Ni_4Ti_3 Precipitates in NiTi Shape Memory Alloys: Effect of Diffusion Fluxes Driven by Elastic Energy Gradients

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The formation of coherent Ni_4Ti_3 precipitates in bulk and grain boundaries of NiTi shape memory alloys controls subsequent martensitic phase transformations and therefore the shape memory effect. Nucleation and growth of these precipitates occurs under the dual influence of concentration and stress. In this study, we investigate stress-driven diffusion which adds to normal diffusion, as outlined by Larche and Cahn [1]. There is a composition dependence of i) lattice parameters (Vegard's law) and ii) elastic coefficients. Although the first term is discussed in detail in the literature, the second one is widely neglected. We show that the effect of compositional dependency of elastic constants is strongly correlated to solutal diffusion and may play an important role on the precipitation process. We employ the phase field simulation to study the effect of simultaneous concentration and stress fields variations. The coefficients of the elastic matrix, in particular their dependence on composition are determined from first principles calculations. This model predicts the existence of stress stabilized solutal gradient around the precipitates which in contrast to previous models is closer to the experimental observations.

Reference:

[1] F.C. Larche, J.W. Cahn. Acta metall, 30:1835â€“1845, 1982.