Impurity Diffusion

The expression for the concentration $C(x,t)$ in one-dimensional diffusion when the tracer or impurity slab is much thinner than the diffusion length (i.e., $h \ll 2\sqrt{Dt}$) is:

$$C(x,t) - C_1 \approx (C_0 - C_1)\frac{h}{\sqrt{\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right) \tag{1}$$

For impurity diffusion, C_0 is the impurity in the as-coated impurity layer, and C_1 is zero for pure materials. Assuming that the concentration is proportional simply to the intensity as measured by SIMS,

$$I(x,t) \approx \frac{I_0 h}{\sqrt{\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right) \tag{2}$$

Unfortunately, I_0 is not readily available after diffusion takes place and also because surface effects influence the measured intensity. We can let the product $I_0 h$ be a fitting parameter. Experimental data can be fitted to (2) by minimizing the sum of the square of the residuals and letting $I_0 h$ and D be fitting parameters:

$$\sum_x \left\{I(x,t) - \left[\frac{I_0 h}{\sqrt{\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)\right]\right\}^2 . \tag{3}$$

Since $I(x,t)$ can vary due to drift in incident ion-beam intensity, it may be corrected using the Mg-24 signal for diffusion into Mg alloys.

$$\sum_x \left\{\frac{I(x,t)}{I_{\mathrm{Mg}}(x,t)} - \left[\frac{I_0 h}{\sqrt{\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)\right]\right\}^2 \tag{4}$$

In experimental practice using SIMS depth profiling, some further broadening of the diffusion profile is expected by roughening and mixing. Schultz et al. 2003[1] include a σ term to account for this effect, which leads to a further modified form of (4):

$$\sum_x \left\{\frac{I(x,t)}{I_{\mathrm{Mg}}(x,t)} - \frac{I_0 h}{\sqrt{\pi Dt}}\exp\left[-\left(\frac{x}{2\sqrt{Dt+\sigma^2}}\right)^2\right]\right\}^2 \tag{5}$$

[1] Olaf Schulz, Manfred Martin, Christos Argirusis and Günter Borchardt. 2003. "Cation tracer diffusion of ^{138}La, ^{84}Sr and ^{25}Mg in polycrystalline $La_{0.9}Sr_{0.1}Ga_{0.9}Mg_{0.1}O_{2.9}$" *Phys. Chem. Chem. Phys.* **5**, 2308–2313.