

Figure 5.7 Composition profile after the entire rod of Figure 5.6 has solidified, illustrating normal solidification at two different values of k_0 , $k_{0-1} = 0.35$ (upper curve) and $k_{0-2} = 0.05$

melt has a uniform composition and (3) negligible diffusion takes place in the solid, a composition profile like the one in Figure 5.6 is obtained when equilibrium prevails at the interface.

A horizontal cylinder of liquid alloy of initially uniform composition X_0 is cooled at the left end (see Figure 5.6b). Let a small amount of solid form so that the solid–liquid interface is located at position 1. When a small volume has solidified, the composition in that volume has dropped from X_0 to k_0X_0 . A mass of solute proportional to the crosshatched area to the left of position 1 has been removed from the solid and rejected into the remaining liquid. This will increase the liquid composition to a level above *X*0. If we consider that local equilibrium prevails at the solid–liquid interface during solidification, the liquid and solid compositions at the interface are tied together by the equation $X_s = k_0 X_1$. So when the composition of the liquid is raised, the solid composition must also rise as solidification proceeds. When the solid–liquid interface has moved to position 2, the solid composition will have gradually increased, as shown in Figure 5.6(b).

It is shown in Figure 5.7 that k_0 will have a marked effect on the distribution of impurities in solid silicon. Values of *k*⁰ for different elements are given in Table 5.7 [24, 25]. For impurities having a low value of k_0 , for example, $k_{0,Fe} = 8 \times 10^{-6}$, the solidification process has a large purifying effect: only one Fe atom out of about 100 000 in the melt will enter the solid when solidification starts. For elements in which k_0 is near to 1, no marked change in the concentration of impurities will appear between the melt and the solid silicon.

During the solidification process, the impurity concentration at the interface varies with the fraction of melt solidified and $k₀$. If the solute rejected into the boundary region is not transported immediately into the melt in front of the interface, solute will build up at the boundary. As the solute builds up, however, its concentration gradient across the boundary layer becomes steeper and the rate of transport through the boundary layer by diffusion increases until a balance is obtained between the solute being rejected into and