Thus, it may be important to include impurity gettering and hydrogen passivation in TF-Si solar cell fabrication [88–92].

The impurities of most interest in PV-Si are the transition metals (TM), particularly Fe, Cr, and Ni. They are typically present in concentrations as high as $10^{14}/cm^3$ in the as-grown substrates. In the dissolved state, these impurities are highly mobile with diffusivities close to 10^{-6} cm^2/s at typical process temperatures [93]. They produce deep level electronic states within the bandgap which act as efficient recombination sites. For example, at room temperature, the interstitial iron (Fe_i) introduces a donor level at $E_T \approx E_V + (0.375 \pm 0.015)$ eV. The hole capture cross section of interstitial iron can be written as (in cm^{-2})

$$\sigma_p(\mathrm{Fe_i}) = (3.9 \pm 0.5) \times 10^{-16} \times \exp\left(-\frac{0.045 \pm 0.005\ \mathrm{eV}}{k_B T}\right), \qquad (8.8)$$

where k_B stands for the Boltzman constant and T is the temperature. The electron-capture cross-section of Fe at room temperature was measured as $\sigma_n = 4 \times 10^{-14}/\ cm^2$. Because of near-mid gap energy and a large-capture cross-section, it is expected that Fe will produce high-recombination or low minority-carrier lifetime.

TMs in Si also have the ability to form complexes with each other. For example, B can form Fe–B and B–O pairs. B–Fe forms a donor level at $E_v + 0.1$ eV ($\sigma_n = 4 \times 10^{-13}/cm^2$ at the room temperature) and an acceptor level at $E_c - 0.29$ eV. At low injection levels, the recombination rate caused by the Fe–B pair is lower than that of interstitial Fe. Recent studies have also shown that B–O pair formation occurs in some solar cells. This effect is manifested as a decrease in the minority-carrier diffusion length (MCDL) of the cell under sunlight. This mechanism has a pronounced effect of reducing the efficiency of a Si solar cell.

Impurity gettering is used in microelectronic device fabrication to trap impurities away from the active region of the device by oxygen precipitates. This leaves a very clean, denuded surface region, while the impurities are driven into the bulk. For this reason, it is often referred to as *internal gettering*. Because microelectronic devices use only the near-surface region of the wafer, internal gettering works well for them. Solar cells, being minority-carrier devices, use nearly the entire thickness for the device. Hence, it is necessary to apply external gettering techniques to clean up the bulk of the material. In external gettering, a surface region serves as a sink for impurities. Fortunately, phosphorous diffusion and Al alloying are some of the processes that have worked well for efficient gettering in solar cells. Because these processes are extensively used in solar cell fabrication for junction and contact formation, all Si solar cells experience a certain degree of gettering. In a typical junction formation or Al alloying process, the Fe concentration can be reduced by two orders of magnitude. Theoretical and experimental details of P and Al gettering are reviewed in several papers [94, 95]. For a typical multicrystalline Si wafer, P diffusion for formation of an n^+p solar cell can lead to an improvement in the average MCDL from a value of about 50 μm to 75 μm. This increase in the MCDL is caused by removal of fast-diffusing transitional metal impurities from the bulk of the substrate into the P diffused region. Similar results are obtained with the Al-alloying used for formation of the backside p^+ region and back metallization.