

One can certainly anticipate continuing refinements of such empirical potentials. So far, they have been mainly, though not exclusively, fitted to some experimental quantities relating to perfect or nearly perfect metallic crystals, e.g. equilibrium lattice spacing, cohesive energy, elastic moduli, plus some particular phonon characteristics. But one would envisage, in refinements (see also Heine, 1994) information about unusual bonding geometries (e.g. at reconstructed metal surfaces) or perhaps an interstitial atom at the maximum of its migration barrier, also being embodied.

1.9. *Pair Potentials*

Simulations using empirical interatomic potentials can often supply efficient and usually inexpensive routes for studying ionic structure and dynamics in metallic systems. For a long time, pair potentials were used very extensively in such simulation studies. They can reproduce usefully total energies for many systems. But when one turns to elastic properties, deficiencies begin to emerge (e.g. their inability to reproduce the so-called Cauchy discrepancy: see for instance Johnson, 1972). This situation can be remedied by the addition to the pair potential contribution of a volume-dependent, structure independent energy (the reasons being set out in Chaps. 6 and 7). But in specific examples, such as fracture of surfaces, where the volume is ambiguous, pair potential models need transcending. A further difficulty in the (simplest) pair potential scheme comes up in the determination to the vacancy formation energy E_v (compare Johnson, 1987). It is found empirically that this energy E_v is typically about 1/3 of the cohesive energy. In contrast, the straightforward pair potential models predict that, excluding the contribution from relaxation which is modest in close-packed metals, these two energies are equal. These limitations of the simple pair potential approximation have been addressed by the development of empirical many-body potentials which is the major theme of Chap. 8.

1.10. *Grain and Twin Boundaries*

Most solids do not occur as single crystals. Usually, they are assemblies of small crystallites randomly oriented with respect to one another. The boundaries between them are referred to as grain boundaries (Mclean, 1957; Kê, 1947, 1990). Rosenberg (1978) gives a figure (Fig. 3.7, p. 42) of crystallites and grain boundaries in α -brass: the specimen having been first cold-rolled and then annealed. Generally the structure of a grain boundary is complicated, but

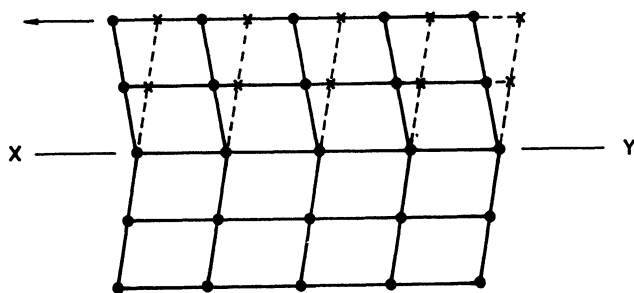


Fig. 1.3. Twinning. The crystal structure is reflected in the plane XY which forms the twin boundary. The vertical sides of the crystal as drawn are no longer smooth.

a special case of importance is that for which the orientation of neighbouring grains is very similar: such cases are termed low-angle boundaries. Their geometry is relatively simple and can be expressed in terms of dislocations.

We shall return to grain boundaries in Chap. 8 when we report atomistic structures with some realistic force laws. However, let us summarize here a few basic facts on twin boundaries.

Crystals are frequently produced with a fault which is such that one region of the crystal is a mirror image of the other part. The atoms in one region are in positions produced by reflecting the atoms in the second part at some symmetry plane of the crystal. Figure 1.3, reproduced from Rosenberg (1992), is an example of twinning. The crystal structure is reflected in the plane XY which forms the twin boundary.

Twinning frequently occurs in metals which have a small stacking fault energy as this fact then implies that the additional energy needed for any small atomic mismatch is small. Twinning can also happen during deformation. Twinning planes can often be seen by optical microscopy, and the presence of twins can be detected by X-ray diffraction. This is due to extra sets of spots which are produced from the twinned regions.

1.11. Alloy Formation: Rules and Models

1.11.1. Solid Solubility: Hume-Rothery Factors

Hume-Rothery *et al.* (1934, 1969) in very early work proposed several factors controlling the extent of solid solubility. Even at the time of writing, these factors form a useful basis for discussing the formation of extensive or restricted solid solutions (see also Alonso and March, 1989).