Table 3.1. *Vectors* $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ *that define the primitive unit cell of simple crystals.*

Only crystals with one or two atoms per unit cell are considered; the position of one atom in the PUC is always assumed to be at the origin; when there are two atoms in the PUC, the position of the second atom $\mathbf{t}_2$ is given with respect to the origin. All vectors are given in cartesian coordinates and in terms of the standard lattice parameter a, the side of the conventional cube or parallelpiped. For the HCP lattice, a second parameter is required, namely the c/a ratio. For graphite, only the two-dimensional honeycomb lattice of a single graphitic plane is defined. d_{NN} is the distance between nearest neighbors in terms of the lattice constant a. These crystals are illustrated in Fig. 3.1.

Lattice	$\mathbf{a}_1$	$\mathbf{a}_2$	$\mathbf{a}_3$	$\mathbf{t}_2$	c/a	d_{NN}
Cubic	$(a, 0, 0)$	$(0, a, 0)$	$(0, 0, a)$			a
BCC	$(\frac{a}{2}, -\frac{a}{2}, -\frac{a}{2})$	$(\frac{a}{2}, \frac{a}{2}, -\frac{a}{2})$	$(\frac{a}{2}, \frac{a}{2}, \frac{a}{2})$			$\frac{a\sqrt{3}}{2}$
FCC	$(\frac{a}{2}, \frac{a}{2}, 0)$	$(\frac{a}{2}, 0, \frac{a}{2})$	$(0, \frac{a}{2}, \frac{a}{2})$			$\frac{a}{\sqrt{2}}$
Diamond	$(\frac{a}{2}, \frac{a}{2}, 0)$	$(\frac{a}{2}, 0, \frac{a}{2})$	$(0, \frac{a}{2}, \frac{a}{2})$	$(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$		$\frac{a}{4\sqrt{3}}$
HCP	$(\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0)$	$(\frac{a}{2}, -\frac{\sqrt{3}a}{2}, 0)$	$(0, 0, c)$	$(\frac{a}{2}, \frac{a}{2\sqrt{3}}, \frac{c}{2})$	$\sqrt{\frac{8}{3}}$	$\frac{a}{\sqrt{3}}$
Graphite	$(\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0)$	$(\frac{a}{2}, -\frac{\sqrt{3}a}{2}, 0)$		$(\frac{a}{2}, \frac{a}{2\sqrt{3}}, 0)$		$\frac{a}{\sqrt{3}}$

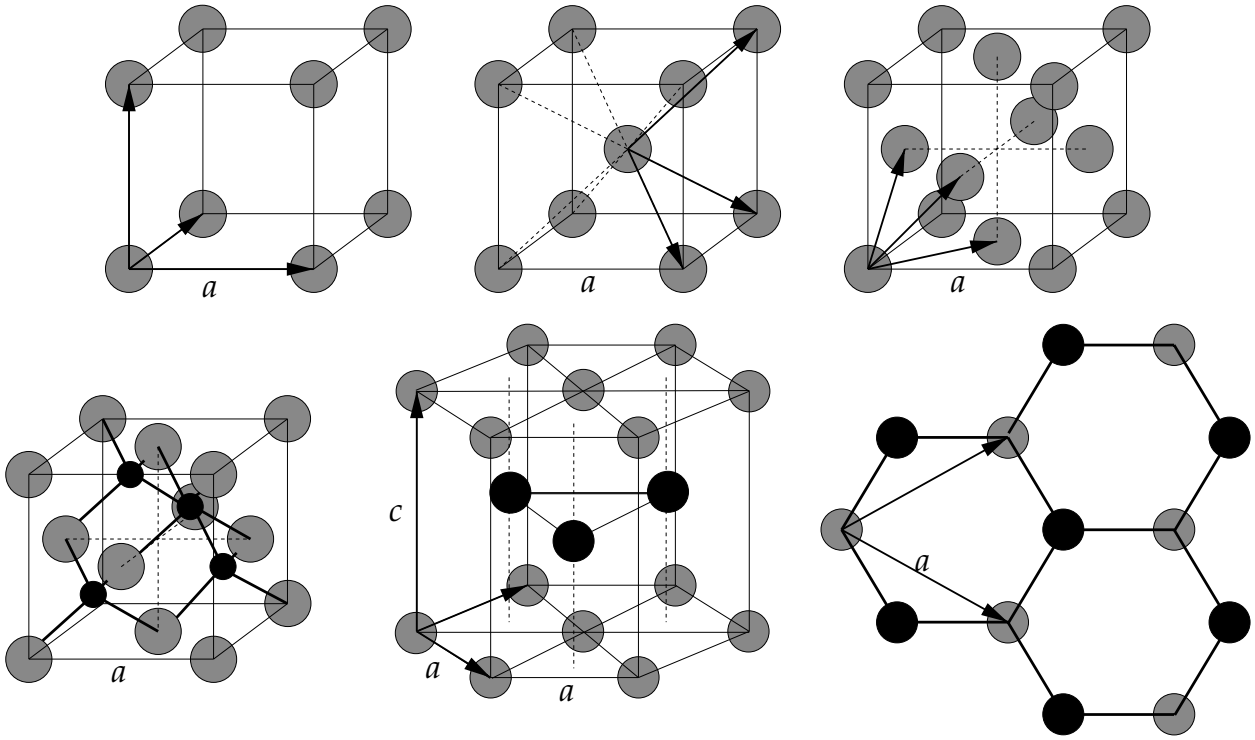

Figure 3.1. The crystals defined in Table 3.1. **Top**: simple cubic, BCC, FCC. **Bottom**: diamond, HCP, graphite (single plane). In all cases the lattice vectors are indicated by arrows (the lattice vectors for the diamond lattice are identical to those for the FCC lattice). For the diamond, HCP and graphite lattices two different symbols, gray and black circles, are used to denote the two atoms in the unit cell. For the diamond and graphite lattices, the bonds between nearest neighbors are also shown as thicker lines.