Grain growth in thin films – when the third dimension matters

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Abstract

Grain boundary motion is a complex three-dimensional process driven by a reduction of the Gibbs free energy. While the case of a spherical grain embedded in a larger matrix grain is easy to calculate, two- or three-dimensional polycrystalline structures are much more complex. In this case, the evolution of the grain structure is the result of an interplay between total volume conservation and a preservation of the local balance in the grain boundary network regarding, e.g., dihedral angles along triple lines. Historically, grain growth has mainly been investigated in two dimensions. Two-dimensional sections have been analysed experimentally and corresponding numerical 2D simulations have been employed. For thin films, in particular, this practice has survived even until recent times. In our current study we show that two-dimensional considerations cannot mimic the three-dimensional grain boundary motion. To that aim, we model a three-dimensional grain structure in a highly textured thin film with one added, particularly large grain of deviating orientation. The migration of its boundary depends strongly on both, the location of the particular grain and the morphology of the matrix grains. Such a dependence can indeed only be captured in three dimensions. The implications for texture evolution in thin films are discussed.

Keywords: grain boundary motion, thin films, polycrystalline structure, texture, simulation

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