

Microstructure prediction of light weight steel using probabilistic Cellular Automata

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ABSTRACT

Microstructure evolution during thermo-mechanical treatment of steel is of significant importance to obtain the desired mechanical properties in the final product for various applications. Cellular Automata model in mesoscale is one of the most important simulation methodologies for studying the recrystallization and grain growth processes in materials. In the present work, temporal evolution of microstructure in austenitic light weight steel has been simulated using probabilistic Cellular Automata technique. Two dimensional microstructural maps have been generated to visualize growth kinetics at various temperatures. The simulation time step has been calibrated to the physical time of the process in order to compare the model prediction with experimental data of grain growth kinetics for austenitic Fe-Mn-Al-C steel and have been found in good agreement. It has been found that the average grain size increases with time and the number of grains decreases resulting grain coarsening at a fixed isothermal holding temperature. The predicted grain growth exponent is corroborated well with the published literature data. The grain size distribution has been found to be self-similar, indicating that the average grain size has shifted to larger grain size which closely resembles experimental results.

Keywords: Cellular Automata simulation, grain growth, average grain-size, steel, microstructure evolution

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I. INTRODUCTION

Low density steels have become a paramount consideration for automobile applications to reduce environmental burden and fuel consumption [1-3]. The properties of these steels are highly influenced by the evolution of microstructures which may be austenitic, ferritic or duplex based, according to the phase constituents of the matrix. The austenitic alloys are very promising for their high strength, high formability and good toughness. Therefore, controlling the evolution of microstructures through processing is very crucial to optimize the performance of these materials. The material properties, specifically the mechanical behavior significantly depend on grain size and thus, the grain growth phenomenon has tremendous technological importance for materials application point of view. For example, in structural applications at low temperatures, generally a smaller grain size is required to optimize strength as well as toughness, whereas for high temperature creep resistance requirements, a large grain size is preferable. Further, in steels, the kinetics of austenite transformation

during cooling is sensitive to the prior austenite grain size. Therefore, a sound understanding of grain growth phenomenon is required to control the microstructures and properties of materials during its processing. This also necessitates to control a large number of variables associated with microstructure evolution which makes the problem challenging.

Grain growth predominantly occurs when a material is exposed to a high temperature. The driving force for grain growth comes from the reduction of free energy of the total area of the system. Over the last few decades, a number of analytical and numerical approaches have been developed to describe the evolution of grain growth process [4-6]. Mesoscale modelling is an emerging computation tool to simulate the evolution of microstructure and extensively used in the area of physical phenomena such as solidification, grain growth, recrystallization and phase transformation. This modelling technique includes methodologies such as Potts Monte Carlo (MC) models, cellular automata (CA), Ginzburg-Landau-type phase field kinetic model etc [7-10]. In both the Monte Carlo and

Cellular Automata methods, the microstructure is discretized on a regular grid and both are successfully applied to simulate the recrystallization and grain growth processes. The Monte Carlo model is successful due to its flexibility and computational simplicity [7,9]. But, an important shortcoming of MC model is the absence of temperature dependence of average grain size as well as correspondence between Monte Carlo steps and real time. This inability makes this method inappropriate when comparing characteristics of simulated grain growth data with experimental investigation. In contrast to the MC method, the dynamics governed by the CA method are deterministic and variables like temperature are better defined [10-13]. Further, the CA method use only local rules and avoid the need to generate high quality random numbers for the simulation of microstructure evolution. In current times, the phase-field modeling is very promising for simulating various processes at the mesoscale level. The gamut of applicability of phase field method is growing rapidly because of high performance computing technique. The phase field model has been applied successfully in the areas of solidification, solid-state phase transformations, grain growth etc [14-15]. However, the computational effort involved in simulating an evolving microstructure using phase field method is time consuming.

In this investigation, a Cellular Automata modelling framework has been developed to understand the grain growth behavior of austenitic steel during annealing. The grain growth models incorporate some of the thermodynamic parameters like grain boundary energy, activation energy of grain boundary diffusion etc. These parameters are not always easily obtainable from open literature for different alloy systems. In spite of the intensive studies in the simulation of microstructure evolution, spatial and temporal evolution of complex microstructure in materials still remains a challenging problem. In cellular automata, the system evolves by applying a set of deterministic rules which depend on some of the specific variable as well as neighboring cells of a lattice system. In spite of such simplicity of CA, it shows a significant complexity in their behavior that emerges from simple rules and hence, fascinated materials researchers. In materials modelling, people often faced with very complex behavior based on physical mechanisms that cannot be modelled directly. With cellular automata, such complex behavior can be modelled with very simple rules and computations, which can yield behavior that is very similar to known materials phenomena. In traditional CA modeling, a time step is determined by the previous time step. In probabilistic CA, deterministic rules are replaced by stochastic rules that depend on randomly changing a state from one

configuration to other. Probabilistic Cellular automata have been applied successfully to simulate the evolution of grain growth in polycrystals. However, this modelling technique has no real time of physical system owing to its probabilistic nature. Therefore, difficulties arise during conversion of simulated time (CA step) to real time and thus verifying that the model correctly captures the underlying physio-chemical processes is not straight forward.

Although, CA model has been developed long ago, however, it found wide applications in the diverse areas of science and engineering in the last few decades [16-21]. The model has been used extensively to simulate mesoscopic behaviour of materials, such as solidification [18-19], grain growth, recrystallisation [10-13, 16,17], texture evolution [20] and phase transformation [21]. In particular, it was very successful in describing grain growth kinetics in polycrystalline materials. Initially, Hesselbarth et al. [10] proposed CA method to simulate recrystallization behavior in 2-dimensions. Thereafter, the method has been applied in many material behavior processes such as static and dynamic recrystallization and the influences of texture and precipitates on grain growth process. Although this methodology has been applied widely in materials science, however, some of the critical issues have not yet been taken into consideration in depth using CA technique. Except very few [22], in most of the simulations the spatial dimensions and time interval employed are not calibrated by a characteristic physical length or time scale but investigated in a generic manner and the literature information in this domain is rather scanty.

In this paper, grain growth kinetics of low density steel during annealing has been studied using Cellular Automata simulation framework. Temporal evolution of microstructure in two dimensions has been simulated at different temperatures to study the effect of temperature on grain growth kinetics. In the simulation, the anisotropy of the grain boundary energy and mobilities of grain boundaries have been incorporated in the model. The conversion of Cellular Automata step to real time is attempted based on curvature-driven grain growth mechanism and the simulation results have been calibrated to real time of the grain growth process in order to compare with the experimental data. The simulation results have been analyzed and validated in the light of experimental data obtained from literature [23].

1.1 THE CELLULAR AUTOMATA METHOD

In Cellular automata, system can be divided into regular finite number of cells (square, triangular or hexagonal) where each cell may have a definite

number of states. During the evolution of the system a set of homogeneous local rules are obeyed through discrete time steps which represent the dynamics of the systems. These local rules are defined so that the required governing laws are fulfilled. The updated state of each cell is determined using these states switching rules which depend on the previous configuration of the selected site as well as configuration of the neighboring sites. Fig. 1(a, b) shows a two dimensional square cellular automata grid, the neighborhood is typically defined to be the four (Von Neumann) or eight (Moore) adjacent neighboring cells [11].

In this method, the microstructure is mapped onto a discrete two dimensional square lattice system. In two dimensions, the cell neighbourhood is defined using either the Von Neumann or Moore method. To produce the initial microstructure, the orientation of lattice sites is initialized randomly by assigning an integer number, S_i between 1 and Q to each lattice site, where S_i is the number of a grain orientation and Q is the maximum number of possible grain orientations in the system. All sites within a grain have the same orientation number S_i , and the grain boundaries are interfaces between two neighboring sites with different orientation numbers. Periodic boundary conditions are used to avoid the finite size effects. In this boundary condition, a site on the edge of the domain is connected to sites on the opposite edges. The simulation steps are as follows:

- (i) A lattice site is selected which takes the orientation of one of its neighborhood following a given transition rule.
- (ii) A cell must overcome the energy barrier, which is a function of temperature, to attain its new state. The probability (P) of successful transition of the state in a cell is given by a simple equation (Equation 1) [24]:

$$P = \exp(-\Delta E / RT) \quad \text{----- (1)}$$

where ΔE is the energy barrier, T is temperature in absolute scale and R is the universal gas constant.

- (iii) The transition of atoms depends on the free energy difference (ΔG_A) of atoms as well as on the energy barrier before and after jumping.
- (iv) The energy of a cell is given by the sum of thermal energy (G_T) and grain boundary energy (G_B). The thermal energy of the cells is assumed to follow the Maxwell-Boltzmann distribution. According to Maxwell-boltzmann statistics, the thermal energy ΔG_T can be defined as [25]:

$$\Delta G_T = -RT \ln(\text{RAND}()) \quad \text{----- (2)}$$

where RAND() is any random number between 0-1. The grain boundary energy is given by the Hamiltonian, as represented in Equation 3:

$$G_B^i = G_B(\theta) \Sigma(\delta_{s_i, s_j} - 1) \quad \text{----- (3)}$$

where $\Sigma(\delta_{s_i, s_j} - 1)$ is the count of non-similar neighbour sites of the selected site. From the Read-Shockley equation (Equation 4) the grain boundary energies are calculated.

$$G_B(\theta) = G_0 \sin \theta [1 - \log(\sin \theta)] \quad \text{----- (4)}$$

where, $G_B(\theta)$ is the boundary energy as a function of the misorientation angle, θ , the G_0 is the maximum grain-boundary energy seen at a high angle. The misorientation angle is calculated based on Equation 5:

$$\theta = \frac{\pi}{2} * \left(\frac{\Delta Q}{Q} \right) \quad \text{----- (5)}$$

where ΔQ is the difference between the orientation numbers of two adjacent grains.

In the CA model [24], the energies are compared directly. If the thermal energy is greater than the difference between the activation free energy and the total boundary energy of the cell then the grain boundary moves.

$$G_T > G_A - \Sigma G_B^i \quad \text{----- (6)}$$

Equation 6 represents the transition rule. If Equation 6 is satisfied, the boundary passes through the cell and the selected site is replaced with the random neighbour site.

The unit of time is defined as one Cellular Automata Steps (CAS) per site, which corresponds to N re-orientation attempts where N is the total number of sites.

1.2 SIMULATION METHODOLOGY

The microstructure of polycrystalline material consists of grains of different sizes and is depicted by an average grain size and a grain size distribution. The average grain size under normal isothermal grain growth conditions obeys power law growth kinetics of the form [23]:

$$d^m - d_0^m = kt \quad \text{----- (7)}$$

where d and d_0 are the final and initial average grain size, respectively, m is the growth exponent and depends on many parameters including alloy composition and annealing temperature, t is the annealing time and k is a constant which exhibits Arrhenius temperature dependence. In the case of $d \gg d_0$, the kinetics is reduced to

$$d = kt^n \quad \text{----- (8)}$$

where the grain growth exponent, n , is equal to $1/m$.

To obtain one-to-one correspondence between CA technique and real parameters of grain size and time, it has been assumed that the real grain size is related to the CA grain size as

$$d_R = k_1 d_{CA} \quad \text{-----(9)}$$

where d_R is the real grain size, d_{CA} is the simulated grain size, and the constant, k_1 is a scaling factor. The relationship between real time and CAS is defined [26] as

$$CAS = k_2 t \quad \text{-----}$$

---(10)

The quantity, k_2 , in the Equation 10 represents temperature-dependent boundary mobility given by

$$k_2 = k_0 \exp\left(\frac{-Q_A}{RT}\right) \quad \text{-----(11)}$$

where k_0 is the pre-exponential factor, Q_A is the grain growth activation energy, T is the temperature on absolute scale, and R is the universal gas constant.

In the present work, the Cellular Automata technique has been used to simulate the grain growth kinetics in austenitic steel (Fe-30.8Mn-9.2Al-0.7Si-1.0C-0.5Mo, wt%) under isothermal conditions. In this simulation, the initial grain structure was generated randomly using a 2-D square lattice system of size 200×200 with grid size of $2 \mu\text{m}$. In order to avoid frequent impingement of grain of similar orientation, a large value has been assigned to Q ($Q = 256$) [12]. The value of activation energy has been taken as 467 kJ/mol [23], which is the activation energy for grain growth in the lightweight steel considered in this paper. In this simulation, average grain size has been computed over a time range, which is fixed at 1800 s . In order to verify the predictive capability of the present model and to validate the simulation results with experimental data, the Cellular Automata Steps have been calculated using Equation 10 and the CA simulation were run for predetermined CAS for different temperatures and the corresponding grain size have been considered. The mobility values for the steel at varying annealing temperatures have been obtained from literature and are shown in Table 1 [23]. The atomic mobility values can be calculated from the change in grain diameter squared [26]. Table 2 lists the values of the parameters used in the developed code used to implement the grain growth model based on CA algorithm.

II. RESULTS AND DISCUSSION

In the present work, input parameters are initialized on the basis of experimental data to define the starting microstructure (Table II). The average

grain size as a function of CAS for different values of Q is shown in Fig.2. It may be observed that grain size variation shows a dependence on Q values of 4, 8 and 16. However, for higher Q values ($Q \geq 32$) this dependence sharply diminishes as Q value increases. The low Q configurations consist of irregular and asymmetric grains and the irregularity is enhanced with reduced Q values. On the other hand, the grains in the high Q configurations are considerably compact and equiaxed. These predictions and their trend are validated and are in agreement with the data published in literature [12]. Fig. 3 depicts the variation of number of grains as a function of CAS which shows that grain numbers in the simulation system reduced progressively. This is in accordance with the published literature [25].

In Figures 4 and 5 the computed microstructural evolution maps are shown at different CAS considering both Von Neumann and Moore neighborhood for different temperatures, $400 \text{ }^\circ\text{C}$ and $600 \text{ }^\circ\text{C}$, respectively. In these maps, multiple colours represent various crystallographic orientation of the lattice. Temporal evolution of grain growth has been clearly elucidated in Figures 4 and 5 as a function Cellular Automata time. It has been found that Moore neighborhood consideration gives better resolution, kinetics of grain growth remaining the same. Hence, throughout the simulation we have considered Moore neighborhood. Coarsening of large grains by absorption of small grains can be observed during the grain growth process with the advancement of CA time. It has been observed by experimentally that the distribution of grain size on normalizing by average grain size remains more or less constant during the growth phenomenon. This definitely implies that during the process some grains grow, while others shrink, the grain ensemble remains self-similar.

Fig. 6 shows the grain size distribution at temperature $600 \text{ }^\circ\text{C}$ for different CAS. The result indicates the time invariance of the grain size distribution when plotted as a function of the normalized grain size, which is in agreement with the published literature [23]. Fig. 7 shows temporal evolution of grain size as a function of CAS over the temperature range 1000 , 1050 and $1075 \text{ }^\circ\text{C}$. The simulation has been run for duration up to 1800 s and the corresponding CAS has been computed using Equation 10. The data represented in the figure is the average value of at least five simulation runs. The relationship of CAS and real time depends on number of factors such as grain growth activation energy and temperature. It may be observed (Fig. 7) that the evolution process follows power law growth kinetics [12] and grain growth is faster at elevated temperatures. The grain size of the product phase also depends on the relative rates of nucleation and growth. The value of grain growth exponent (n) has been extracted from the

slope of the plot of logarithm of grain size versus Cellular Automata time and obtained as 0.367, 0.394 and 0.390, respectively (refer Fig. 7). Fig. 8 shows temporal evolution of grain size as a function of CAS at different temperatures, namely, 900, 950, 975, 1000, 1050 and 1075 °C. The plot is obtained based on Equation 8 after estimating the values for 'n' and 'k'. Hillert [26] predicted the value of n to be 0.5 using an analytical model for pure metals. The present CA simulation estimated the value of n in the range 0.37-0.41 over the temperature range of 900 – 1075 °C, which is in agreement with the Hillert model.

Fig. 9 shows the variation of average grain size as a function of temperature. For comparison purpose, the experimental data obtained from literature is also included in the figure superimposed on it. The solid line represents the best fit to the simulated data and the broken line represents the best fit to the experimental data. To verify the predictive capability of the present model, all the pertinent parameters used in the simulation has been kept similar to the experimental data and shown in Table 1. Fig. 9 clearly demonstrates that present Cellular Automata computations are in good agreement with the experimental data for austenitic steel. Fig. 10 depicts variation of grain growth exponent as a function of temperature, which is nearly constant with respect to the temperature. The model constant k as a function of temperature has been shown in Fig. 11. It may be observed that k increases with the increase in temperature, which is consistent with respect to Arrhenius temperature dependence functionality.

III. CONCLUSIONS

The temporal evolution of grain growth has been simulated using Cellular Automata method. Two dimensional microstructural maps have been generated to visualize the growth kinetics at various temperature levels which captures the grain coarsening phenomena. The average grain size variation with CAS for different values of grain orientation (Q -value) has been found to be less sensitive to higher Q -values (≥ 32). However, the average grain size variation shows a dependence on lower Q -values. The average grain size variation as a function of CAS has been computed. It has been found that grain size increases with the increase in temperatures and steady state grain size distribution is self-similar and follows log-normal distribution. The grain growth exponent ' n ' has been determined by constructing a graph of the logarithm of average grain size against time for each temperature and have been found as 0.4 ± 0.04 , which is in reasonable agreement with the literature data. It has been found that grain size increases at elevated temperature.

Understanding the evolution of microstructure as well as grain size distribution and morphology of microstructure during annealing is very important. The grain size obtained using CA simulation has been validated with the experimental data for light weight steel and has been found in good agreement.

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Conflict of interest

The authors declare that they no conflict of interest.

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Table 1: Mobility values for the lightweight steel at varying annealing temperatures.

Annealing Temperature	Mobility($\mu\text{m}^4/\text{J.hr}$)
1173 K (900°C)	0.194×10^2
1223 K (950°C)	0.350×10^3
1248 K (975°C)	1.95×10^3
1273 K (1000°C)	5.63×10^3
1323 K (1050°C)	8.01×10^3
1348 K (1075°C)	10.9×10^3

Table 2: Input parameters for simulation [23]

Parameters	Values
$G_A = Q_A$	467 kJ/mol
G_0	25 kJ/mol
Q	256
R	8.314 J/mol.K

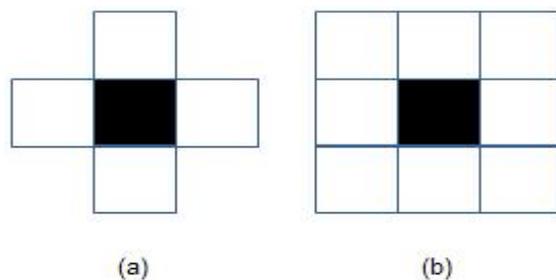


Figure 1: Two types of neighborhood (a) Von Neumann, (b) Moore neighborhood in CA

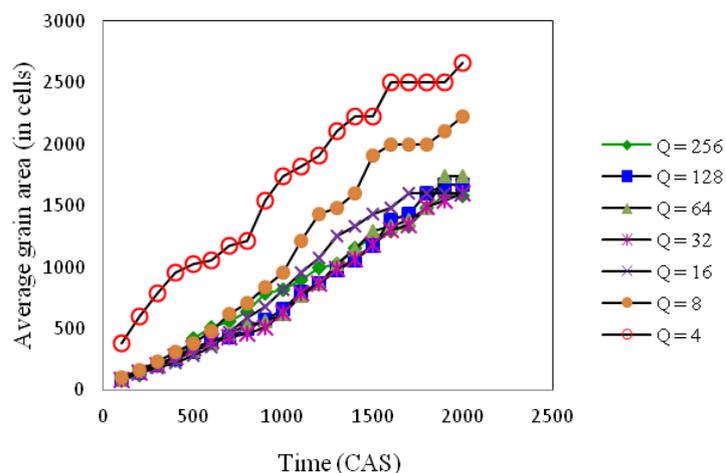


Figure 2: Average grain size as a function of CAS for different values of Q at 600°C

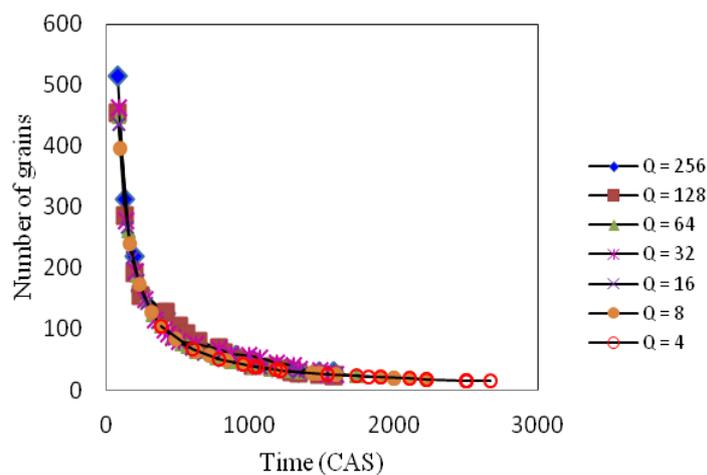


Figure 3: Number of grains as a function of CAS at 600 °C

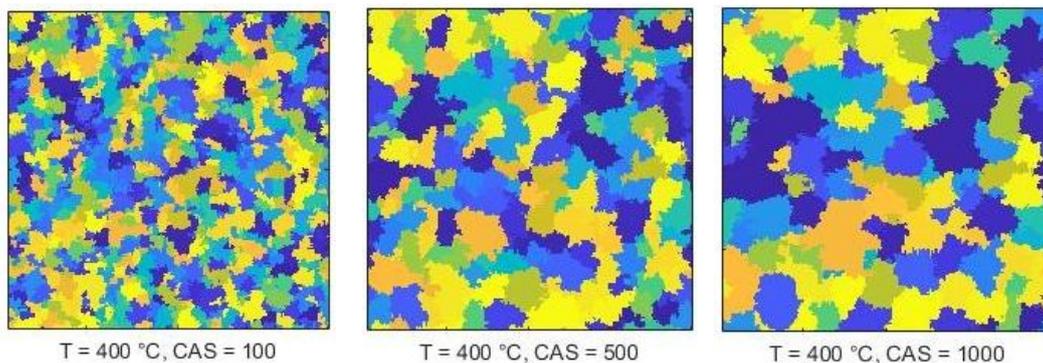


Figure 4: Temporal evolution of microstructure for 200×200 square lattice at temperature 400 °C for different CAS (Von Neumann neighborhood)

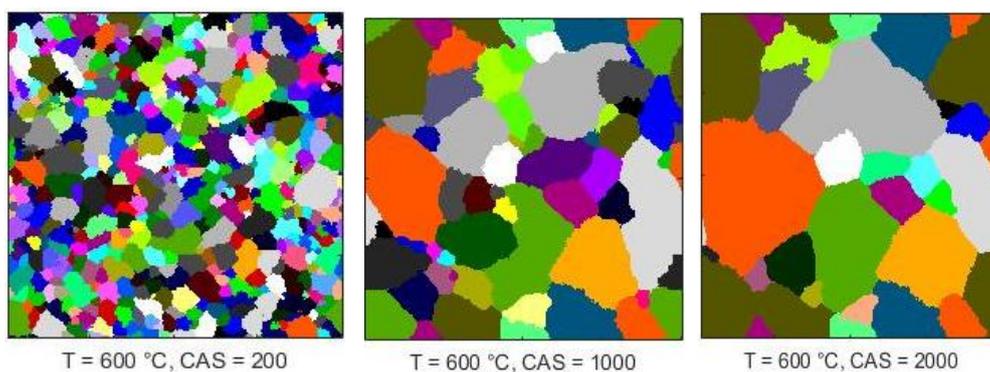


Figure 5: Temporal evolution of microstructure for 200×200 square lattice at temperature 600 °C for different CAS (Moore neighborhood)

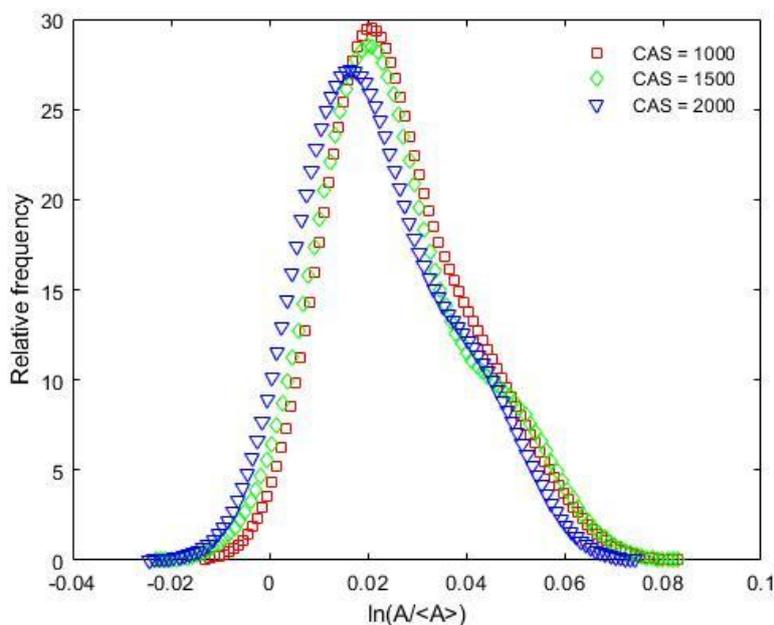


Figure 6: Grain size distribution at temperature 600 °C for different CAS on 200×200 square lattice.

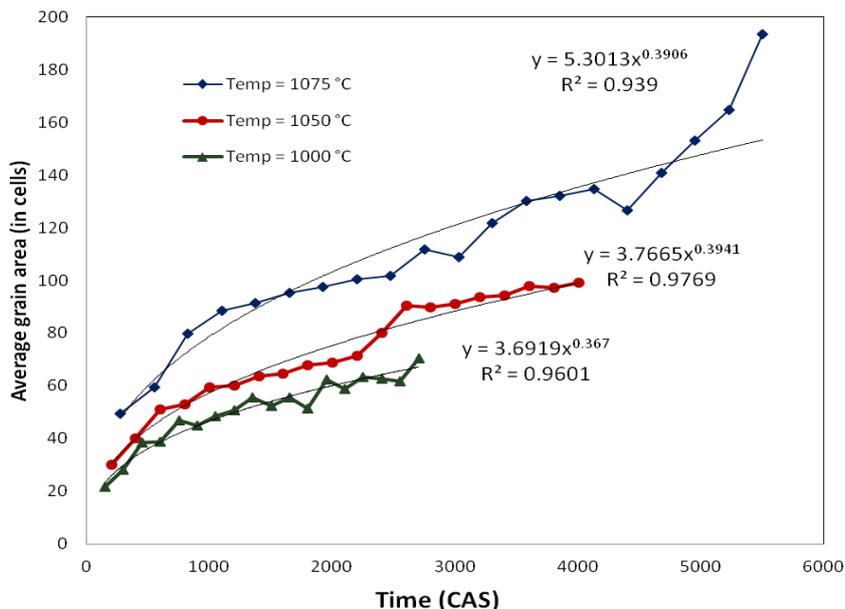


Figure7: Average grain size as a function of CAS for different temperatures

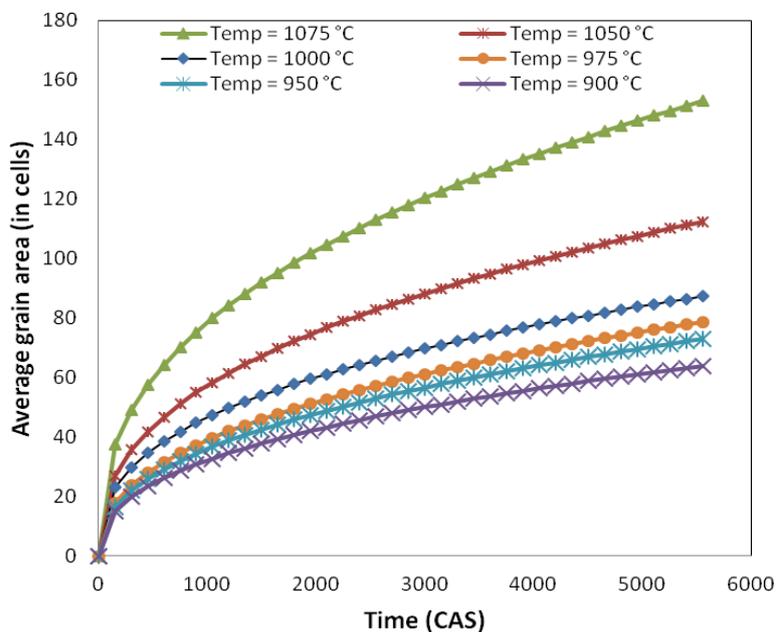


Figure 8: Average grain size as a function of CAS for different temperatures

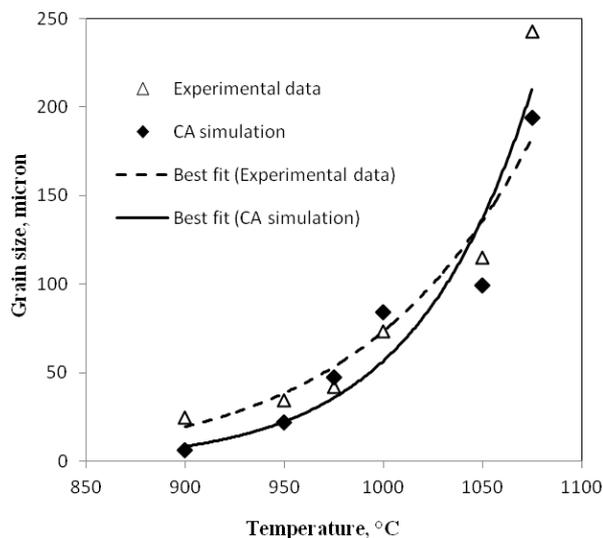


Figure 9: Average grain size as a function of time for different temperatures

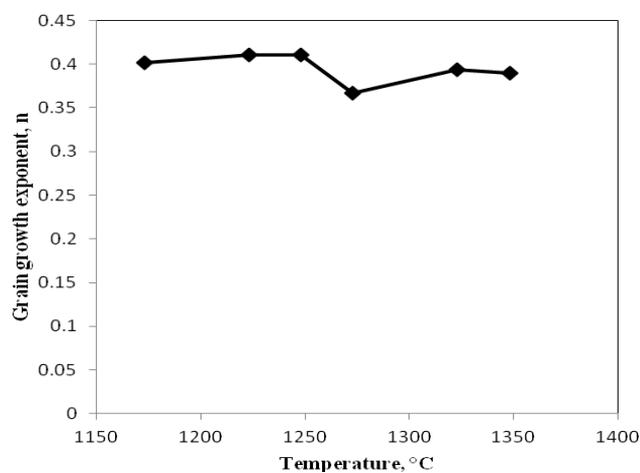


Figure 10: Variation of grain growth exponent, n as a function of temperature

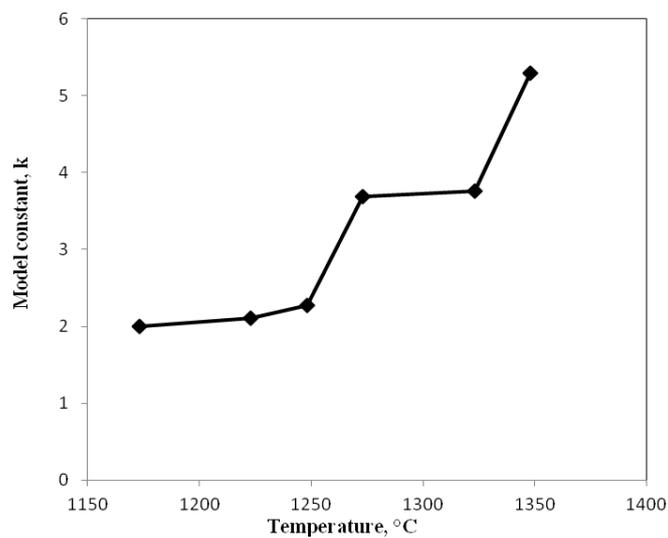


Figure 11: Variation of model constant, k as a function of temperature