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Grain-boundary grooving and agglomeration of alloy thin films: phase-field simulations MATHIEU BOUVILLE, DONGZHI CHI, Institute of Materials Research and Engineering, DAVID J. SROLOVITZ, Yeshiva University — A common failure mode in polycrystalline thin films is grain- boundary grooving through the thickness of the film. This can bring the surface in contact with the substrate, leading to film agglomeration. Although grain-boundary grooving has received a great deal of attention over the past half-century, the extant models are too idealized to be useful to predict agglomeration in most technologically interesting materials, such as multicomponent alloy films. We relax many of the assumptions made in the classical analysis, thereby finding unprecedented richness in the problem. Our approach employs a phase-field model for grain-boundary grooving and agglomeration of polycrystalline alloy thin films. In particular, we study the effects of slow-diffusing species on grooving rate. As the groove grows, the slow species becomes concentrated near the groove tip so that further grooving is limited by the rate at which it diffuses away from the tip. At early times the dominant diffusion path is along the boundary, while at late times it is parallel to the substrate. This change in path strongly affects the time- dependence of grain boundary grooving and increases the time to agglomeration. The present model provides a tool for agglomeration-resistant thin film alloy design.

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