MONTE CARLO SIMULATION OF TEMPERATURE DEPENDENCE OF GRAIN GROWTH KINETICS IN C-Mn STEEL PRIOR TO HOT ROLLING

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Abstract

A Monte Carlo simulation framework has been proposed to characterize grain growth phenomena during microstructural evolution of plain C-Mn steel under reheating condition prior to hot rolling. The effect of deformation temperature on the temporal evolution of the grains has been analyzed during reheating operation prior to hot rolling.

Keywords: *Monte Carlo simulation, C-Mn steel, grain growth evolution, average grain-size, reheating temperature*

1.0 Introduction

Grain growth is the process in which the average grain size increases after primary recrystallisation is complete. The driving force results from the decrease in free energy which accompanies reduction in total grain boundary area. Normal grain growth kinetics have been described by

$$d = kt^n \tag{1}$$

where d is the average grain diameter, n is referred to as the growth exponent, t is the annealing time and k is a constant which exhibits Arrhenius temperature dependence.

In the present work, a Monte Carlo (MC) simulation framework has been developed to study the grain growth behaviour of plain C-Mn steel slab during reheating operation in the furnace prior to rolling.

2.0 Methodology

In this simulation, the grain structure of single phase materials was initialized with a two dimensional square lattice of size 400X400 and site orientation (Q). The evolution of the microstructure is modeled by picking a site and choosing a new orientation at random from the set of allowable values. The change in total system energy (ΔE) for reorienting the site is computed, and the reorientation is implemented with a Boltzmann transition probability. The total energy, E, of the system is defined as:

$$E = J \sum_{i=1}^{nn} (1 - \delta_{s_i s_j}) \tag{2}$$

where, J is a positive constant which sets the scale of the grain boundary energy, S_i and S_j are the orientation numbers of site i and one of its neighbor sites j, respectively and $\delta_{s_i s_j}$ is the Kronecker delta.

3.0 Results and Discussions

A typical grain growth process is shown in Fig 1. A color of a lattice point represents the crystallographic orientation of the grain. Fig 2 shows the variation of the grain size distribution for the simulated microstructure. The average grain size as a function of Monte Carlo time steps (MCS) for different values of Q (8, 16, 32, 48, and 64) is shown in Fig.3. The simulation results do not depend significantly on the value of Q, while Q is greater than 32. The value of grain growth exponent (n) has been extracted from the slope of the plot of logarithm of grain size versus Monte Carlo time (Fig. 4). It may be observed from this figure that the evolution process follows power growth kinetics [1]. Figure 5 shows the validation of current Monte Carlo prediction with Yoshie model [2] for C-Mn steel. Figure 6 depicts the logarithmic variation of k as a function of 1/T. As k follows Arrhenius law with regard to temperature variation, the slope of the line gives the activation energy for grain growth. The value of activation energy (order of magnitude) obtained form this model for C-Mn steel is found to be in close agreement with the value cited in the literature [3].
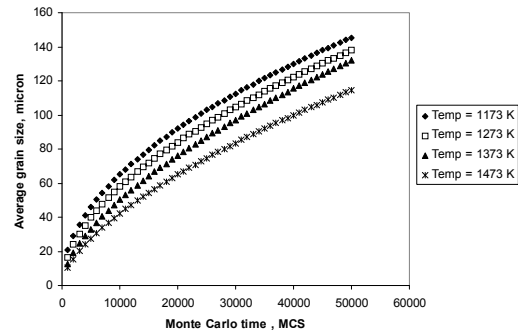
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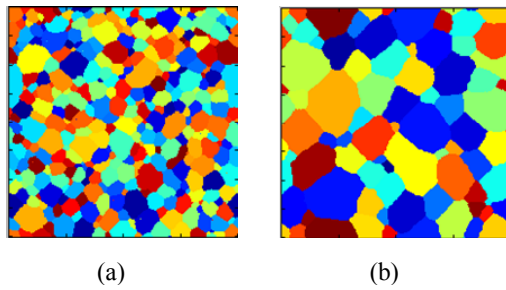
Fig 1: Temporal evolution of grain boundary at temp1173 K and Q = 48 a) 1000 MCS, b) 5000 MCS
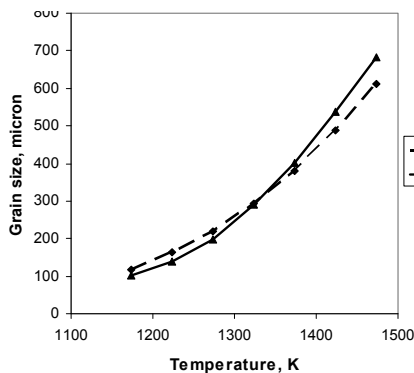

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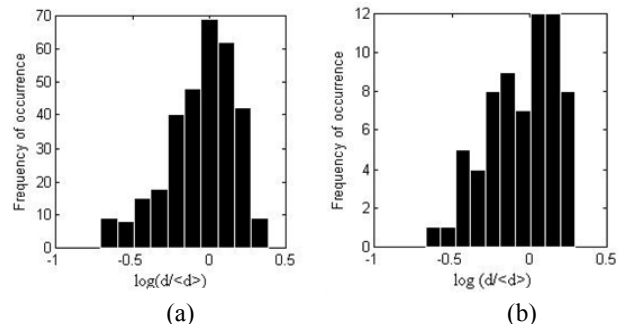
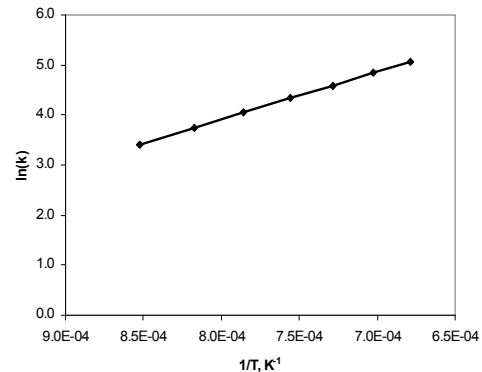**Fig 2: Grain size distribution at temp 1173 K for different MCS, a) 1000 MCS, b) 5000 MCS**
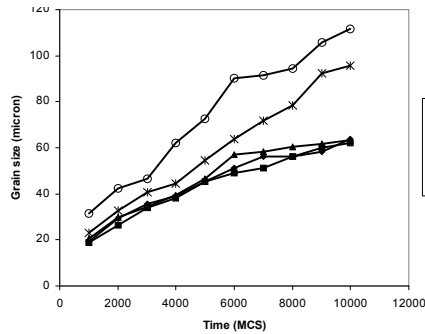
Fig 3: The grain growth behavior as a function of number of grain orientations (Q)

Fig 4: Average grain size variation with Monte Carlo time step at different temperatures

Fig 5: Validation of Monte Carlo grain growth simulation with Yoshie model [2]

Fig 6: Logarithmic variation of model constant (k) as a function of reciprocal temperature

4.0 Conclusions

The present model assumes an isotropic distribution of grain boundary energy. The average grain size, grain size distribution, simulated microstructure as a function of MCS and activation energy of grain growth have been predicted for various operating temperatures. The Monte Carlo predictions are found to be in excellent agreement with published literature and consistent with power law growth kinetics.

5.0 References

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