1.4. *Dislocation Core and Atomic Force*

Early development of dislocation theory, and related theoretical treatment of metallic properties controlled by dislocations, focussed most attention on the effects of long-range elastic fields. In the present context (see also Vitek, 1995) mechanical properties were frequently analyzed in terms of long-range dislocation-dislocation, dislocation-point defects, etc interactions. The attitude prevailing in the late 1960s that dislocation cores were of but secondary importance in the plastic deformation of metals was radically altered in the next two decades. It became widely recognized then that dislocation core phenomena could play a role at least as important as long-range interactions in the deformation behaviour of many materials. As emphasized in the studies of Vitek and co-workers (Vitek, 1985) clear signatures of core effects are to be found in deformation modes and slip geometry, strong orientation and temperature dependences of the yield stress, and also in anomalous temperature dependence of the yield and flow stresses (see also Duesbery and Richardson, 1991).

Significant impetus for such atomistic modeling has been the marked improvement in experimental techniques (see Appendix 2.1), such as high resolution electron microscopy (HREM), that are capable of atomic resolution.

1.5. *Stacking Faults*

Rosenberg (1992) discussed how close-packed planes of hard spheres can be stacked to form, say, an fcc structure, Fig. 1.2 being reproduced from his account.

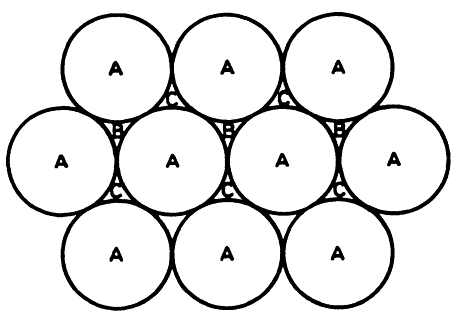

Fig. 1.2. The close-packed array of spheres. Note the three different possible positions. A, B and C for the successive layers.

The first and second layers can be in positions labelled A and B while the third layer can be placed above the C positions. The pattern continues as ABCABC..., the pattern repeating at every third layer.

A stacking fault* in such an fcc structure occurs if this sequence gets disturbed, as in ABCBCABC.... Here a layer A is missing, while in the sequence ABCABACABC... an extra A layer has been introduced. While stacking faults can, at least in principle, extend through the entire crystal, they usually occupy only a part of the plane. In this last case, of a stacking fault which terminates within the crystal, the configuration at the termination is referred to as a partial dislocation.

1.6. *Glissile and Sessile Dislocations*

Dislocations that can move by pure slip are called glissile. Dislocations which cannot glide, but have to move by some form of mass transport are called sessile (Read, 1953).

In crystals, the dislocation core spreads to certain crystallographic planes containing the dislocation line. If the core spreads into one of such planes, the core is planar and is glissile. If the core spreads into several non-parallel planes of the zone of the dislocation line, it is non-planar and is sessile. In the former case the dislocation moves easily in the plane of the core spreading, while in the latter case, it moves only with difficulty (Vitek, 1992). A Shockley partial is a partial dislocation, the Burgers vector of which lies in the plane of the fault. Then, Shockley partials are glissile. A Frank partial is a partial dislocation, the Burgers vector of which is not parallel to the fault. Then, Frank partials are sessile.

1.7. *Concept of Fractals*

Over a decade or more, diverse scientists have recognized that many of the structures common in their experiments have a quite special kind of geometrical complexity. The pioneering work was that of Mandelbrot (1977, 1979, 1982, 1988) who drew attention to the particular geometrical properties of such things as the shore of continents, tree branches, or the surface of clouds.

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*Stacking faults remain a challenge for interatomic force fields. A novel system which might test N-body force lows discussed in Chapter 8 has arisen from the study of S. A. de Vries *et al.*, (Phys. Rev. Lett. *81*, 381, 1998). These authors have studied the influence of Sb on the formation of stacking faults due to Ag(111) growth using X-ray scattering (see also related theoretical studies of S. Oppo *et al.*, Phys. Rev. Lett. *71*, 2437, 1993).