A Sharp-Interface Approach for Diffusion-Controlled Phase Transformations with Application to Cu_6Sn_5 Growth

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The formation and growth of intermetallic compounds (IMCs) are common in soldering and electroplating applications. In many cases, IMC growth is diffusion-controlled. At the atomistic scale, composition typically varies rapidly but continuously across phases. However, at the *mesoscale*, interfaces can be effectively treated as discontinuous, motivating the use of a sharp-interface formulation, which forms the basis of the present work.

We present a model that consistently couples mechanical deformation with atomic diffusion. The thermodynamic formulation treats the bulk material, grain boundaries, and phase interfaces within a unified framework, following [1]. The theoretical development follows a consistent structure in which general thermodynamic principles are clearly separated from constitutive assumptions. In the bulk, the framework allows for elasto–plastic deformation. At grain boundaries, the framework provides a thermodynamically consistent description of stress-driven grain boundary sliding and diffusion. Grain boundary diffusion and sliding are implemented through a three-field variational formulation, while phase interfaces are evolved using a level-set method known as the Voronoi implicit interface method.

A binary Cu–Sn system is considered, in which a Sn layer is deposited on a Cu substrate, leading to the formation of the IMC Cu_6Sn_5 at the interface. The evolution of biaxial stress in the Sn layer is shown in Figure 1 for both columnar and equiaxed microstructures. The results indicate that grain boundary diffusion significantly enhances stress relaxation in the equiaxed microstructure, while its effect is negligible in the columnar case. These findings suggest that grain boundary diffusion is a plausible mechanism for explaining the increased stress relaxation observed experimentally in equiaxed microstructures [2].

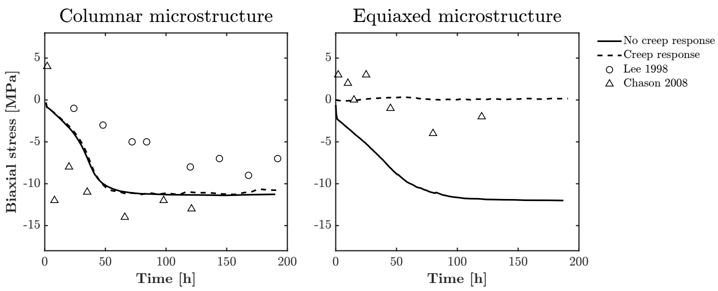

Figure 1. Biaxial stress in the Sn film for a columnar (left) and an equiaxed (right) microstructure.

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[1] Eliot Fried and Morton E Gurtin. Coherent solid-state phase transitions with atomic diffusion: a thermomechanical treatment. *Journal of statistical physics*, 95(5):1361–1427, 1999.

[2] E Chason, N Jadhav, WL Chan, L Reinbold, and KS Kumar. Whisker formation in Sn and Pb–Sn coatings: Role of intermetallic growth, stress evolution, and plastic deformation processes. *Applied Physics Letters*, 92(17), 2008.