

Mandelbrot used the word ‘fractal’ for these complex shapes, in order to emphasize that they are to be characterized by a non-integer (fractal) dimensionality.

Our interest here is the fractal aspects of fractured surfaces. Mandelbrot *et al.* (1984) gave an elegant route for determining the fractal dimension D of the fractured surface. Their work pointed to a correlation between toughness and D . Further studies were performed by Lung (1986), Pande (1987), Lung and Mu (1988) and Xie and Chen (1988). Bouchaud *et al.* (1990) later reported their findings that for a variety of rupture modes and materials the observed fractal dimensions were the same to within the error bars. Dauskardt *et al.* (1990) reported a fractal dimension $D \cong 2.2$, which, when combined with the studies of Bouchaud *et al.* (1990) may turn out to be a universal value (but also see below).

Though it is known that cracks in nature can have fractal character, at the time of writing it is still difficult to specify just how this fractal nature arises. For it is certainly true that the mechanisms leading to fracture are highly material dependent (see Liebowitz, 1984). This, we will discuss further in Sec. 4.17.

Progress has resulted from modelling the growth of a single, connected crack. With the assumption of central forces numerical simulations of media with a breaking probability proportional to the elongation of springs revealed that the cracks resulting are fractal (Louis *et al.*, 1986; Hinrichen *et al.*, 1989). The fractal dimension of such cracks appears to be sensitive to the type of external force (e.g. uniaxial tension, shear, uniform dilatation) but since only rather small cracks can be grown, more precision is lacking. Herrmann (1989) has considered therefore deterministic models.

1.8. ‘Glue’ and Related Models of Interatomic Force Fields

Ab initio simulation of complex processes is fairly commonplace at the time of writing. But it is still eminently worth while (compare Heine, 1994) to ask whether empirical models for accounting for interatomic bonding can be refined so as to make them, even if not completely satisfactory, at least widely useful.

In the field of interest of our book, namely metals and metallic alloys, the various types of ‘glue’ models (Finnis and Sinclair, effective medium, embedded atom, etc.) developed since the early 1980s embody metallic many-atom bondings and therefore are major advances over earlier models.

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