CA 모델을 통한 동적재결정 예측에 있어서의 재료상수 선정

Alexander R. Bandar[#] · Weitsu Wu[1] · 이경훈[2] · 강경필[2]

Determination of Materials Constants for Dynamic Recrystallization Prediction by Cellular Automata Modeling

Alexander R. Bandar, Weitsu Wu, Kyunghoon Lee, Gyeongpil Kang

Abstract

Physics based Cellular Automata model is developed and implemented into FEM code. CA model can predict microstructure evolution based on physical phenomena, such as hardening, recovery and recrystallization. This paper outlines the methodology to determine the materials constants for these different phenomena from simpler measurements.

Key Words : Cellular Automata Algorithm, Recrystallization, Recovery, Grain Growth, Microstructure Evolution

Introduction

Finite element modeling simulations of metal forming processes are becoming very reliable at predicting part shape and state variables. The next major improvement for metal forming simulations is now to improve part property prediction, such as ductility, failure strength and fatigue resistance. In order to make these predictions, it is necessary to model microstructure evolution, and then to compute physical properties from the predicted microstructure. Johnson-Mehl-Avrami-Kolmogorov (JMAK) empirical equations are quite good at predicting grain size and volume fraction recrystallized during deformation and heat treatment, as long as sufficient testing and characterization were performed. However, the next stage of microstructure prediction should be more physics-based, not empirical, so that predictions can be made without necessarily having to test the entire range of the thermomechanical processing envelope, which is costly and time-consuming. Additionally, physics-based microstructure prediction will permit physics-based structure-property relationships, and allow for more realistic property prediction. Towards this goal, a more phenomenological (physics-based) model, based on a virtual microstructure represented by a Cellular Automata infrastructure, has been developed and implemented into DEFORM-3D. This model, rather than relying on empirically interpolating thermomechanical histories onto previously mapped microstructure, attempts to predict microstructure evolution based on physical phenomena, as hardening, recovery, recrystallization and growth. The challenge with such a model is to determine the appropriate materials constants for these different phenomena. It requires sophisticated testing and characterization equipment (such as mechanical testing machines, EBSD analysis, TEM and stepped annealing experiments). Rather than to explicitly measure these constants, it would be helpful to have a quantitative method to back-calculate these values from simpler measurements, such as a flow curve from a compression test and LOM analysis. This paper outlines such a methodology.

1. Scientific Forming Technology Corporations(SFTC)
2. (주)마케팅랩
교신저자: SFTC, E-mail: abandar@deform.com

Cellular Automata Model

The following assumptions are necessary to backwards-calculate microstructure evolution constants from macroscopically measurable features:

1) *microstructure can be computed as a function of thermomechanical state variables (strain, strain rate, stress, temperature, time, etc)*

2) *flow stress can be computed as a function of microstructure*

3) *true stress-true strain curves can be extracted from the experimental load-stroke measurement of a compression test*

4) *recrystallized grain size as well as volume fraction recrystallized can be measured experimentally by Light Optical Microscopy (LOM)*

Details follow:

1) Flow stress can be given by:

$$\sigma = \sigma_0 + \alpha G b \sqrt{\rho} \qquad (1)$$

where σ_0 is the Peierls stress, also called the "natural" flow stress or the "friction" stress of the material (it is a function of temperature); α is a tuning constant, G is the shear modulus of the material, b is the Burgers vector of the matrix, and ρ is the dislocation density of the material. During deformation, the dislocation density increases as a result of Orowan hardening, and reduces as a function of dynamic recovery. The hardening term is given by:

$$\rho^+ = \frac{d\varepsilon \sqrt{\rho}}{nb} \qquad (2)$$

where $d\varepsilon$ is the strain increment per FEM step, n is the number of dislocation "families" which a dislocation crosses during its lifetime, and b is the Burgers vector of the matrix.

The recovery term is given by:

$$\rho^- = d\varepsilon \cdot R \sqrt{\rho} \qquad (3)$$

where R is the dynamic recovery parameter. The values of n and R can be back-calculated from the true stress - true strain curve (Fig. 1) which can be derived from the load-stroke curve.
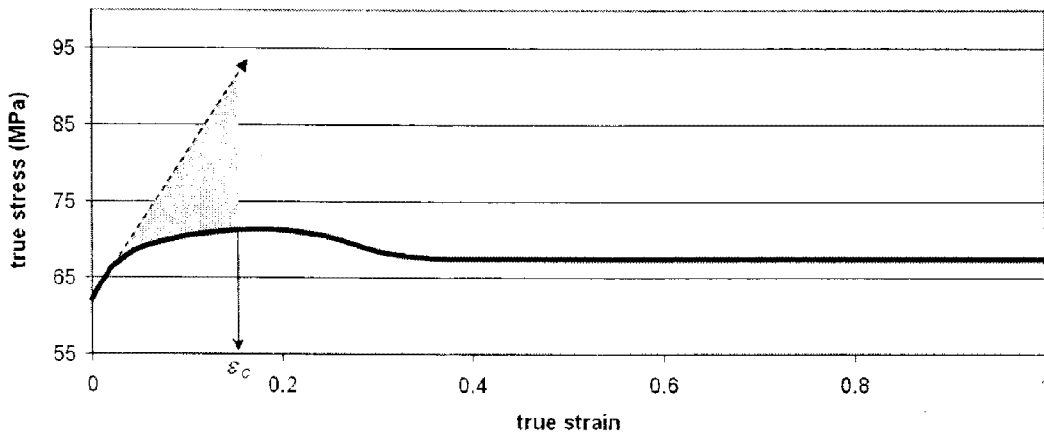

Fig 1. Example flow stress curve, demonstrating hardening slope (dotted line), dynamic recovery region (grey area), and critical strain to recrystallization (ε_c)

The linear portion of the true stress-true strain curve (dotted line) can be used to determine the hardening parameter. The portion of the true stress-true strain curve which deviates from linear hardening (grey area), but prior to recrystallization-induced softening, can be used to determine the recovery parameter. The critical strain, ε_c, can be used to compute the critical dislocation density, ρ_{crit}, necessary to initiate recrystallization. In this manner, constants related to the hardening, recovery and recrystallization behavior of the material may be quantified from experiment. A Cellular Automata microsctructure model has been developed and integrated into DEFORM-3D. This model takes the state variables predicted in a DEFORM-3D FEM simulation, and feeds those thermomechanical histories to a physics-based CA microstructure model, and predicts dislocation density, recrystallization, grain growth, flow stress, and more (Fig. 2).
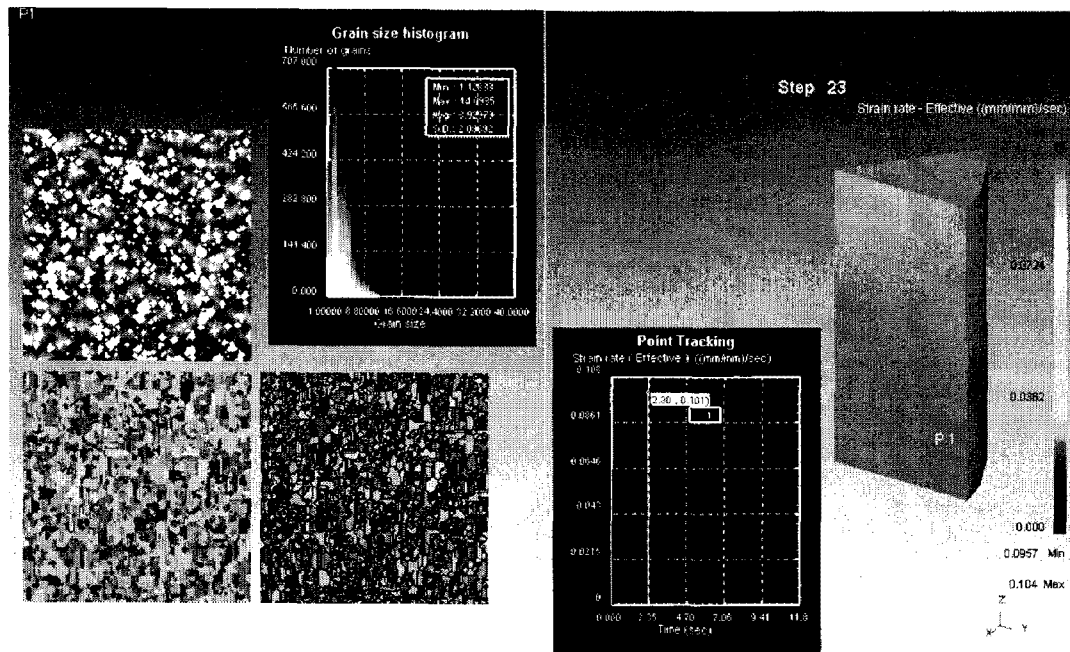

Fig. 2 FEM and microstructure simulation of cylindrical compression test. Left: recrystallized regions (top left); grain crystallography (bottom left); grains + grain boundaries (bottom right); and histogram of grain size (top right). Right: specimen(1/8th symmetry) and plot of strain rate for point tracked on point P1.

Fig. 2 demonstrates an FEM and CA microstructure simulation of a compression test. Microstructural data are plotted and state variable data can be viewed. Fig. 3 contains screen capture of the microstructure evolution during the simulation. Values for hardening, recovery and recrystallization materials constants have been taken from published literature.
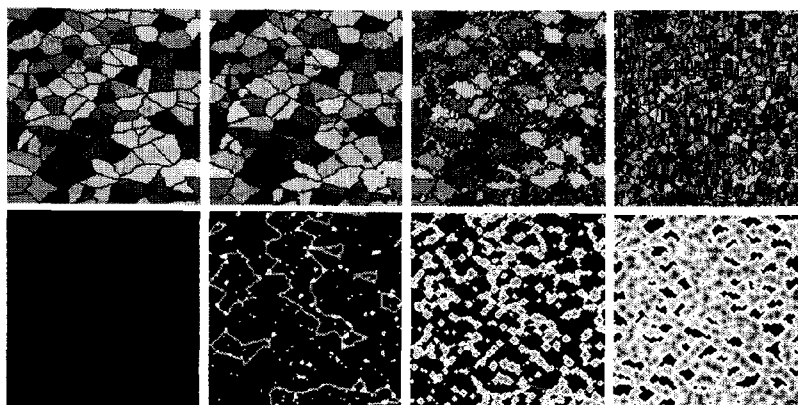

Fig. 3 Cellular Automata microstructure model of dynamic recrystallization. Top: grains, color-coded by crystallographic orientation. Bottom - dislocation density, indicating recrystallization (light = recrystallized).
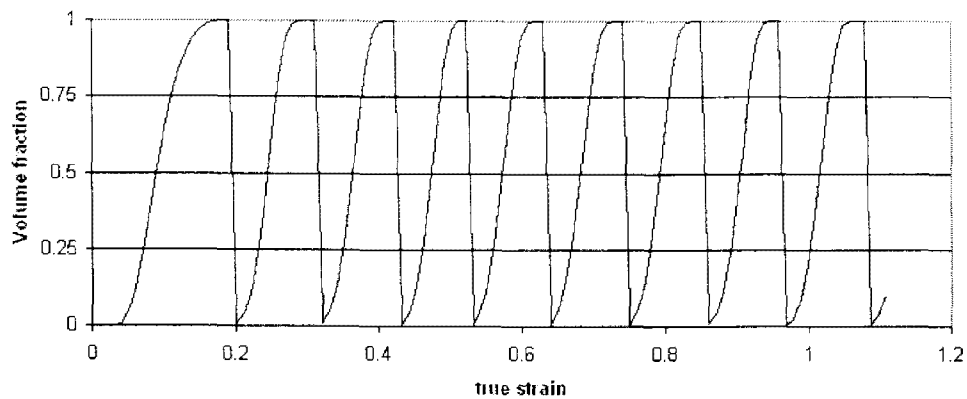
Fig. 4 Graph of volume fraction recrystallized during deformation of a cylindrical compress

Fig. 4 demonstrates the cyclic nature of dynamic recrystallization during deformation. It is this cyclic nature which produces a "steady-state" flow stress past the critical strain to recrystallization.
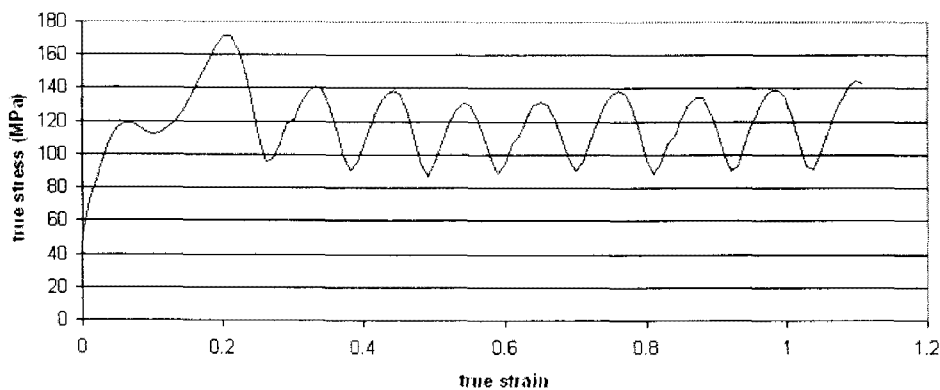

Fig. 5 Flow stress predicted via CA microstructure evolution modeling.

Fig. 5 plots the flow stress predicted by the microstructural evolution. Note that there is a "bump" in the flow stress after the first round of recrystallization - this is due to the Hall-Petch strengthening effect of a fine-grained microstructure (this term was not included in the flow stress equation presented earlier).

Current work involves analyizing experimental test data (load-stroke curves converted to true stress-true strain curves; LOM microstructures of progressively dynamically recrystallizing samples to show the volume fraction recrystallized as a function of strain). The methodology described earlier is employed, backwards-calculating the hardening, recovery, and recrystallization parameters. The results of the CA microstructure model will then be compared to the experimental data, and the constants or model evaluated for further tweaking / development.

References

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