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Monte Carlo modelling of the recrystallization kinetics

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In the paper the influence of different values of the degree of stored energy *H/J* and different models of the nucleation on the primary, static recrystallization kinetics modelled by the Monte Carlo simulation has been shown. The sigmoidal time dependence of recrystallized volume fraction observed in the simulation is often emphasized in the literature and finds its justification in the experiment. The Avrami exponent *n=2* is properly reproduced by the simulations. It has been shown that the model correctly responds to the change in the degree of stored energy *H/J*.

INTRODUCTION

Prediction of microstructural parameters of the structure exposed to plastic deformation and heat treatment such as recrystallization kinetics, grain size, and texture, is required to optimise processing conditions and properties of the finished products.

An analytical model of recrystallization able to describe it completely would be an ideal and highly desired solution to the discussed problem. However, such a model has not yet been created due to the complexity of grain interactions.

Computer simulations of grain growth and recrystallization may contribute to a better understanding of the phenomena and enable prediction of the final microstructures.

SIMULATION RESULTS

In the paper the Monte Carlo algorithm has been applied to model the primary recrystallization of a variable nucleation rate.

The algorithm employed in the simulation of recrystallization is similar to that described by Anderson et al. [1] and Srolovitz et al. [2] and was described in details in [3,4].

On the basis of classification given by Christian [5] five types of nucleation were simulated:

a) decreasing nucleation rate I – every *10 MCS* (Monte Carlo Step – is a time unit for the simulation) *I-(n(i-1)/10)* nuclei were randomly placed on the lattice; *I=100*, *n=10* and *i=1*, *11*, *21*, ... *MCS*,

b) decreasing nucleation rate II – as above but *I=200*, *n=10* and *i=1, 11, 21*, ... *MCS*,
c) site saturated – *I=200* nuclei were randomly placed on the lattice at *t=0* and no additional nuclei were created,
d) increasing nucleation rate – *I=n(i-1)/10* new nuclei were placed on the lattice every *10 MCS* until *I=100*; *n=10*, *i=1, 11, 21, …101 MCS*,
e) continuous nucleation rate – *I=10* nuclei randomly placed on the lattice every *10 MCS*.

Each nucleation type was simulated using four degrees of stored energy *H/J=1*; *1.5; 2* and *2.5*. [3,4]

It can be noticed from figures 1- 4 that for the small values of stored energy *H/J=1* and *H/J=1.5* the fastest model of recrystallization is the decreasing nucleation rate II (b) and I (a) followed by the site saturated model (c), continuous nucleation rate model (e) and the model of increasing nucleation rate (d).

For higher values of *H/J=2* and *2.5* the material simulated with the site saturated nucleation model recrystallized first. It is because for the higher values of the degree of the stored energy *H/J*, the time of completed recrystallization is *50 MCS* for models a), b) and d) and in such a short time the amount of nuclei introduced into microstructure at *t=0* is crucial.

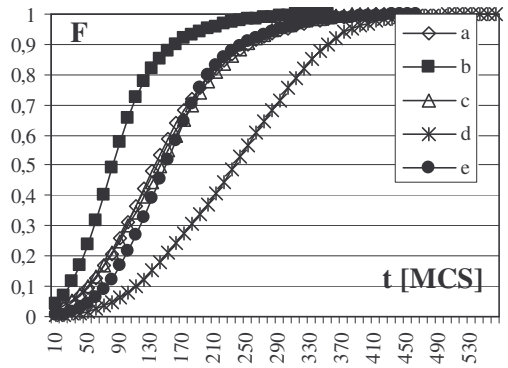

Fig. 1. Recrystallized volume fraction *F(t)* for the degree of stored energy *H/J=1* and different models of nucleation: a) decreasing nucleation rate I, b) decreasing nucleation rate II, c) site saturated, d) increasing nucleation rate and e) continuous nucleation rate.

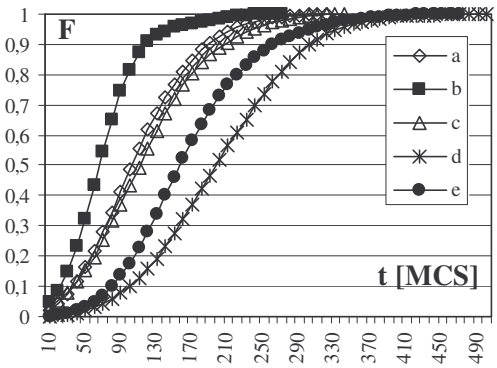

Fig. 2. Recrystallized volume fraction *F(t)* for the degree of stored energy *H/J=1.5* and different models of nucleation: a) decreasing nucleation rate I, b) decreasing nucleation rate II, c) site saturated, d) increasing nucleation rate and e) continuous nucleation rate.

For the site saturated nucleation as well as for the decreasing nucleation rate II the amount of the nuclei at *t=0* is *200* that is e.g. twice as much as for the decreasing nucleation rate I. In a longer time these proportions change. Setting higher energy causes a significant increase in the nucleation rate. Comparing data from fig. 1- 4 it can be noticed that for *H/J=1* recrystallization was completed at *t=350 MCS* for the decreasing nucleation rate II while for the increasing nucleation rate at *t=560 MCS*. For *H/J=2* the times are *t=50 MCS* and *t=110 MCS* respectively. It is assumed that the degree of the stored energy *H/J* reflects both the amount of deformation and the recrystallization temperature. Thus it can be observed that higher values of *H/J* result in a higher recrystallization rate. It is in agreement with the recrystallization rules formulated by Burke and Turnbull in 1952 and cited by Byrne [6].

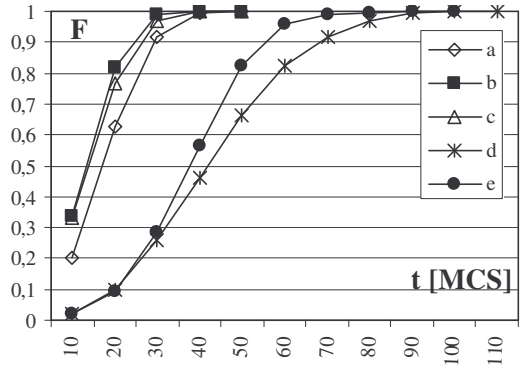

Fig. 3. Recrystallized volume fraction *F(t)* for the degree of stored energy *H/J=2* and different models of nucleation: a) decreasing nucleation rate I, b) decreasing nucleation rate II, c) site saturated, d) increasing nucleation rate and e) continuous nucleation rate.

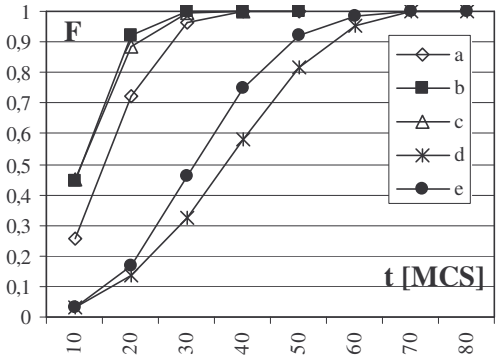

Fig. 4. Recrystallized volume fraction *F(t)* for the degree of stored energy *H/J=2.5* and different models of nucleation: a) decreasing nucleation rate I, b) decreasing nucleation rate II, c) site saturated, d) increasing nucleation rate and e) continuous nucleation rate.

The Avrami exponent n (1) is determined by the slope of the Avrami plot:

$$n = \frac{\partial \log\left(\ln\left(1/\left(1-F\right)\right)\right)}{\partial \log t} \tag{1}$$

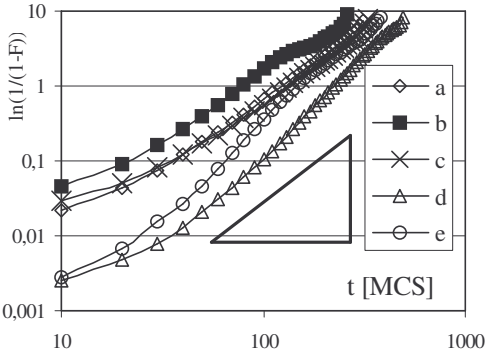

Fig. 5. The Avrami plots for the degree of stored energy *H/J=1* and different nucleation models: a) decreasing nucleation rate I, b) decreasing nucleation rate II, c) site saturated, d) increasing nucleation rate and e) continuous nucleation rate.

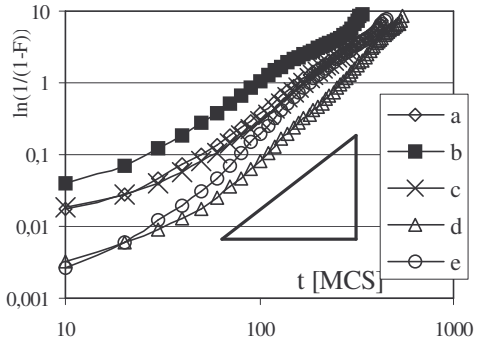

Fig. 6. The Avrami plots for the degree of stored energy *H/J=1.5* and different nucleation models: a) decreasing nucleation rate I, b) decreasing nucleation rate II, c) site saturated, d) increasing nucleation rate and e) continuous nucleation rate.

The Avrami plots for different nucleation models and *H/J=1* are shown in figures 5-8. The Avrami exponent *n=2*, expected for the *2D* recrystallization, is indicated by the slope of the triangle. The Avrami plot is expected to be linear with a slope equal to the Avrami exponent *n*. The departure from linearity observed in the simulation results, especially for the initial period, might be caused by putting a relatively large number of nuclei into the initial matrix at *t=0*. In the classical recrystallization theory the same constant growth rate for all the recrystallized grains is assumed. In the present simulation that assumption is not satisfied. Furthermore many authors [1,2] stated that this linear behaviour is never observed in experiment.

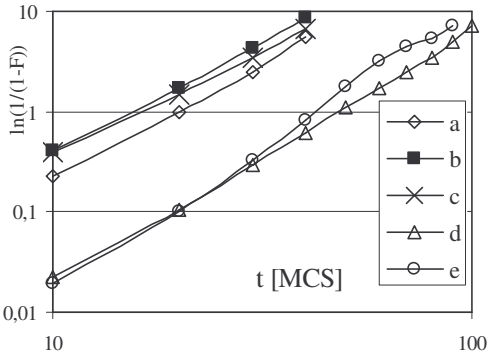

Fig. 7. The Avrami plots for the degree of stored energy *H/J=2* and different nucleation models: a) decreasing nucleation rate I, b) decreasing nucleation rate II, c) site saturated, d) increasing nucleation rate and e) continuous nucleation rate.

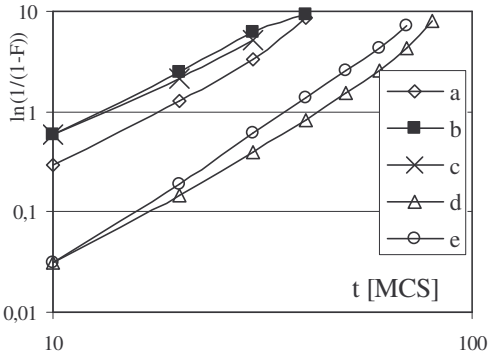

Fig. 8. The Avrami plots for the degree of stored energy *H/J=2.5* and different nucleation models: a) decreasing nucleation rate I, b) decreasing nucleation rate II, c) site saturated, d) increasing nucleation rate and e) continuous nucleation rate.

SUMMARY

In the paper the influence of different values of the degree of the stored energy *H/J* and different models of the nucleation on the recrystallization kinetics modelled by the Monte Carlo simulation has been shown. The results of the simulations of the primary static recrystallization confirm correctness of the models concerning the curves of the recrystallized volume fraction *F(t)*. The sigmoidal time dependence of recrystallized volume fraction observed in the simulation is often emphasized in the literature and finds its justification in the experiment (fig. 1-4). The Avrami exponent *n=2* is properly reproduced by the simulations (fig. 5-8). It has been shown that the model correctly responds to the change in the degree of stored energy *H/J* and remains in agreement with theoretical and experimental works of other authors.

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