

To be able to control the level of doping, the concentration of unwanted elements from the Groups IIIA and VA must be well below the concentration of the doping element.

Our theoretical understanding of the properties of impurities in silicon other than those from the Groups IIIA and VA is less well developed. However, as new instrumentation has become available, a lot of experimental results of high scientific standard have been published.

5.6.3.2 Carbon

Carbon is a common substitutional impurity. Like silicon it has four valence electrons and is therefore electrically neutral. The carbon atom is smaller than the silicon atom and may therefore be involved in precipitation of species expanding the lattice like silicon oxide.

The solid solubility limit is $C_S = 3.5 \times 10^{17}$ atom/cm³ at the melting point or $C_S(T) = 4 \times 10^{24} \exp(-2.3 \text{ eV}/kT)$ atoms/cm³, where k is the Boltzmann's constant [89, 91].

In metallurgical grade (MG) silicon, carbon is present at levels above the solid solubility limit and SiC precipitates are commonly present. In electronic grade (EG) the concentration of carbon is low. But in contact with the crucible and the carbon-rich atmosphere (graphite), it is difficult to avoid contamination of the melt.

As a substitutional element, carbon diffuses rather fast [$D = 1.9 \exp(-3 \text{ eV}/kT)$ cm²/s], but much slower than interstitial impurities.

5.6.3.3 Oxygen

The subject of oxygen atoms in silicon has been studied for many years. Since results from experiments performed under different thermal histories have varied, the discussion goes on.

Oxygen atoms in solid solution are electrically inactive and predominantly enter interstitial sites. The equilibrium value of the solid solubility at the melting point is generally accepted to be 1×10^{18} atom/cm³. However, the results from measurements of solid solubility as a function of temperature differ markedly. The value of k_0 will therefore vary (see Table 5.7).

In a work by Itoh and Nozaki [32] an important point was made that the concentration of oxygen at equilibrium at a given temperature was determined by the type of oxide that was stable at that temperature. So if the type of oxide varied, it would be expected that bends in solid solubility curves at temperatures at which the silicon oxides change would be observed. However, up to 1200°C, SiO₂ is the stable chemical form and the solubility $L = \exp(\Delta S/R) \exp(-\Delta H/kT)$ will have constant values of ΔS and ΔH .

On cooling, super saturation is easily obtained and oxygen precipitates at a rate that depends on oxygen content, temperature, and time at temperature and nucleation sites. Carbon is also found to influence the precipitation of silicon oxides, possibly because the carbon atoms reduce the expansion of the lattice when silicon oxide is growing.