EFFECT OF LATTICE AND NEIGHBOURS IN THE 2D AND 3D MONTE CARLO GRAIN GROWTH SIMULATIONS

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Abstract:

Grain growth is largely studied both theoretically and by computer simulations in two dimensions. but it represents as yet a challenge in three dimensions because the difficulty to studying the gain growth from physical experiments. Usually, microstructure studies are performed for cross-sections of experimental specimens, thus providing only 2D microstructure information's. Therefore. computer simulation is actually the most effective tool for studying the 3D grain growth process. In this paper, three and two dimensional Monte Carlo simulations are conducted to study the isotropic gain growth. This technique involves representing the microstructure on a discrete set of regular space grid. In this paper we investigate the *effect* of lattice that represents the discrete microstructure by using a square grid for 2D and a simple cubic network for 3D. Grain growth kinetics and their topology are analyzed with the 1^{st} , 2^{nd} and 3^{rd} neighbour's consideration both on 2D and 3D. 1t can be seen that a compact grain structure was developed. Various microstructural features of normal grain growth commonly observed in 2D Monte Carlo simulations were also seen in the microstructure in the cross-section planes. The first results show that the lattice symmetry and the neighbour's number have a fundamental influence on the results of grain growth simulation. Also the average grain size is a very important parameter because it is closely related with many properties of simulated microstructures. The mean grain size increases as a power law of the time both in 2D and 3D simulations but microstructure evolutions on 2D cross-sections starting from 3D simulation give better results compared to a direct 2D simulation.

Keywords: Monte Carlo; grain growth; topology; lattice; neighbours; 3D; 2D