INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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Capturing the complex physics behind universal grain size distributions in thin metallic films

Grain growth experiments on thin metallic films have shown the geometric and topological characteristics of the grain structure to be universal and independent of many experimental conditions. The universal size distribution, however, is found to differ both qualitatively and quantitatively from classical curvature driven models of Mullins type, which reduce grain growth to an evolution of a grain boundary network, with the experiments exhibiting an excess of small grains (termed an “ear”) and an excess of very large grains (termed a“tail”) compared with the models. While a plethora of extensions of the original Mullins model have been proposed to explain these characteristics, none have been successful. In this work, large-scale simulations of a model that resolves the atomic scale on diffusive time scales, the phase field crystal model, are used to examine the complex phenomena of grain growth. The results are in remarkable agreement with the prior experimental results, recovering the characteristic “ear” and “tail” features of the experimental grain size distribution. The simulations also indicate that, while the geometric and topological characteristics are universal, the dynamic growth exponent is not.