Incorporating grain boundary curvature-driven growth mechanisms into the random cellular automata dynamic recrystallization model

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Abstract

Numerical simulations can help predict microstructure morphology evolution under hot forming conditions and support the determination of final material properties. In the case of microstructure evolution occurring under high deformation degrees, especially during dynamic recrystallization (DRX), the full-field random cellular automata method (RCA) can be successfully used (1). As is known, grain boundary curvature plays a certain role in determining the driving energy of microstructural evolution processes that involve grain boundary migration under grain growth. Similar mechanisms should also be considered in the DRX process to make the predictions more reliable.
However, unlike in the classical cellular automata, the random arrangement of CA cells in the RCA method makes curvature determination more complex and requires a series of sophisticated numerical approaches. This challenge is further compounded by the need for an in-depth analysis of the stability of proposed solutions, which must account for varying cell arrangements and discretization levels of the investigated computational domain. Such analyses are essential to ensure accuracy and consistency in curvature estimation across diverse configurations.

In this study, established methods for curvature determination (i.e., Kremeyer (2), Mason (3)) were adapted to the RCA method, and an original approach based on the convex hull algorithm was also developed. The implemented solutions were evaluated using custom software designed to simulate microstructure evolution during the DRX process, with particular attention to examine the influence of discretization and deformation levels on the results. The results of the implemented algorithms and their computational efficiency were also analysed and compared.

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