Cellular automaton calculation for dynamic recrystallization

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Abstract. Since the mechanical behavior of superalloys can be optimized by tailoring the microstructure, the evolution of microstructure should be carefully controlled by thermo-mechanical treatments. To study the microstructure evolution of Ni-Cr-Fe based 718 alloy during hot forging, computational simulation and microstructure prediction model can be combined with experimental observation. It is necessary to establish a microstructure prediction model considering the recrystallization during the hot working process. In this work, cellular automaton (CA) method was used to simulate the dynamic recrystallization phenomena of 718 alloy during hot compression. The strain rate and temperature were considered as the processing variables. CA stress strain curves were compared with the experimental results and the prediction for the grain nucleation and growth were presented.

1. Introduction
Creep property of superalloys which are based on many alloying components depends on their microstructure such as grain size and diameter [1] [2]. In this regard, process parameters of hot forging need to be carefully controlled in respect to the recrystallization and grain growth. The recrystallization behavior during the hot forging is influenced by process variables such as the forming temperature, strain rate, initial grain size and amount of deformation [3]. The aim of this research is to establish a methodology during hot deformation process. Microstructural changes of Ni-Cr-Fe based 718 alloy was investigated with processing variables of temperature and strain rate during high temperature compression test. Recrystallization fraction and grain size change were predicted by cellular automaton (CA) technique. In this paper, nucleation rate was considered by the Arhenius type probability rule compared to the reference [6] in which dislocation accumulation was considered. These microstructural considerations lead to the optimum process condition at high temperature compression.

2. Numerical modeling
Many dislocations are accumulated and work-hardening behavior occurs during hot compression process. The increased dislocation density is reduced by dynamic recovery and recrystallization process if the temperature is higher than annealing temperature in the hot compression process.
The recrystallization includes the nucleation and growth process of new grains. In dynamic recrystallization, as opposed to static recrystallization, the nucleation and growth of new grains occur during deformation rather than afterwards as part of separate heat treatment. In this section, a brief summary of numerical modeling of dynamic recrystallization is given.

2.1. Nucleation of grain
In hot forging, new grains appear preferentially at highly energetic sites such as cell boundaries of the polygonized structure or grain boundaries, eliminating most of the dislocations. The process of formation of new grains is known as recrystallization. The driving force for recrystallization comes from the stored energy of work. If a region reaches a certain strain, enough driving force is stored, and the site is eligible for the nucleation of a new small grain. Some amount of activation energy will be required for the nucleation of the new grains in the physical point of view. If the dislocation density of the region is \( \rho \), then the strain energy by the line tension of one dislocation line will be \( \tau \rho \) per unit volume. If the activation energy for the nucleation is \( Q_n \) and the region has the enough dislocation energy to overcome the activation energy, then a nucleus will be created. The probability for the nucleation for one attempt will be

\[
p = \exp \left( -\frac{Q_n - \tau \rho V/2}{RT} \right)
\]

where \( V \) is the molar volume. If there are \( f_n \) attempts per one second for the nucleation, then the total probability during time interval \( \Delta t \) is

\[
p_+ = \exp \left( -\frac{Q_n - \tau \rho V/2}{RT} \right) f_n \Delta t = f_n \Delta t \exp \left( \frac{\tau \rho V}{2RT} \right) \exp \left( -\frac{Q_n}{RT} \right)
\]

Similarly, there can be the reverse transformation to nullify the nucleation, and the net probability will be

\[
p_{\text{total}} = p_+ - p_- = f_n \Delta t \left[ \exp \left( \frac{\tau \rho V}{2RT} \right) - \exp \left( -\frac{\tau \rho V}{2RT} \right) \right] \exp \left( -\frac{Q_n}{RT} \right)
\]

when \( \tau \rho V \ll RT \).

In the compression work, the dislocation density will increase by work hardening. In Kocks-Mecking (KM) approach the equation for the evolution of \( \rho \) reads [8]

\[
\frac{d\rho}{d\epsilon} = \left( k_1 \rho^{1/2} - k_2 \rho + \frac{1}{bd} \right)
\]

The production term \( k_1 \rho^{1/2} \) is associated with the athermal storage of moving dislocations and the second term \( k_2 \rho \) is associated with dynamic recovery (stage III). Therefore \( k_2 \) depends on temperature and strain rate \( k_2 = k_2 (\dot{\epsilon}, T) \). It can be evaluated that \( k_1 = 2 \theta_{II}/(G \alpha b) \) where \( \theta_{II} \) is the slope of the stress-strain curve in stage II or \( \theta_{II} \approx G/200 \). Using the steady state stress \( \sigma_s \), one can evaluate \( k_2 = \alpha G b k_1/\sigma_s \). The third term is due to geometrically determined quantities such as particles or grains with constant mean free path \( d \). The initial condition of the dislocation density is zero.
2.2. **Grain growth**

After small new grains are nucleated, there can be driving force for the motion of the grain boundary. The driving force can be grouped into the volumetric part and the surface energy part. We will follow the procedure in the literature [6]. When the driving force is defined by the Gibbs free energy change by the motion of the grain boundary, it will turn out

\[ F = \frac{dW}{dr} = 4\pi r^2 \tau [\rho] - 8\pi r \gamma. \]

where \( r \) is the radius of the grain and \( \tau \) is the dislocation line energy \( \mu b^2 / 2 \) and \( [\rho] \) is the difference of the dislocation densities on both sides and \( \gamma \) is the unit surface energy per area. The driving force density per unit surface area will be

\[ P = \frac{F}{4\pi r^2} = \tau [\rho] - 2\gamma r. \]  \hspace{1cm} (2)

Then the velocity of the grain boundary will be \( v = MP \). The mobility \( M \) is a function of temperature \( M(T) = M_0(T) \exp \left( -\frac{Q_m}{RT} \right) \). The grain boundary energy can depend on the orientation mismatch between the two grains as shown in [6].

2.3. **Cellular automaton**

In the CA calculation [4] to [7], the material is divided by many cells and each cell has state variables. Grain orientation number, dislocation density, grain size, nucleation probability, strain and stress were stored as the state variables in this study. The evolution or change of the state variables are determined by the local state or neighborhood. Moor neighborhood was considered. Dislocation density, strain, and stress are determined by local states by the governing equations, and grain nucleation and grain boundary motion are determined by the neighborhood as well as itself.

Whether a grain is nucleated or not will be decided by a probabilistic transition rule. If a cell is contiguous to a grain boundary, the average dislocation density of two cells across the grain boundary was used in \( \rho \) to compute the nucleation probability given in (1) and then the probability was compared with a random number. If the probability is larger than the random number the cell will be given a new state variable for the grain orientation and its dislocation density will drop to zero. Because the dislocation density is the average of neighboring two cells, if one cell has a very low dislocation density, it will be hard to nucleate a new grain at that position.

The size of the time increment will be determined from a characteristic equation which reads

\[ l_c = dx = v_c \cdot \Delta t_c \]

\( v_c \) is a characteristic speed of the grain boundary, so if the velocity \( v \), determined by \( v = MP \), is different from \( v_c \), then the CA time step will be reduced or increased by

\[ v \cdot \Delta t = v_c \cdot \Delta t_c \]  \hspace{1cm} (3)

2-dimensional simulation was carried out and the number of CA cells was 250×250. The size of one cell was \( dx^2 = 1\mu m \times 1\mu m \). The index for the planar grain orientation can vary from 1 to 256. The misorientation between adjacent grains can be determined by the difference of the grain indices.
Table 1. Material parameters for cellular automaton.

| Parameter       | Value                                      |
|-----------------|--------------------------------------------|
| $M_0$ Mobility  | $100 \times 10^{-6} \text{ m}^{-3}/\text{ N/s}$ |
| $Q_m$ Mobility activation energy | 126000 J/mole |
| $R$ Gas constant | 8.314 J/mole |
| $b$ Burgers vector   | 0.256 nm |
| $f_n$ Frequency     | $1 \times 10^{-13} \text{ s}^{-1}$ |
| $Q_n$ Nucleation activation energy | 180000 J/m$^3$ |
| $k_1$ Hardening constant | $600 \times 10^6 \text{ m}^{-1}$ |
| $k_2$ Softening constant | 40 |
| $V$ Molar volume   | $1 \times 10^{-8} \text{ m}^3$/mole |
| $\epsilon_c$ Critical strain | 0.005 |
| $\Delta t_c$ Characteristic time | 0.146 s |
| $v_c$ Characteristic velocity | 4.3 $\mu$m/s |

Table 2. Temperature dependence shear modulus.

| Temperature T | Shear modulus $\mu$ |
|---------------|----------------------|
| 1000 °C       | 200 GPa              |
| 1150 °C       | 150 GPa              |

It is necessary to compute the curvature or radius of the grain to obtain the surface driving force for the grain boundary motion in (2). We used a procedure to compute 2-dimensional curvature in [6].

$$r = a_r \frac{n + 1}{n_k - n_i}$$

In Moor neighborhood, $n = 48$ and $n_k = 24$ were used and $n_i$ is the number of neighbors that belong to the grain. The fitting parameter was $a_r = dx/4$. The material parameters used in CA are listed in Table 1 and Table 2. The critical strain [9][6] is the minimum strain for the initiation of the grain nucleation by the accumulation of the energy.

3. Cellular automaton results

Figure 1 shows the stress strain curves computed by CA for different strain rates and temperatures. The results show accordance with the experimental curves in Figure 2 obtained from Ni-Cr-Fe based 718 alloy. The stress was computed from the CA calculation by using the average dislocation density, $\sigma = \alpha \mu b \sqrt{\rho}$. The strain is obtained by multiplying time and a fixed strain rate. The annihilation of dislocations was rapid in the case of low strain rate and higher temperature and the stress did not increase to higher values. The computed stress strain curves at low strain rates show fluctuation. The reason may be that the number of grains is small as shown in Figures 5 and 6 and nucleation occurs during the time period for the slow strain increment. The hardening observed in the experiment for $\dot{\epsilon} = 10 \text{s}^{-1}$ and $T = 1000 \degree \text{C}$ is lower significantly, and the reason needs to be investigated in the future.
Figures 3 ∼ 6 show the dislocation density and the grain microstructures at strain $\varepsilon = 0.5$ for each strain rate and temperature. The dislocation density is uniform in each grain. The distribution of the dislocation density in $250^2$ cells is shown in Figures 7 and 8. When the strain rate is high, small recrystallized grains exist in contrast to the results of the slow strain rates. It was observed that small number of grains were nucleated inhomogeneously and made growth to large grains for a longer time until it reached $\varepsilon = 0.5$ in the case of the slow loading rates as shown in Figures 5 and 6. It was reported that at lower temperatures, there was a tendency for necklace patterns of new grains along the pre-existing grains. [6]

4. Conclusion
Cellular automaton was used to simulate recrystallization of hot compression of 718 superalloy. Nucleation rate was considered by the Arhenius type probability rule. Effects of strain rate and temperature were investigated. It was shown that the stress strain curves during the hot compression can be replicated by CA method. The stress level was lower for small loading rate and high temperature. The grain size was smaller for high strain rate and low temperature. It will be necessary to study the effects of the initial grain size and mesh size in the future research.

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References
[1] J.T. Yeom, C.S. Lee, J.H. Kim, N.K. Park. 2007 Finite-element analysis of microstructure evolution in the cogging of an Alloy 718 ingot Mater. Sci. Eng. A. 448–451 722. doi:10.1016/j.msea.2006.02.415
[2] V. Balasubramanian, Y. Li, T. Stotler, J. Crompton, N. Katsube, W.O. Soboyejo. 1997 Numerical simulation of inertia welding of Inconel 718 Asme-Publications-Pvp. 369 289
[3] R.D. Doherty, D.A. Hughes, F.J. Humphreys, J.J. Jonas, D.J. Jensen, M.E. Kassner, W.E. King, T.R. McNelley, H.J. McQueen, A.D. Rollett. 1997 Current issues in recrystallization: a review Mater. Sci. Eng. A. 238 219. doi:10.1016/S0921-5093(97)00424-3
[4] Rappaz M. and Gandin Ch.-A. 1993 Probabilistic modelling of microstructure formation in solidification process Acta Metall. Mater. 41 345
[5] Raabe D. 1999 Introduction of a scalable three-dimensional cellular automaton with a probabilistic switching rule for the discrete mesoscale simulation of recrystallization phenomena Philosophical Magazine A 79 2339
[6] Hallberg H, Wallin M, Ristinmaa M 2010 Simulation of discontinuous dynamic recrystallization in pure Cu using a probabilistic cellular automaton *Computational Materials Science* **49** 25
[7] Hallberg H, Svendsen B., Kayser T. and Ristinmaa M 2014 Microstructure evolution during dynamic discontinuous recrystallization in particle-containing Cu *Computational Materials Science* **84** 327
[8] Estrin Y, Mecking H 1984 A unified phenomenological description of work hardening and creep based on one-parameter models *Acta Metallurgica* **32** 57
[9] Roberts W. and Ahlblom B. 1978 A nucleation criterion for dynamic recrystallization during hot working *Acta Metallurgica* **26** 801

**Figure 3.** CA microstructure and dislocation density at $\varepsilon=0.5$ for $\dot{\varepsilon}=10\text{s}^{-1}$ and $T=1150^\circ C$.

**Figure 4.** CA microstructure and dislocation density at $\varepsilon=0.5$ for $\dot{\varepsilon}=10\text{s}^{-1}$ and $T=1000^\circ C$.

**Figure 5.** CA microstructure and dislocation density at $\varepsilon=0.5$ for $\dot{\varepsilon}=0.1\text{s}^{-1}$ and $T=1150^\circ C$.

**Figure 6.** CA microstructure and dislocation density at $\varepsilon=0.5$ for $\dot{\varepsilon}=0.1\text{s}^{-1}$ and $T=1000^\circ C$.

**Figure 7.** Dislocation density at $\varepsilon=0.5$ for $\dot{\varepsilon}=10\text{s}^{-1}$ and $T=1150^\circ C$.

**Figure 8.** Dislocation density at $\varepsilon=0.5$ for $\dot{\varepsilon}=0.1\text{s}^{-1}$ and $T=1150^\circ C$. 