Oxygen has a high diffusion coefficient, $D = 0.13\ \exp(-2.53/kT)$ [36]. By heat treatments, the distribution of oxide particles may change since particles may get dissolved when heated and grow when cooled. Oxygen atoms are found to change the effect of other impurities, a process known as internal gettering.

One important oxygen source is the crucible. Silicon is normally melted in high-purity-fused quartz (SiO_2) crucibles (single crystals) or quartz crucibles coated with high-purity Si_3N_4 (multicrystalline ingots). If holes appear in the coating, quartz will easily dissolve in the melt and raise the level of oxygen in the solid.

The variety of effects observed with oxygen in silicon will truly stimulate further research for a long time.

5.6.3.4 Transition metals

Properties of transition-metal impurities in silicon have been reported in a large number of articles, reviews and books [28–30, 33]. The transition metals are presented by the symbols 3d, 4d and 5d, which specify the outer electron configuration of a neutral atom. Most of the metals forming deep energy levels ("midway" between the conduction band and the valence band) in silicon belong to this group and have therefore a large influence on the electronic properties of silicon.

The main impurities found in silicon belong to the 3d transition metals (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu). In general, these are present as interstitial impurities.

The diffusivity increases with increasing atomic number in the 3d row (see Figure 5.8), with Ni and Cu having the largest diffusion coefficients known in silicon.

The concentration of vacancies is very low in silicon. The high diffusion coefficients of 3d elements can therefore only be explained by interstitial diffusion mechanisms independent of vacancies.

The 3d transition metals have a steep temperature-dependent solid solution limit that make them easily supersaturated during cooling (see Figures 5.9 and 5.10). They therefore frequently form complexes/precipitates at dislocations, grain boundaries or other lattice defects.

The solubility at room temperature is very low, of the order of 1 atom/cm^3. However, some 3d impurities are mobile even at room temperature. So the atoms with the highest mobility (Co, Ni, Cu) will be out of the solid solution during or just after the cooling. The 3d metal atoms with a low diffusivity may remain in the solid solution at interstitial sites for a much longer time after cooling. This may depend upon crystal perfection, which determines the diffusion length to reach sinks such as dislocations, grain boundaries and precipitates.

The solid solubility of the 3d transition metals in silicon is shown in Figure 5.10.

A severe deterioration of the electrical properties is expected from solid solution impurities capturing the minority carriers (being electrons on the *p*-side of a *p-n*