Part II : Interfaces
Module 1: Structure of interfaces

Interfaces

In this part, we discuss the structure and energetics of interfaces, a simple bond breaking model for surface energies, and, Wulff construction for the equilibrium shape of crystals.

We assume that the user of this module has undergone a structure of materials course. In this chapter, we only discuss in detail certain concepts that are needed in the study of phase transformations. Our discussion is primarily based on Porter, Easterling and Sherif [1]. We refer the interested reader to the following textbooks for more information: [2–6].

1 Structure of interfaces

1.1 Motivation

What are the different types of interfaces? How do we classify interfaces?

1.2 Structure of interfaces

In this module, we are concerned with crystalline solids and the three types of interfaces that they form, namely, solid-solid, solid-liquid and solid-vapour interfaces. The surface of a single crystal (of a pure element) is an example of a solid-vapour interface. The solidification front is an example of a solid-liquid interface. Any engineering material, if looked under the microscope, is teeming with solid-solid interfaces: grain boundaries, twin boundaries, precipitate-matrix interfaces and so on.

Interfaces like the twin and grain boundaries separate the same phase (albeit with different crystal orientations). Hence, they are called homophase interfaces. In contrast, the solid-vapour or precipitate-matrix interface is called a heterophase interface.

Many engineering properties of interest are decided by the structure of the solid-solid interfaces in the material. Hence, a classification of solid-solid interfaces in crystalline systems according to the structure of the interface itself is important.

Based on the structure of the interface, a (crystalline) solid-solid interface can be classified into three broad categories. They are as follows:

1. **Coherent interfaces**

   An interface across which the lattice planes are continuous are called coherent interfaces.

2. **Incoherent interfaces**

   An interface across which there is no lattice plane continuity is called an incoherent interface.

3. **Semi-coherent interfaces**

A typical interface in an engineering material is neither fully coherent nor completely incoherent. There are continuous lattice planes interspersed with regions of discontinuity. Such interfaces are called semi-coherent interfaces.

1.3 Coherent interfaces

Coherent interfaces, as defined earlier, are interfaces across which the lattice planes are continuous. In some cases, the continuity can be maintained without any distortion of lattice planes; see Figure. 1 for a schematic. However, in most of the coherent interfaces, the lattice planes are elastically strained to maintain continuity; see Figure. 2 for a schematic. These elastic strains play a crucial role in determining the properties of the material containing such coherent interfaces.

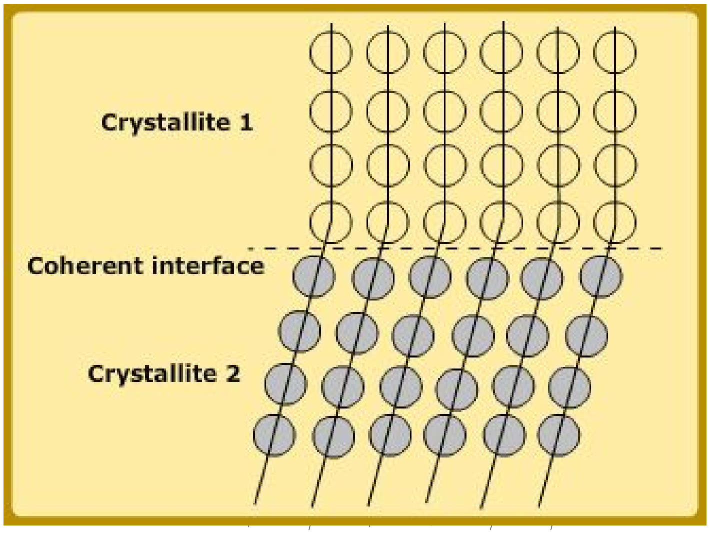

Figure 1: Coherent interface with little elastic strain.

The Ni_3Al precipitates in Ni-base superalloys form coherent interfaces with the Ni-rich matrix. Al-Li and Al-Cu are some of the other systems in which coherent precipitates are seen.

Certain twin boundaries can be coherent; they are known as coherent twin boundaries.

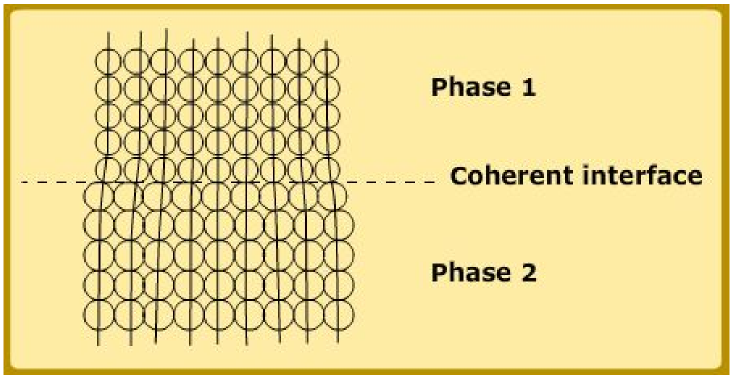

Figure 2: Coherent interface with elastic strain.

The epitaxial growth of thin films on substrates also lead to coherent interfaces between the film and substrate.

1.4 Incoherent interfaces

Incoherent interfaces, as defined earlier, are interfaces across which there is no continuity of lattice planes. In Figure. 3, we show, schematically, an incoherent boundary. There is an elastic energy associated with incoherent boundaries, which is due to the difference in the volume of the particle without any constraints and the volume of the matrix available for the particle.

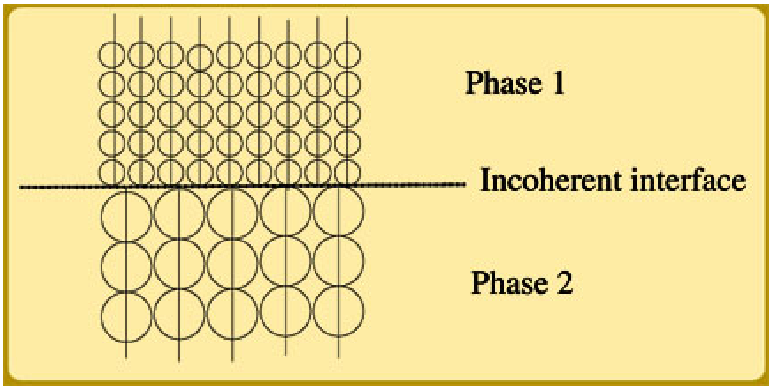

Figure 3: An incoherent interface: there is no lattice plane which is continuous across the interface.

Generic high angle grain boundaries are typically incoherent. Similarly, the inclusions in alloys (for example, MnS in steel) have incoherent interfaces.

1.5 Semi-coherent interfaces

Interfaces across which some planes are continuous and some are not are knwon as semi-coherent interfaces.

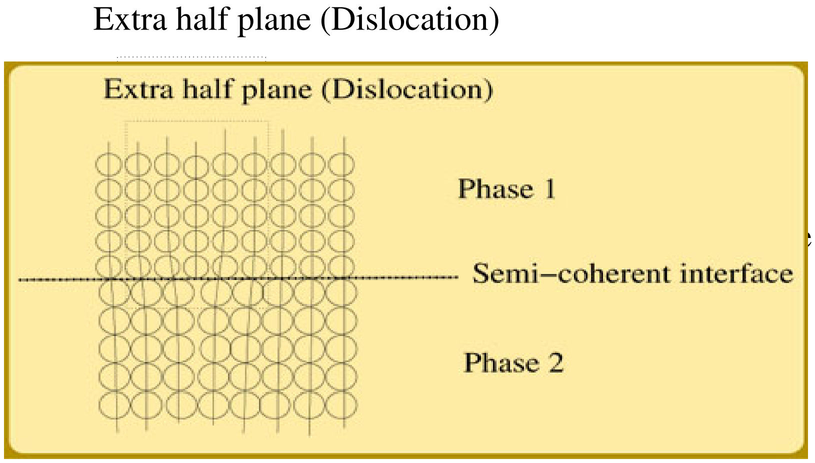

Figure 4: A semi-coherent interface: regions of lattice plane continuity are punctuated by discontinuities in the form of dislocations.

The small angle grain boundaries which are made up of a wall of dislocations and CSL (conicident site lattice) grain boundaries are classic examples of semi-coherent boundaries.

1.6 Tutorial problems and questions

1. Is the antiphase boundary in an ordered alloy a homophase boundary or heterophase boundary?
2. In an ordered alloy, the interface between two differently ordered domains (known as antiphase boundaries) exist. Are they coherent or incoherent interfaces? Why?
3. Coincident site lattice: is it coherent, semi-coherent or incoherent? Why?

1.7 Solutions to the tutorial

1. The antiphase boundary in an ordered alloy is a homophase boundary because it separates two different domains of the same ordered phase.
2. In an ordered alloy, the interface between two differently ordered domains (known as antiphase boundaries) exist. These are typically coherent interfaces. This is because across the antiphase boundary the lattice planes are continuous and only the site occupancy is different. For example, across an antiphase boundary in a B2 ordered structure, the body centers are occupied by A type of atoms instead of B type of atoms and cube corners are occupied by B type of atoms instead of A type of atoms.
3. Coincident site lattices are semi-coherent; this is because any Σ boundary has certain number of continuous lattice planes across the boundary; f or example, in a $\Sigma 5$ boundary, once in every five lattice boundaries are continuous. (In general, a Σn boundary means, every n-th lattice plane is continuous across the interface).

1.8 Supplementary information

The structure of interface plays a key role in determining its energy. The coherent and semi-coherent interfaces have strain energies associated with them. In the case of coherent interfaces for example, the elastic energy associated with the interface along with the interfacial energy determines its equilibrium shape. The system will choose that shape which minimizes the total interfacial energy. In some cases, the shape preferred by interfacial energy could be different from that preferred based on elastic energy considerations. In general, for very small sizes, the interfacial energy considerations play a dominant role while at higher sizes, the elastic energy dominates. This is because interfacial energy scales with interfacial area while elastic energy scales with the volume of the phase.