Inverse determination of interdiffusion coefficients in Si-Al-Fe alloys

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Diffusion of silicon and aluminium in steel in an important topic in electrical steels. In a macro-model approach, the relevant diffusion equations are, with $i = 1$ (Si), 2 (Al),

$$\frac{\partial n C_i^3(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(D_{i1}^3\left(C_1^3, C_2^3\right)\frac{\partial C_1^3(x,t)}{\partial x} + D_{i2}^3\left(C_1^3, C_2^3\right)\frac{\partial C_2^3(x,t)}{\partial x}\right), \quad (1)$$

where $0 \leq x \leq L$, $0 \leq t < \infty$, and the superscript 3 indicates the dependent element (Fe). Appropriate boundary conditions are imposed.

We show how to determine practically the four interdiffusion coefficients $D_{ij}^3,\ i,j = 1,2$, from experimental measurements of concentration profiles at discrete timesteps, thus avoiding separate interdiffusion determining experiments. An unbiased approach is chosen, comparing a Levenberg-Marquardt type of approach with a costate (adjoint) approach.