

Figure 13.23: Illustration of various types of steel in terms of tensile strength and corresponding ductility.

13.4.2 Gum Metal

Gum metal is my example of a metal alloy designed and optimized for specific properties on the basis of first-principle calculations. Given that the material of interest was a multi-component alloy, the many experimental parameters would have made it impractical to evaluate a sufficient number of material compositions by experimental trial and error. Based on the modeling, the material was synthesized, and it confirmed the predicted properties. "Gum metal" is a registered trademark of Toyota Central R&D Labs and was initially developed there. The results of this research were first published in 2003.

Gum metal is a cubic Ti alloy with ultra-low elastic modulus, ultra-high T.S., very large elasticity, and very high plastic deformation at room temperature which occurs without work-hardening. Hence, plastic deformation must take place via a dislocation-free mechanism. In addition, with a suitable heat treatment after cold work, some elasticity can be sacrificed for even greater strength. Yield strengths close to 2000 MPa have been achieved, which is comparable to the strongest steels.

The Toyota researchers sought to optimize the mechanical properties of Ti alloys by varying the composition of several constituents. Optimal properties were achieved for alloys of the approximate composition $Ti_{0.75}X_{0.25}$ where X was another transition metal (Fig. 13.24).

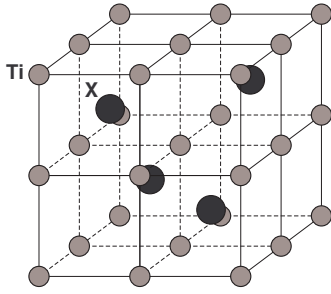


Figure 13.24:
Unit cell of gum metal

In Fig. 13.24 the Ti atoms are on a simple cubic grid, and the X atoms are in the center of every other cube, whether you go in the x-, y-, or z-direction.

The optimal mechanical properties were a result of the alloy's electronic structure, specifically of three "magic numbers" related to the effective number of valence electrons and the atom-atom bond order. The alloy properties could be further improved by adding small amounts of additional elements including oxygen. A practical example is Ti-23Nb-0.7Ta-2Zr-0.1O (mol%).

13.4.3 Metallic Glasses

In our discussion of metals, I made the point that it is almost impossible not to end up with a crystalline material. Specifically, this means that it is very difficult to cool molten metal fast enough not to form crystals, especially a pure metal or a simple alloy.

Therefore, if one is interested in amorphous metals, one has two options: 1) develop an experimental method to cool the molten metal fast enough or, 2) figure out a different way to prevent the molten metal from crystallizing. Both these approaches have been implemented, and it is indeed possible to produce amorphous, i.e. glassy, metals.

What is at issue can be illustrated with a crystallization curve similar to the one we discussed in Chapter 10 on ceramics (cf. Fig. 10.4).

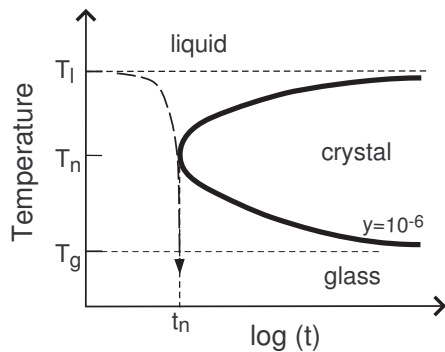


Figure 13.25:
Generic crystallization (TTT) curve for a metal alloy. The critical continuous cooling curve is indicated by the dashed line.

The time-transformation curve in Fig. 13.25 indicates how long it takes for crystallization to begin as a function of temperature. In order that crystallization is avoided entirely, the cooling rate must be larger than the critical cooling rate $r_c = (T_l - T_n)/t_n$, where T_l is the liquidus temperature and T_n the temperature of the nose for the given alloy composition. T_g is the glass transition temperature, below which the amorphous material has become rigid, i.e. essentially solid.

Research on metallic glasses began in the early 1960s with simple binary and ternary alloys. It became evident quickly that very large cooling rates, typically $r_c > 10^5$ K/s, were needed to produce amorphous metals. Such cooling rates were achievable by a process called splat-cooling. This basically involved dropping a small drop of molten material onto a cold surface. As the molten drop spread into a thin splat, it cooled down extremely quickly.

Early experiments involved binary alloys consisting of a transition metal and a non-metal (B, N, C, Si, P). These showed, for example, that alloys of Au, Pt, and Pd yielded ductile glasses, whereas Fe- and Ni-based glasses were brittle. It was also clear that the very high cooling rates made these materials rather impractical, although it was demonstrated that thin metallic glass wires and ribbons could be produced. In addition, there were indications that it may be easier to prevent crystallization in ternary alloys, an example being $\text{Pd}_{78}\text{Si}_{16}\text{Cu}_6$ vs. $\text{Pd}_{80}\text{Si}_{20}$.

The search for more practical materials has been ongoing, and still is. Generally, a multi-component alloy is necessary. Many of the investigated alloys have four or five components. The fundamental question is, of course, what properties of the alloy constituents make it likely that the material will form a glass. You are in a position to appreciate at least in broad outline the important parameters.

First, we can go back one more time to our approach to forming metals by packing spheres. A useful way of visualizing an amorphous alloy is to start with a random packing of spheres of the main constituent and then try to fill the holes in-between these main atoms with other, smaller atoms. It also helps if atoms interact more strongly with the other type rather than with their own kind. Both these characteristics stabilize the amorphous structure. Second, compositions near a eutectic point with a deep eutectic, i.e. with a large temperature difference between the liquidus and the eutectic lines, are favorable for glass formation. A deep eutectic indicates a stable liquid phase.

Since one has to deal with a multi-component system, it is clear that in terms of potentially useful compositions, the range is enormous. Hence, modeling approaches based on thermodynamic and kinetic considerations are being developed so that more compositions can be evaluated quickly, at least in an approximate fashion. Fig. 13.26 gives an example of a set of theoretical TTT curves. The figure is meant to illustrate how sensitive these curves are to small variations in composition. The numerical details, for example the exact conditions for the nose, depend on the model assumptions.

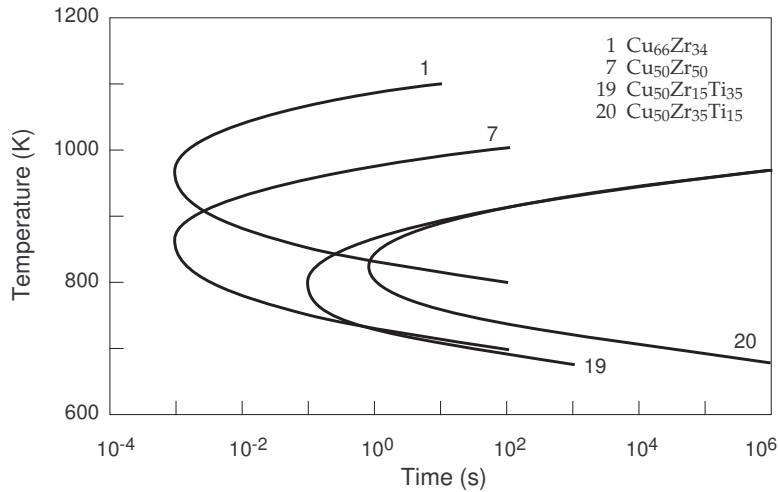


Figure 13.26: Calculated TTT crystallization curves for some CuZr alloys.

An experimental TTT curve for a $\text{Zr}_{58.5}\text{Nb}_{2.8}\text{Cu}_{15.6}\text{Ni}_{12.8}\text{Al}_{10.3}$ alloy is displayed in Fig. 13.27.

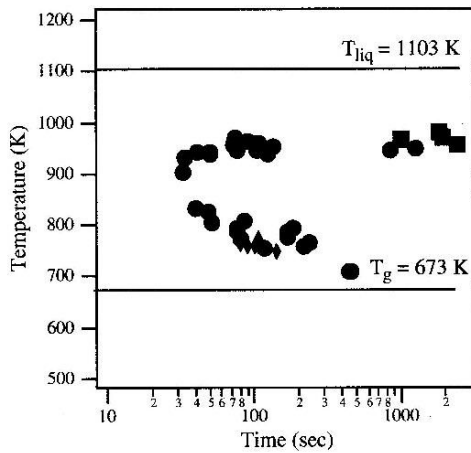


Figure 13.27: Experimental TTT curve for a $\text{Zr}_{58.5}\text{Nb}_{2.8}\text{Cu}_{15.6}\text{Ni}_{12.8}\text{Al}_{10.3}$ alloy.

The mechanical properties of a metallic glass are of special interest compared to polycrystalline metals. From the point of view of structure, the metallic glass is the same type of material as a silicate glass, namely amorphous. But the bonding between the atoms is totally different: metallic in the metallic glass vs. covalent in the silicate glass. Hence, the metallic glass is structurally amorphous, but not a network. The consequence is that a metallic glass is not brittle, but has a very high ductility. Furthermore, its plastic deformation is not by dislocation motion because, being a glass, it does not form dislocations. The

mechanism giving rise to plastic deformation in a metallic glass is complicated but more similar to homogeneous shear. In terms of the elastic modulus and the tensile strength, a metallic glass shows behavior that is typical of a metal.

Recent developments in the application of metallic glasses have taken advantage of TTT curves such as the one in Fig. 13.27 implementing a process called thermoplastic forming. This involves plastic deformation of a metallic glass at a temperature above T_g but below the crystallization curve. Fig. 13.27 suggests that for the right kind of alloy, there will be sufficient time for the material in the viscous state to be formed into a desired shape while remaining amorphous. The deformations achievable under these conditions are, of course, much larger than at room temperature. There are companies offering this type of process as a commercial service.

13.5 Photonic Crystal Optical Fibers

The next case study I wish to present concerns optical fibers, and in particular recent developments in fibers involving a so-called photonic crystal. This will be more a study in advanced materials processing, but the achieved structures are equivalent to new man-made materials. Optical fibers have, of course, become a mainstay of modern communications.

The key feature of optical fibers is that they are able to guide light over long distances. The principle of optical fibers can be illustrated as follows:

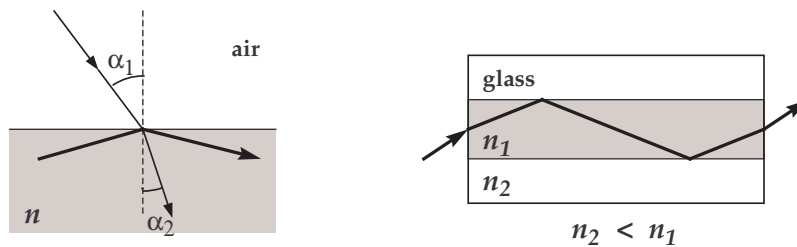


Figure 13.28: Refraction of light at a material interface, and guiding of light inside a fiber by internal reflection.

In the panel on the left, we consider light waves impinging from the air on a piece of planar glass. The optical properties of the glass are indicated by the so-called **refractive index** n , sometimes also called **index of refraction**. The refractive index is the factor by which the propagation velocity of the light wave is reduced in the glass compared to air (or vacuum). The refractive index n is related to the dielectric constant ϵ_r (see Eq. 12.28) by

$$n = \sqrt{\epsilon_r} \quad (13.9)$$