8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

MICRO-SCALE SIMULATION OF RECRYSTALLIZATION THROUGH CELLULAR AUTOMATA

N.Yazdipour[1], C. H. J. Davies[2], P. D.Hodgson[3]

[1] Deakin University
Centre for Material and Fibre Innovation, Geelong, Victoria 3217, Australia
nyaz@deakin.edu.au

[2] Monash University
School of Physics and Materials Engineering, Victoria 3800, Australia
Chris.Davies@eng.monash.edu.au

[3] Deakin University
Centre for Material and Fibre Innovation, Geelong, Victoria 3217, Australia
phodgson@deakin.edu.au

Key Words: *micro-scale simulation, cellular automata, static recrystallization.*

ABSTRACT

Dynamic recrystallization (DRX) improves the final microstructure during a hot deformation process and computer simulation can be used as a powerful tool to predict the evolving microstructure during dynamic recrystallization. Various models have been suggested to predict dynamic recrystallization but they were unable to incorporate the local details of the process. Cellular Automata (CA), as one potential solution to simulate recrystallization successfully.

In this study, a CA model is developed to model dynamic recrystallization utilizing a comprehensive data set for Type 304 austenitic stainless steel [1] for validation. Initial grain size, initial grain orientation and dislocation density were used as input data to the CA model. Flow curve, dislocation density, final grain size and orientation, and volume fraction of dynamic recrystallization were the output data that was then compared with the experimental data to validate the model.

In the current model, an initial microstructure composed of 100×100 cells was used to reduce the running time and memory space usage and the initial neighbourhood radius was defined as 3; both of these input variables can be altered. The initial microstructure with prescribed average grain size and equiaxed grain structure was generated by running the CA model for the condition of homogeneous recrystallization with site-saturated nucleation. From this a fully impinged microstructure was obtained, with the grain size as a function of the nucleation density. In the current model, three different initial microstructures were generated for comparison with the experimental results (d_0=20, 35, 60 μm) (Fig.1) [2].

Figure 1: Different initial microstructures applied in the CA model in which each grain has its own orientation (θ).

As deformation continues beyond the peak stress, the difference between the dynamic recovery and recrystallization curves will increase. If we assume that the stress difference between dynamic recovery and dynamic recrystallization curves is a

function of the recrystallization fraction (S), then it is possible to obtain "S" as a function of deformation. Firstly, the critical and steady state stresses were determined from the work-hardening curve under various thermomechanical conditions. By having these points, it is possible to plot the dynamic recovery curve. By running the CA model, recrystallization initiated and continued up to the point where the whole microstructure would be fully recrystallized. So, it would be possible to measure the recrystallized fraction in each time step demonstrating a sigmoidal configuration [3]. By combining the dynamic recovery curve and the curve of recrystallized volume fraction obtained from running the CA model, the dynamic recrystallization curve can be acquired.

It is shown that deforming samples with different initial grain sizes at a similar thermomechanical condition (constant temperature and strain rate) will produce a similar final grain size [3]. To verify the CA model, three different initial microstructures (D_0=20, 35 and 60 μm) were simulated (Fig.1).

The simulation and experimental results have excellent agreement up to the peak stress for the different initial microstructures (Fig.2). However, the simulations deviated from the experimental results at large strains and the difference increased as the initial grain size increased (Fig.2a). The deviation can originate from the initial grain size. This means that the large initial grain size microstructure was not fully recrystallized [1] and the un-recrystallized grains receive more dislocations due to further deformation and work hardened. Since the flow curves shown in Fig.2 are the representative of the average dislocation densities in the whole microstructure, the work hardened grains increase the average dislocation density and cause the deviation in the flow curve.

The dynamic recrystallization kinetics in the simulation has been verified by the measured volume fraction of the recrystallized microstructure obtained using EBSD (Fig.2b) [1]. Overall there is good agreement. The key difference in the CA model is that the steady state stress is not constant, whereas experimentally it approaches a similar value, as expected.

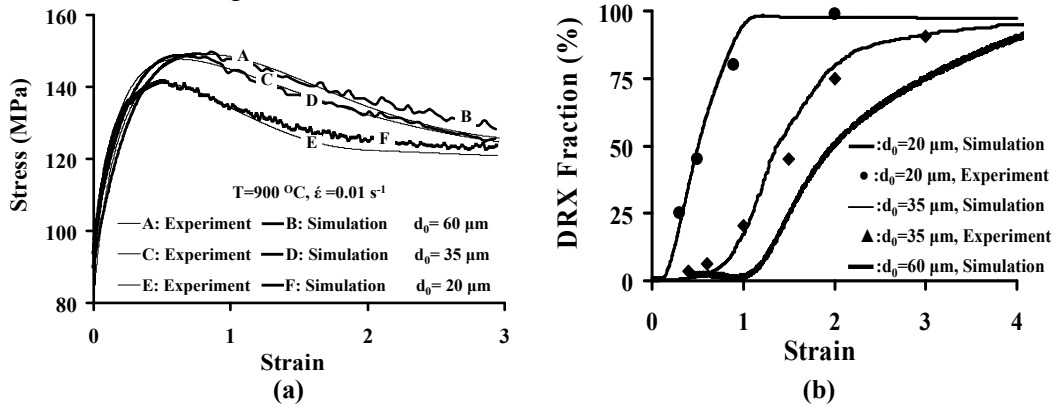

Figure 2: Simulation results from three different initial microstructures.

[1] A. D. Manshadi, "The Evolution of Recrystallization During and Following Hot Deformation", PhD thesis, pp. 37, 2007.

[2] N. Yazdipour, C. H. J. Davies, P. D. Hodgson, "Simulation of Dynamic Recrystallization Using Random Grid Cellular Automata", Computer Methods in Materials Science, Vol. **7**, pp. 168, 2007

[3] D. Raabe, "Cellular Automata in materials Science with Particular Reference to Recrystallization Simulation", Annu. Rev. Mater. Res, Vol. **32**, pp. 53-76, (2002).