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MODELING THE DYNAMIC RECRYSTALLIZATION: A MODIFIED CELLULAR AUTOMATON METHOD

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Abstract

The paper presents a modified cellular automaton (CA) model for quantitative and topographic prediction of dynamic recrystallization (DRX) of Ni-based superalloy during hot deformation. To describe the effect of deformation on grain topology, an updated topology deformation technique was used in the model, in which a cellular coordinate system and a material coordinate system were established separately. The cellular coordinate system remains unchangeable in the whole simulation. The material coordinate system and the corresponding grain boundary shape change with deformation. The grain topography, recrystallization fraction and average grain size were also predicted. The simulated results agree well with the experimental data in terms of average grain size and flow stress, suggesting that the modified CA model is a reliable numerical approach for predicting grain evolution during dynamic recrystallization.

Introduction

The mechanical properties of a metallic component such as high temperature alloy are largely depended on their chemical composition and microstructures resulted from processing and heat treatment history in industrial production. Accurate prediction and precise control of the microstructural evolution is of great importance for designers to achieve excellent mechanical properties for metals and alloys through hot working. Up to date, DRX has been recognized as a powerful mechanism for grain refinement under hot plastic deformation. In this context, in-depth understanding of microstructural evolution during DRX would help develop more accurate prediction methods to simulate microstructural characterization and mechanical properties in the hot deformation of metals and alloys.

With the rapid development of computer technology and a thorough understanding of microstructural evolution thermodynamics and kinetics, mesoscale methods, i.e. the CA method, Monte Carlo (MC) method, vertex models, phased field approach and level set modelling, have been successfully used to simulate microstructural evolution in hot working. Mesoscale models can not only predict the general average microstructure properties, but are also able to visually provide the virtual microstructural evolution during hot deformation. Compared with the other methods, CA method can provide an alternative approach, describing the spatial and temporal microstructure evolution on a mesoscale. There is no doubt some shortcomings of CA method. For example, CA has poor representation of grain boundary curvature compared to the phase fields model and level sets model. The first attempt to model of microstructural evolution during

DRX by CA method was made by Goetz and Seetharaman [1]. Up to now, there have been many cases of successful application of CA in modeling microstructural evolution. In these studies, Ding et al [2], Raabe et al [3], Kugler and Turk [4], Xiao and Zheng [5] and Jin and Cui [6] contributed greatly to the development of the CA method for the simulation of DRX from the aspects of optimization algorithm, grain morphology change and parameter identification. Recently, based on the work of Ding et al [2] and Kugler and Turk [4], Yazdipour et al [7] simulated DRX during thermomechanical deformation in a 304 austenitic stainless steel by the CA method. In this case, initial grain size, initial grain orientation and dislocation density are used as input data to the CA model; the flow curve, dislocation density, finial grain size and orientation and recrystallized fraction are the output data. Hallberg et al [8] employed the CA model with probabilistic cell switches in the simulation DRX of pure Cu. Ding et al [9] investigated the hot compression behavior of the Mg-9Al-1Zn alloy using EBSP analysis and the CA method. Chen et al [10] predicted microstructural evolution during DRX of an ultra-super-critical rotor steel. In addition, the DRX behavior of TRIP steel, C-Mn micro-alloy steel and Ti-alloy were studied by using improved CA models. Furthermore, the three-dimensional (3D) CA model was also put forward to simulate the grain evolution during DRX by Svyetlichnyy [11] and Hallberg [12]. Compared with traditional 2D version, the 3D CA model best reflects the processes of nucleation and grain growth, because the microstructure evolution is obviously three dimensional during dynamic recrystallization. However, 2D CA model has fewer elements. For every element, there are fewer neighbours which need to be considered. In other words, 2D CA models require significantly less memory and time for calculation. Therefore, developing 2D CA model is also an effective way to predict microstructure evolution for balancing accuracy and computational efficiency. To date, studies in the field of CA modeling of DRX mainly based on Ding and Guo's method [2]. However, in order to perfect the classical CA model for DRX, the following two aspects still need further investigation. On the one hand, it is highly necessary to develop reasonable and practicable method to calculate CA simulation constants such as nucleation parameter. On the other hand, it is desirable to introduce the mechanisms of grain morphology change on the nucleation and grain growth during DRX in either two-dimensional or three-dimensional.

In this study, a CA model coupling with the topology technique was developed. In order to verify the applicability of the model, the DRX behavior of IN718 superalloy was simulated by using the modified CA model. The effects of a wide range of thermomechanical parameters on the DRX kinetics and austenite grain size were investigated.

Modeling of CA

Mechanism of CA simulation of DRX

When CA method is adopted, the evolution of the microstructure can be represented by some basic microstructural constituents such as the grain orientation. This means that the actual microstructures can be predicted at mesoscale and the statistical information of internal variables used in the macro-scale models are just the inevitable results. The interaction mechanism between mesoscopic and macroscopic evolution for CA simulation is illustrated in Fig. 1. Actually, the dislocation density provides a link of multi-scale modeling to bridge the macroscopic thermo-mechanical parameters and the mesoscopic microstructures. Fig. 1a also schematically shows the variation of flow stress as well as the mean dislocation density of the

material and instantaneous dislocation density at a single cell of CA. In the case of none recrystallization, the flow stress depends on the combined effects of work hardening and dynamic recovery, showing a monotone increase towards a saturated stress. But in fact, DRX takes place once the dislocation density reaches a critical value, resulting in a significant decrease of the dislocation density in the recrystallized zone. The difference between the dislocation density of recrystallized grain and the matrix supplies the thermodynamic driving force for the growth of recrystallized grain. In continuous deformation, the dislocation density of a particle changes as the strain increases and the recrystallization happens, which shows a decreased mean dislocation density and a decreased flow stress. Therefore, when the CA method is adopted, one of the most important issues is to track the changes in dislocation density. Fig. 1b also shows the details of CA simulation of nucleation and grain growth during DRX.

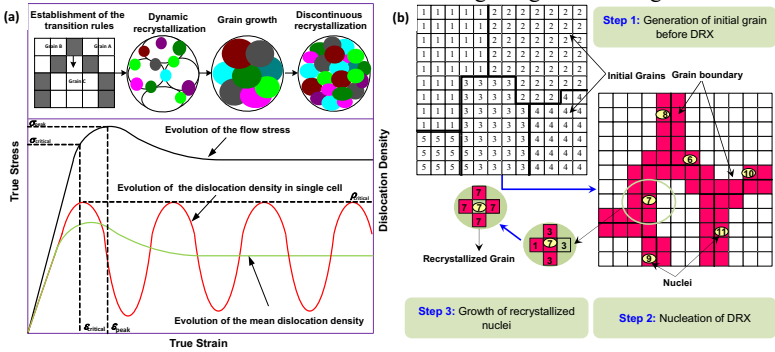

Figure 1. (a) Interaction mechanism between mesoscopic and macroscopic evolution for CA simulation. (b) Illustration of nucleation and recrystallized grain growth during DRX by CA.

Consideration of grain geometry of real deformation

The deformation of grain geometry makes change of grain boundary and consequently affects nucleation and growth of nuclei during DRX. To describe the effect of compression on the grain shape more accurately, a 2D CA model incorporation of a grain morphology deformation technique was adopted in this study. In the modified CA model, a cellular coordinate system and a material coordinate system were established separately. The cellular coordinate system was used to describe the nucleation of DRX and the growth of new recrystallized grains, the size of the cell remains unchangeable. The material coordinate system and the corresponding grain boundary shape change with deformation during a CA simulation. A detail description of grain morphology mechanism in CA simulation can be found in Fig. 2. As shown in this figure (step 1), the original matrix were compressed in the compression direction and elongated in the perpendicular direction during DRX. Then, the grain boundary will be mapped from the material coordinate system to the cellular coordinate system before the appearance of DRX (step 2). The dislocation density increases gradually and when the value reaches a critical density (ρ_{critical}), new nucleus appear on the grain boundaries and continue to grow with the model of equiaxed growth in the cellular coordinate system (step 3). Finally, the grain boundary will be mapped back to the material coordinate system for the next round of the simulation.

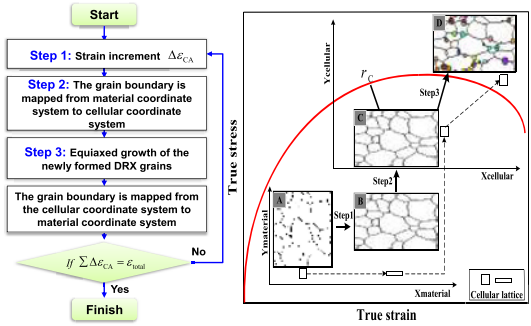

Figure 2. A schematic representation showing the mapping of the grain boundary through material cellular coordinate transformation.

Simulation results and discussion

In the developed CA model, the simulation mesh is 512×512 square lattice, and periodic boundary conditions are used. The size of every cell represents 2μm of the real dimension of the material. In order to balance the accuracy and computational efficiency, the increment of strain is 0.2 during coupling with the effect of grain morphology change on DRX. Fig. 3 shows a comparison of predicted true stress-strain curve and experimental one. It also gives the microstructural evolution of DRX at a strain rate of $1s^{-1}$ and temperature of 1060°C with consideration of grain morphology deformation. The different color regions represent the recrystallized grains and the orange regions denote the deformed matrix, and the black lines denote the grain boundaries (GBs). The initial microstructure (D_0=210μm) is obtained by running the initial microstructural generation module. As shown in the figure, the grains which have not completed the DRX in each round are compressed in the vertical direction with the continuous deformation, and the newly formed recrystallized grains grow with the type of equiaxed growth in the cellular coordinate system. The recrystallized fraction increases with the increase of the strain from 0.62 to 0.93.

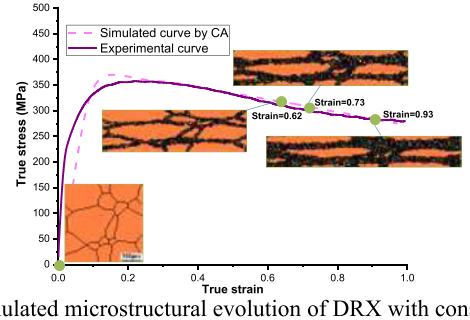

Figure 3. The simulated microstructural evolution of DRX with consideration of grain morphology at a strain rate of $1s^{-1}$ and temperature of 1060°C.

Fig. 4 gives the simulated microstructures without considering the grain morphology change of the initial matrix at the temperature of 1060°C and the strain rates of $1s^{-1}$ and $0.1s^{-1}$,

respectively. Fig. 5 shows the simulated results by using the CA model with support of the grain morphology technology under the same deformation conditions. Additionally, Fig. 6 illustrates the simulated average grain size and recrystallized fraction using the topological CA model at a strain rate of $1s^{-1}$ and $0.1s^{-1}$ and temperature of 1060°C in comparison with the conventional CA simulation. All in all, there is a reasonable agreement between final average grain size in CA simulations and experiments. Meanwhile, the results also show that the grain morphology deformation has an accelerated effect on the recrystallization process. The recrystallized fractions are 89% and 75% for the strain rates of $0.1s^{-1}$ and $1s^{-1}$ respectively when the grain morphology deformation technique was adopted as compared to only 58% and 46% of recrystallized fractions without the consideration of grain morphology deformation. The simulation results also indicate that the simulated average grain size decreases slightly due to the effect of matrix deformation. The reason for such a difference may be because that the elongated grain boundaries provide more potential nucleation sites for recrystallization due to a higher ratio of the grain boundary volume to grain volume. At the same time the newly formed recrystallized grains impinge earlier with support of the morphology change of the matrix, resulting in a smaller average grain size as compared to the conventional CA simulation. Generally speaking, the CA model with the incorporation of the morphology deformation technique can better reflect the topological characteristics of the deformed grains in the simulation of DRX.

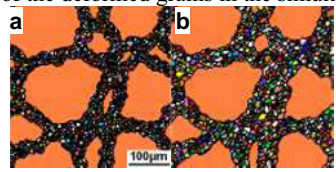

Figure 4. The simulated microstructures without consideration of grain morphology deformation at temperature of 1060°C for different strain rates: (a) $1s^{-1}$ and (b) $0.1s^{-1}$.

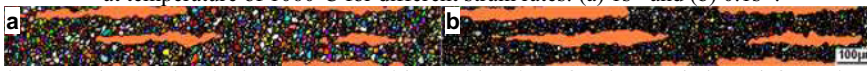

Figure 5. The simulated microstructures with consideration of grain morphology deformation at temperature of 1060°C for different strain rates: (a) $0.1s^{-1}$ and (b) $1s^{-1}$.

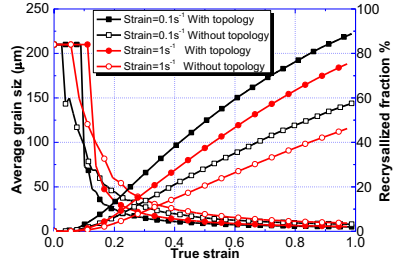

Figure 6. Simulated kinetic curves of DRX using the topological CA model and a comparison with the conventional CA simulation result.

Fig. 7 shows the microstructural evolution during large strain deformation. As shown in the figure, when the strain reaches 1.0, the recrystallized fraction is less than 50%, when the strain reaches 1.5, complete recrystallization takes place, and the initial grains are refined greatly. It is well known that one of the typical characteristic of severe plastic deformation (SPD) is refining

the grain size through the large deformation. Therefore, CA method is capable of predicting microstructural evolution for DRX of IN718 superalloy in SPD process such as multi-direction forging.

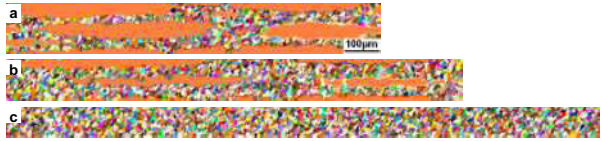

Figure 7. The predation of microstructure evolution at a broad range of strain and the temperature of 940°C and strain rate of $0.001s^{-1}$. (a) ε=1, (b) ε=1.2 and (c) ε=1.5.

Conclusion

By introducing the mechanism of morphology change of grain, a CA model was established to describe the DRX for IN718 superalloy. The CA model is shown to be a new and powerful tool for quantitative and explicit simulation of microstructural evolution during DRX. The established CA model can well describe the DRX behaviors of the studied superalloy. Furthermore, the developed CA model can be also used as an efficient simulation method to investigate the microstructural evolution in large material deformation on a mesoscale under the conditions such as multi-direction forging for IN718 superalloy.

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