Table 5.7 Distribution coefficients, k_0, for some elements in silicon at the melting point [24, 25]

Element	k_0	Element	k_0
B	0.8	Ti	3.6×10^{-4}
Al	0.002	Cr	1.1×10^{-5}
Ga	0.008	Mn	1×10^{-5}
N	7×10^{-4}	Fe	8×10^{-6}
P	0.35	Co	8×10^{-6}
As	0.3	Ni	8×10^{-6}
C	0.07	Cu	4×10^{-4}
O	0.25–1.25	Zn	1×10^{-5}

out of the boundary layer. At this point the ratio $(X_l)_{\text{interface}}/(X_l)_{\text{bulk}}$ becomes constant. The effective distribution function k_{eff} is defined as

$$k_{\text{eff}} = X_{\text{s, interface}} / X_{\text{l, bulk}}$$

and tells a great deal about liquid mixing in front of the interface. Poor mixing in the melt results in $k_{\text{eff}} = 1$. Good mixing (no build-up) means $k_{\text{eff}} = k_0$.

Burton *et al.* [26] have derived an expression for k_{eff} when a rotating crystal is pulled from the melt at a velocity v:

$$k_{\text{eff}} = k_0/[k_0 + (1 - k_0]\exp^{-\Delta})$$

where

$$\Delta = v\delta/D_l \text{ and } \delta = 1.6\ D_l^{1/3} \cdot \nu^{1/6}\ \omega^{-1/2}$$

where δ is the distance from the growing interface to where the concentration in the melt is uniformly equal to $X_{l,\text{bulk}}$, D_l is the diffusion coefficient of the solute, ν is the viscosity and ω the crystal rotation rate.

Kodera [27] has applied this to obtain δ/D_l and D_l values for melts doped with various impurities at different rotating rates, as shown in Table 5.8. For CZ-grown silicon where v is around 1 mm/min, Δ is small and k_{eff} is close to k_0 [24].

The ability to purify molten feedstock by solidification will therefore vary for the different impurities and with solidification velocity. The validity of the assumption of no diffusion in the solid will not be met at a slow solidification rate and some "back" diffusion will take place. In addition, impurities diffuse from the crucible into the solid, the rate depending on temperature and time. Selection of the optimal casting process parameters is complicated and improvements will depend on the ability to model the total solidification process.

5.6.2 Effect of Crystal Imperfections

Silicon has a diamond lattice atomic structure being cubic with atoms joined to four nearest neighbours by covalent bonds at tetrahedral angles. If the atoms are represented