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Modelling the Evolution of Microstructure During Recrystallisation

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This paper discusses the evolution of the microstructure during grain growth and recrystallisation, modelled using the Monte Carlo technique. The properties of alloys and metals subjected to plastic deformation and annealing are significantly influenced by the grain growth and recrystallisation processes. Modelling the recrystallisation process enables the simulation of various driving forces at a fundamental level by defining energy conditions for each individual element. The calculations facilitate the observation of microstructural evolution and the generation of structures consistent with any set of postulates, allowing both the dynamics and the physical processes of grain growth and recrystallisation to be simulated. The paper describes a recrystallisation model based on a two-dimensional array containing 40 000 elements. Each element in the array is assigned a number symbolising the orientation of the grain in which the given element is embedded, along with a value of the free energy of the grain boundary. The internal energy for a given grain is also specified. Four types of nucleation have been modelled. Based on the results obtained, the Monte Carlo technique is considered to be an effective tool for modelling recrystallisation processes, allowing the introduction of many different driving forces. The model presented in the work enables the simulation of the nature of local energy conditions and dynamics.

topics: recrystallisation, numerical simulation, Monte Carlo simulation, evolution of microstructure

1. Introduction

Cold metal forming processes entail heterogeneous plastic deformation leading to material hardening. Microscopically, cold plastic deformation results in increased dislocation and point defect densities. At the macroscopic level, plastic strain is manifested as grain deformation, accompanied by an accumulation of stored energy within the material. This unstable condition necessitates annealing at a specific temperature, known as the recrystallisation temperature.

Recrystallisation is a critical process in metallurgy that transforms a cold-worked structure into a strain-free one through the nucleation and growth of new grains, significantly affecting the mechanical properties and overall performance of the material [1]. This process is essential for softening metals that have been hardened by plastic deformation, allowing further shaping and forming operations without compromising the integrity of the material.

The main driving force behind this phenomenon is assumed to be the stored energy from plastic deformation, which is distributed within the deformed grains, predominantly in the form of point defects and dislocations.

2. Methodology of the simulation

One of the most frequently used numerical methods for modelling the physical phenomena is the finite element method (FEM). Piekarska et al. [2] presented the phase transformation model based on the continuous cooling transformation diagram plotted for welded steel and on the Avrami, Koistinen, and Marburger equations.

The Monte Carlo method is widely recognised as a promising approach for simulating the evolution of microstructures during recrystallisation. It finds applications in a variety of fields, including paramagnetic to ferromagnetic phase transitions, order–disorder transitions, crystal growth [3], solidification, grain growth [4, 5], and recrystallisation [6, 7]. In this study, the Monte Carlo algorithm is specifically used to simulate primary recrystallisation with varying nucleation rates.

2.1. Monte Carlo simulation technique

A two-dimensional Monte Carlo model was used to study the recrystallisation processes. The simulation technique has been detailed in works [8, 9]. In

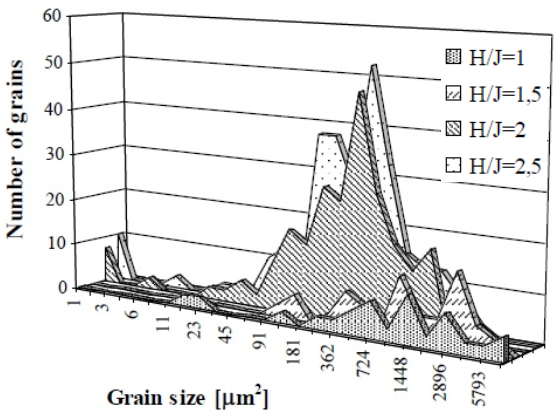

Fig. 1. The logarithmic grain size distribution obtained from the computer simulation of recrystallisation for the site-saturated nucleation model and four different degrees of stored energy $H/J = 1$, $1.5, 2$, and 2.5.

the presented model, the continuum microstructure is discretised into a two-dimensional lattice. Each lattice site (i, j) is assigned a crystallographic orientation represented by an integer from 1 to Q. Initially, the lattice is defined by random assignments of orientations from 1 to Q. To simulate reorientation, a lattice site and a new potential orientation are randomly chosen. The change in energy ΔE associated with this reorientation is computed, and the new orientation is accepted if $\Delta E \leq 0$.

A lattice site is identified as part of a grain boundary if its orientation differs from its neighbouring sites, otherwise it is considered to be part of the grain interior. Successful reorientation of a site from a grain boundary to match the orientation of an adjacent, different site is classified as boundary motion.

In this simulation, n reorientation attempts constitute a Monte Carlo step (MCS). The Monte Carlo model of recrystallisation assumes homogeneous nucleation, i.e., the formation of new recrystallisation nuclei is equally probable at any point within the structure. However, the model exhibits some heterogeneity, i.e., nuclei located inside grains disappear regardless of whether the grain is recrystallised or not. Therefore, similarly to real materials, existing grain boundaries are privileged sites for nucleation in certain locations. To prevent grains of the same orientation from coalescing, Q is set to 48. Recrystallised nuclei are assigned orientations Si ranging from 49 to 64. The initial matrix configuration reflects the desired degree of deformation.

2.2. Simulation parameters

In this study, a comprehensive series of tests on static recrystallisation was performed, incorporating various models of nucleation rates and different levels of stored energy H/J. The initial lattice for the recrystallisation simulation was generated by Monte Carlo grain growth simulation and subsequently deformed.

The frequency of nucleation occurring at grain corners, grain boundaries, and grain interiors was discussed by Saito [6]. It was observed that in the simulation, nucleation within the grain interior is either zero or very low at $H/J = 1$ or 1.5. Under these conditions, nuclei grow only at grain boundaries or at the junctions of three boundaries, which is referred to as heterogeneous nucleation. For $H/J = 2$ and 2.5, critical nuclei can grow when placed anywhere in the lattice, making nucleation within the grain interior dominant, a process known as homogeneous nucleation.

2.3. Nucleation models

Four types of nucleation were simulated in this study:

- site saturated — $I = 200$ nuclei were randomly placed on the lattice at $t = 0$ and no additional nuclei were created;
- constant nucleation rate — $I = 10$ nuclei were randomly placed on the lattice after each Monte Carlo step;
- increasing nucleation rate — new nuclei were placed on the lattice every 10 MCS, where $I = 100$, $n = 10$, and $i = 1, 11, 21, \ldots, 101$ MCS;
- decreasing nucleation rate — nuclei were randomly placed on the lattice every 10 MCS. In this work, $I = 200$, $n = 10$, and $i = 1, 11, 21, \ldots$ MCS were used.

Each type of nucleation was simulated with four degrees of stored energy $H/J = 1, 1.5, 2$, and 2.5.

3. Results and discussion

One of the major advantages of employing the Monte Carlo method for simulating grain growth and recrystallisation is its ability to model and generate complex microstructures based on simple assumptions. This facilitates the effective validation of theoretical hypotheses through comparisons between simulated microstructures and those observed experimentally. Figure 1 illustrates an example of the grain size distribution obtained from the simulation. The calculations were conducted using the site-saturated nucleation model and encompassed all degrees of stored energy examined in this study.

Figures 2–4 show the microstructures simulated with the increasing nucleation rate and stored energy levels and $H/J = 1$, 1.5, and 2, respectively. These figures indicate a strong influence of the H/J value on the recrystallised grain size and its distribution.

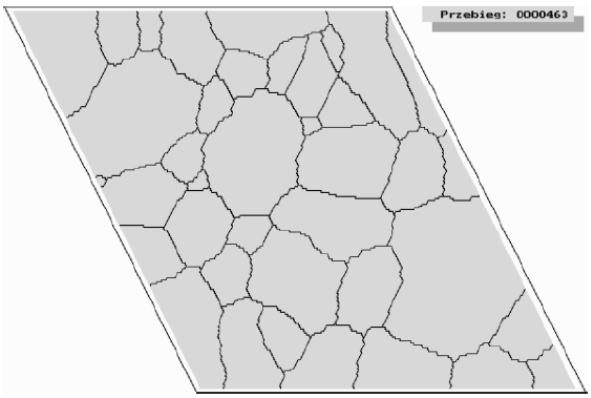

Fig. 2. Microstructure simulated under increasing nucleation rate and degree of stored energy $H/J = 1$.

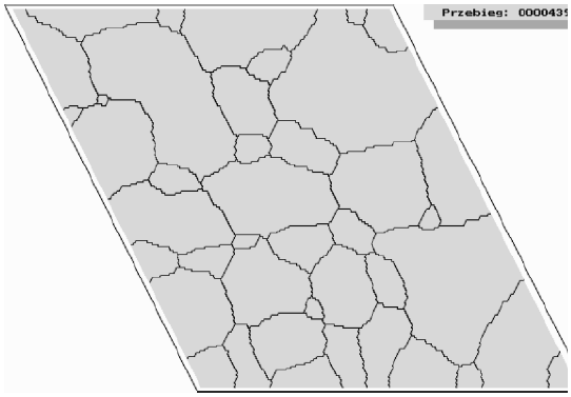

Fig. 3. Microstructure simulated under increasing nucleation rate and degree of stored energy $H/J = 1.5$.

The degree of stored energy H/J is closely related to the extent of cold plastic deformation prior to recrystallisation. A higher H/J value corresponds to greater deformation.

4. Conclusions

The static recrystallisation kinetics is successfully simulated using the Monte Carlo method. The study varied the degree of stored energy H/J and applied different nucleation models. The following key conclusions are drawn from the results:

(i) Impact of stored energy on grain size. The simulations demonstrate that the recrystallised grain size is strongly dependent on the degree of stored energy H/J. Higher H/J values, which correspond to greater plastic deformation prior to recrystallisation, result in finer recrystallised grain sizes.

(ii) Heterogeneous and homogeneous nucleation. The study revealed that at lower stored energy levels ($H/J = 1$ and 1.5), nucleation within the grain interior is minimal, with nucleation occurring primarily at grain boundaries or junctions, indicative of heterogeneous nucleation. At higher stored energy levels ($H/J = 2$ and 2.5) nucleation within the grain interior becomes more prevalent, indicating homogeneous nucleation.

(iii) Nucleation rate models. Various nucleation rate models were simulated, including site-saturated, constant, increasing, and decreasing rates. Each model exhibited distinct effects on microstructure evolution, highlighting the significance of nucleation dynamics in recrystallisation.

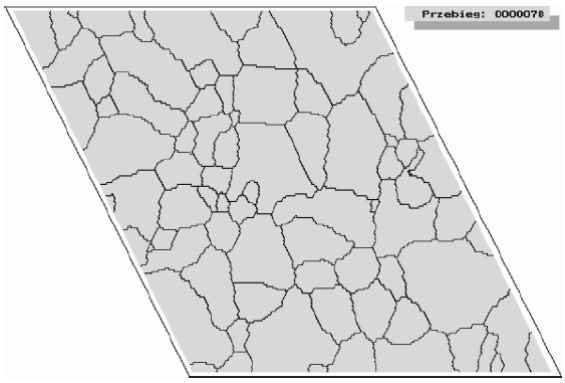

Fig. 4. Microstructure simulated under increasing nucleation rate and degree of stored energy $H/J = 2$.

These findings underscore the effectiveness of the Monte Carlo method in simulating complex microstructural evolutions during recrystallisation and provide a valuable tool for validating theoretical models against experimental data. The strong correlation between simulated and observed microstructures supports the continued use of this technique for studying material behaviour under varying conditions of stored energy and nucleation dynamics.

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