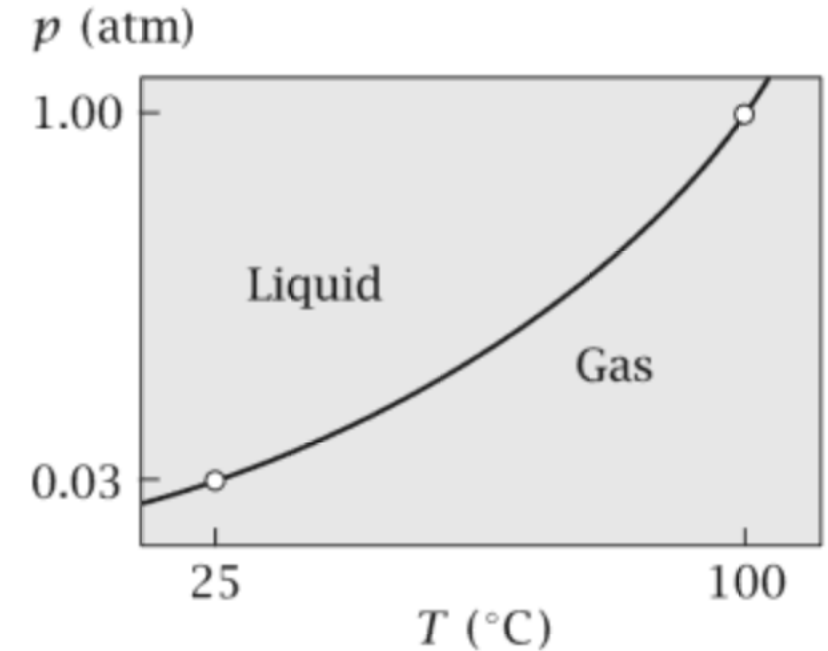
Each line on a phase diagram (also called a phase boundary) represents a set of (p,T) points at which two phases are equally stable. We can mathematically calculate these coexistence lines and then we can construct a phase diagram.



EQUILIBRIUM OF TWO PHASES OF A PURE SUBSTANCE: THE CLAPEYRON EQUATION | CONTINUED



EQUILIBRIUM OF TWO PHASES OF A PURE SUBSTANCE: THE CLAUSIUS CLAPEYRON EQUATION | CONTINUED



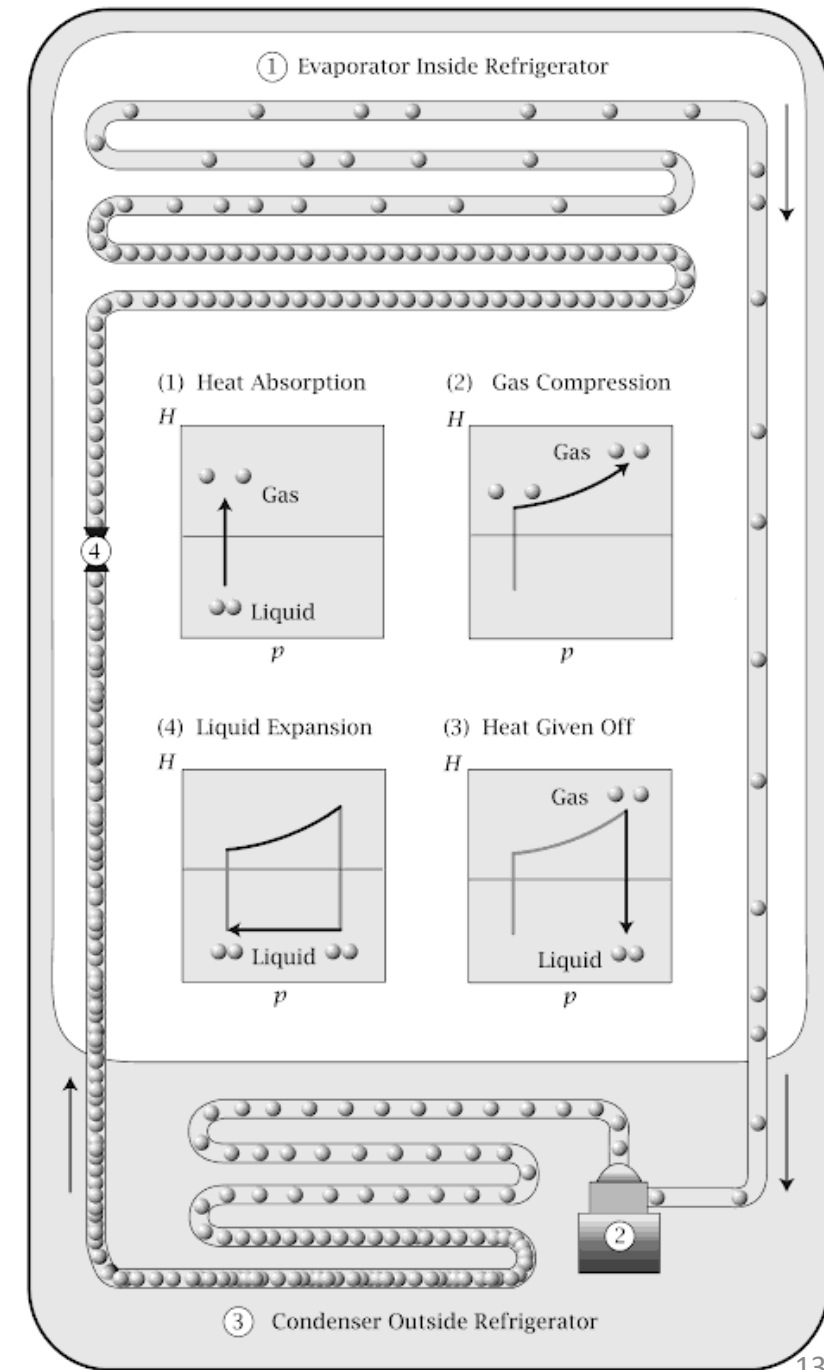
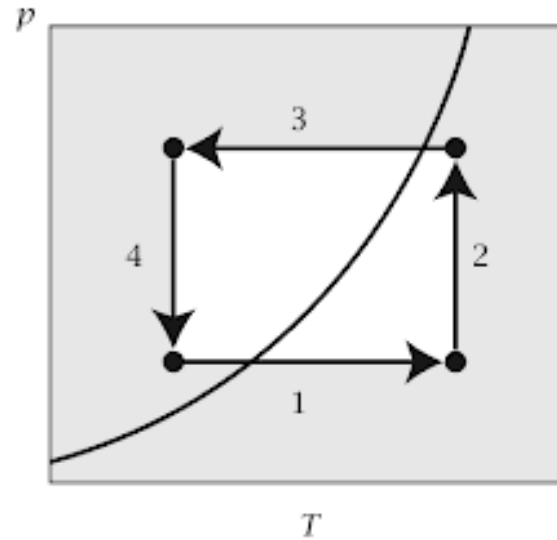
EXAMPLE OF TWO PHASE EQUILIBRIA

THE REFRIGERATOR

In a refrigerator, a “working fluid” is pumped around a system of tubes and undergoes repeated thermodynamic cycles of vaporization and condensation.

Their operation is based on two principles:

- That boiling stores energy by breaking noncovalent bonds and condensation gets that energy back, and
- That a fluid can be boiled at a low temperature and re-condensed at a high temperature by controlling the pressure

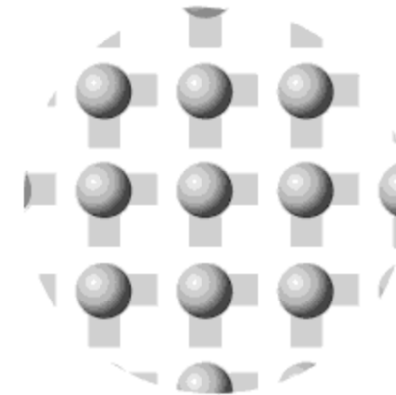
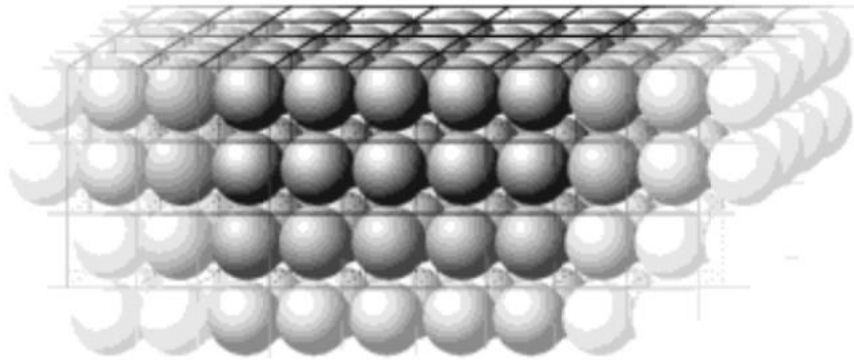


WHY DO LIQUIDS BOIL? | LET'S DEFINE THE SYSTEM

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LATTICE MODEL FOR THE DESCRIPTION OF THE THERMODYNAMIC BEHAVIOR OF LIQUIDS/SOLIDS

We model a liquid (or a solid) as if its particles occupied a crystalline lattice, with every site occupied by one particle. For practical reasons the lattice is considered to be infinite. The main insight represented by the lattice model is that the most important energetic interactions for holding liquids together are the short-range interactions of its particle with its nearest neighbors, and that the number of nearest neighbors has a relatively well-defined average.



CAVITIES IN LIQUIDS AND SOLIDS

Does it matter whether an atom/molecule leaves from the surface or the bulk?

