Computing Class: TTT diagrams

The purpose of this exercise is to illustrate time-temperature-transformation diagrams for steels. A steel is an alloy of iron and a minute amount of carbon. It may also contain other solutes such as manganese, nickel, silicon *etc.*

There are three natural allotropes of pure iron (Fig. 1), of which, ϵ is only stable at some 130,000 atmospheres of pressure and hence does not occur in iron under ambient conditions. The two phases of interest are therefore, austenite (γ) and ferrite (α). Austenite is the stable phase above 911.5 °C, and ferrite below that temperature. There are also a number of magnetic transitions within each of these phases.

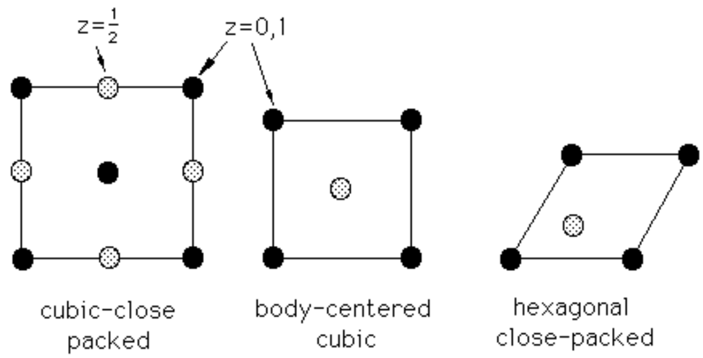

Fig. 1: Projections of the crystal structures of austenite, ferrite and ϵ–iron, along their respective z–axes, which are normal to the plane of the diagram. The dark atoms have z–axis co-ordinates 0 and 1, whereas the lighter atoms are at $\frac{1}{2}z$.

There are two ways in which the austenite can transform into ferrite. The atomic arrangement in a crystal can be altered either by breaking all the bonds and with the help of diffusion, rearrange the atoms into an alternative pattern. This is the *reconstructive* transformation mode in which strain energy is minimised and the atoms are able to partition between the phases in a way which minimises the free energy. However, such a process requires diffusion which may be sluggish at low temperatures.

An alternative mode of transformation which does not require diffusion is known as *displacive* transformation. The ferrite is then generated by homogeneously deforming the austenite into a new crystal structure, Fig. 2. Given the lack of diffusion, the change in crystal structure is accompanied by a change of shape which causes strains and the trapping of solutes. Thus displacive transformations lead to a smaller change in free energy but a more rapid reaction at low temperatures.

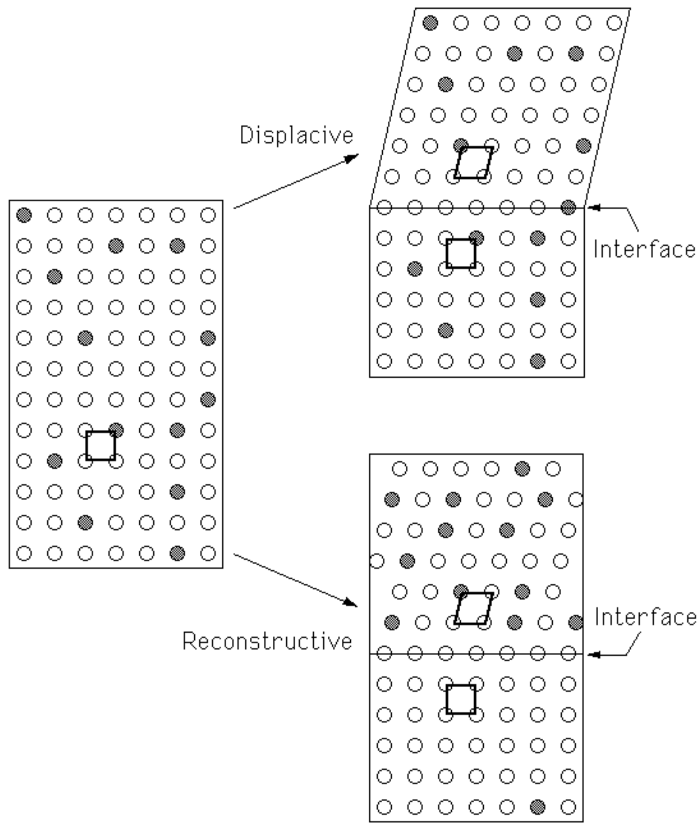

Fig. 2: The main mechanisms of transformation. The parent crystal contains two kinds of atoms. The figures on the right represent partially transformed samples with the parent and product unit cells outlined in bold. The transformations are unconstrained in this illustration.

The Task

The transformation between austenite and ferrite involves nucleation and growth. It can be represented by an Avrami type equation (Lecture MP6–8). We require two such equations, one for the reconstructive transformation which occurs at high temperatures and the other for the displacive transformation which occurs at low temperatures. The Avrami equations can be used to plot a TTT diagram, as illustrated in Fig. 3.

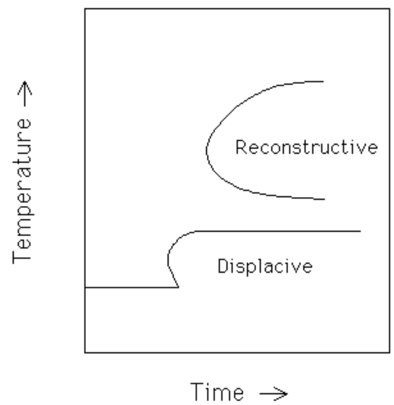

Fig. 3: Schematic TTT diagram showing the time taken to initiate isothermal transformation.

1. Download computer program MAP_STEEL_MUCG46 from the materials algorithms library on www.msm.cam.ac.uk/map/mapmain.html

   This program includes all the thermodynamic and kinetic theory and data needed to calculate a TTT diagram of the type illustrated in Fig. 3. Compile the program and check that it reproduces the output given in the documentation for the standard set of inputs.
2. Repeat the calculation for Fe-0.4C wt% and plot the TTT diagrams. $CTEMP$ is the temperature in degrees Centigrade, $DIFFT$ and $SHEART$ are the times in seconds for the reconstructive and displacive C–curves respectively. You will recall from Dr Manning's lecture that /mphil/examples/plotxy.f is a Fortran program which reads lines of input consisting of x,y coordinates, and then plots them in a box just large enough. /mphil/examples/makefile is the makefile for creating the program.

3. Explain why the time taken to initiate transformation, in each case, shows a C–curve behaviour.
4. Why is the curve for displacive transformations suppressed to lower temperatures when compared with the reconstructive transformations.
5. Repeat the calculation for Fe–0.4C–2Mn wt%. What it the effect of the manganese addition on transformation kinetics, when you compare your results with the corresponding plot for Fe–0.4C wt%?
6. Compare the free energy change for reconstructive ($FPRO$) and for displacive ($FTO400$) transformations at an intermediate temperature. Which leads to a greater reduction in free energy?
7. Is the only effect of the manganese addition through the thermodynamics of transformation? Is the shift in the C–curve following a manganese addition greater for the reconstructive than the displacive transformation?