# *Monte Carlo simulation of microstructure evolution during thermo-mechanical rolling of steel using grid computing technology*

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*Abstract* - **A Monte Carlo (MC) simulation methodology using high performance computing (HPC) has been proposed to characterize grain growth kinetics and recrystallisation phenomena during hot rolling of C-Mn and TRIP steels. The simulation framework comprises of mesoscale modelling of evolution of grain growth and microstructure incorporating the system energetics of grain boundary energy and stored energy which are essentially the driving force for the evolution process. An in-house MC computer code has been developed and implemented in the GARUDA grid. This facilitated achieving faster convergence of the MC algorithm for a given lattice structure. The simulated grain growth and microstructure evolution have been successfully validated with the published data. It is inferred that the MC simulation in conjunction with HPC grid capability can be a powerful tool to simulate material behaviour at mesoscopic scale during thermo-mechanical processing of materials.**

*Keywords* - **Monte Carlo simulation, C-Mn steel, Trip steel, grain growth evolution, average grain-size, recrystallisation kinetics, Grid computing**

## I. INTRODUCTION

Computer based modelling and simulation of microstructural evolution in thermo-mechanical processing has been accepted as one of the most important tools for the efficient design of high-quality steels. The computer simulation models based on first principle approaches, dislocation dynamics, mesoscopic modelling and artificial intelligence techniques have been successfully applied to the prediction of metallurgical phenomena, such as thermo-mechanical behaviour, grain growth and recrystallisation kinetics and evolution of microstructure. However, the modelling of the spatial and temporal evolution of complex microstructure and non-linear interactions during thermo-mechanical treatment still remains a difficult problem in spite of intensive studies in this field. On the other hand, with the advent of HPC, there has been an increasing application of high fidelity computer simulation technology for computational design of materials and processing. Multiscale modelling technique is one of the most promising methods which provide a framework for the design, processing and performance prediction of materials. It provides a linkage from the molecular level up to the macroscopic property level and so permits the assessment of the effect of molecular changes on final properties. While the importance of multiscale modelling in this context is increasingly recognized, however, there is not much work accomplished to address complex and challenging issues in the multiscale materials modelling using HPC.

MC simulation at the mesoscopic scale is one of the most important simulation methodology for studying the recrystallisation, grain growth and microstructure evolution in the materials. Initially, Anderson et al. [1-2] proposed the method to predict grain growth in two dimensions. Subsequently several researchers applied this method to model grain growth, static and dynamic recrystallisation and the influences of texture and particles on grain growth process [3-7]. Although the method has been applied extensively in materials processing operations, however, some of the issues have not yet been addressed comprehensively using stochastic computational techniques, predominantly validation of the model with respect to experimental data and sensitivity of the process and operating parameters on the material properties in prototype industrial system. In particular, the effect of temperature on the austenite grain growth kinetics prior to hot rolling and the effect of strain on the kinetics of recrystallisation and recrystallised grain size of deformed material has not been explored extensively till date. Literature information pertaining to these issues is rather scarce. Majority of the reported MC simulation studies primarily focused on topological aspects and kinetics of recrystallisation and grain growth at temperatures 0 K [1-3] and near 0 K [6]. However, similar investigations have not been reported at elevated temperatures. This is primarily attributed to the limited availability of state-of-the-art HPC facilities and advances in computing technologies.

In the present work, a MC simulation framework has been developed to study the grain growth behaviour of plain C-Mn steel slab during reheating in the furnace prior to hot rolling. The microstructure changes continuously during different processing steps of hot rolling operation. The austenite microstructure after rolling and subsequent cooling on the run out table determines the final grain size and corresponding mechanical properties of the product. Therefore, the model for the prediction of the grain growth of steel during the slab reheating process is arguably the first step for the development of a comprehensive thermo-mechanical predictive model of the rolling process. It not only provides the knowledge of initial grain size but also provide information to control the reheating process parameters. The MC method also has been extended to study the effect of strain on the kinetics of recrystallisation, recrystallised grain size and evolution of microstructure based on a dislocation-strain interaction model. The interaction of dislocations due to different strain and their contribution to the stored energy of the deformed material is calculated. The modelling results have been verified by the experimental data for TRIP steel.

## II. METHODOLOGY

### *A. Semi-empirical grain growth models*

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. According to Hillert's analytical model [8], the normal grain growth exponent $n$ is equal to 0.5 for pure metals.

In his seminal work, Sellars et al [9] arrived at the following general expression for grain growth using previously published data on low carbon-manganese steels

$$d^m - d_0^m = k_1 t \tag{2}$$

$$k_1 = \left[ A_1 \exp\left( -\frac{Q_g}{RT} \right) \right] t \tag{3}$$

where $d_0$ and $d$ represent the initial and the final average grain size respectively, $m$ is referred to as the growth exponent, $A_1$ is a constant which depends on material composition and processing conditions, $Q_g$ is the activation energy for grain growth, $R$ is the universal gas constant and $T$ is the absolute temperature.

Yoshie [10] proposed an empirical approach to predict the grain growth of austenite in as-cast C-Mn steels. The model can be briefly described as follows

$$d^2 - d_0^2 = k_2 t \tag{4}$$

$$k_2 = \frac{\sigma V D_{gb}}{(\lambda RT)} \tag{5}$$

$$D_{gb} = D_{gb}^0 \exp\left( -\frac{Q_d}{RT} \right). \tag{6}$$

where, $\sigma$ is the grain boundary energy, $V$ is the molar volume of austenite, $D_{gb}$ is the diffusion coefficient at grain boundary, $D^0_{gb}$ is the diffusion constant, $Q_d$ is the activation energy for diffusion and $\lambda$ is the thickness of grain boundary.

The activation energy for grain growth, $Q_g$, may be determined by estimating the model constant, $k$ (Eq. 1) at different temperatures and then constructing an Arrhenius plot which is governed by the following logarithmic relationship

$$\ln k = \ln k_0 - \left( \frac{Q_g}{RT} \right) \tag{7}$$

where $k_0$ is the pre-exponential factor.

### *B. Dislocation-strain interaction model*

A dislocation-strain interaction model has been used to estimate the stored energy due to deformation. The stored energy due to work hardening, $H$, is proportional to the total dislocation density. The total dislocation density is the sum of densities of statistically stored dislocations and geometrically necessary dislocations [11]. The density of the statistically stored dislocation, $\rho^s$, is calculated by [7]

$$\rho^s = \frac{M\varepsilon}{\alpha^s b d}. \tag{8}$$

The density of the geometrically necessary dislocation, $\rho^G$, is given by [7]

$$\rho^G = \frac{CM\varepsilon}{bd}. \tag{9}$$

Where, $M$ is the Taylor factor (≈ 3.06), $\varepsilon$ is the macroscopic strain, $\alpha^s$, $C$ are material-dependent constant (≈ 0.5), $b$ the Burgers vector and $d$ is the grain size. Thus, the total dislocation density can be obtained by combining Eqs. 8 & 9 and then the stored energy due to deformation can be calculated [12] as follows

$$\rho = \rho^s + \rho^G \tag{10}$$

$$H = \alpha G b^2 \rho = \frac{\alpha G b M \varepsilon}{d} \left( \frac{1}{\alpha^s} + C \right) \tag{11}$$

where $\rho$, $H$, $G$ and $\alpha$ are the total dislocation density, the total stored energy, the shear modulus and a material-dependent constant, respectively.

### *C. Monte Carlo simulation of recrystallisation and grain growth*

The MC method is used to simulate the evolution of microstructure and grain growth during recrystallisation [1-7]. The recrystallisation model uses stored energy to represent the dislocation content of the materials [2-3]. In this method a continuum microstructure is mapped onto a two dimensional or three dimensional square or triangular lattice systems. Each lattice site is assigned a number, $S_i$, which corresponds to the orientation of the grain in which it is embedded. Lattice sites that are adjacent to sites having different grain orientations are

regarded as being separated by a grain boundary, whereas a site surrounded by sites with the same orientation is in the grain interior. Periodic boundary conditions are used to avoid the singularity of edges in a finite domain. The grain boundary energy is specified by associating a positive energy with grain boundary sites and zero energy for sites in the grain interior, according to

$$E^I = J\sum_{i=1}^{nn}(1-\delta_{s_i s_j}) \tag{12}$$

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 neighbour sites $j$, respectively and $\delta_{s_i s_j}$ is the Kronecker delta. This implies that $\delta_{s_i s_j} = 1$ when $S_i$ and $S_j$ are of like orientation and zero otherwise. The sum is taken over all nearest neighbour sites. In order to incorporate the energy stored within the grain an additional term is added to Eq. 12 such that un-recrystallised regions have a positive energy as described by

$$E^{II} = H\sum_{i=1}^{nn}\theta(Q_u - S_i) \tag{13}$$

where, $\theta(x)=1$ for $x>=0$ and 0 for $x<0$. $H$ is a positive constant which sets the magnitude of the stored energy and $Q_u$ is the number of distinct orientations of un-recrystalllised grains. The recrystallised nuclei are given orientations with $S_i>Q_u$. The total site energy, $E$ of the system is defined as

$$E = E^I + E^{II}. \tag{14}$$

The kinetics of boundary motion is simulated employing a MC technique in which a lattice site is selected at random and its orientation is randomly changed to one of the other grain orientations. The net energy change $\Delta E$ of the system caused by the reorientation is calculated. If the change in energy associated with the change in orientation is less than or equal to zero, the re-orientation is accepted. If the energy change is positive, a random number $R^{'}$ between $0$ and $1$ is generated such that if $R^{'} \le P$, the change will be accepted. The transition probability, $P$, is given by

$$P = \begin{Bmatrix} 1 & if & \Delta E \le 0 \\ \exp\dfrac{-\Delta E}{k_B T} & if & \Delta E > 0 \end{Bmatrix} \tag{15}$$

Here $k_B$ is the Boltzman constant and $T$ is the absolute temperature in kelvin. Thus successful transitions at the grain boundaries with regard to orientations of nearest neighbour grains correspond to boundary migration. The above procedure is repeated $N$ number of times, where $N$ is the total number of sites in the lattice system. The unit of time is defined as one Monte Carlo step (MCS) per site, which corresponds to $N$ re-orientation attempts.

The nucleation of recrystallised grains is achieved by adding new grains to the microstructure at randomly chosen positions. These embryonic grains or nuclei are added periodically in time. Each embryo is assigned a unique orientation number $S$ and initially assigned a stored energy of zero, that is $H = 0$. Two types of nucleation are considered: site saturated and constant nucleation rate. For site saturated nucleation, a fixed number of nuclei are randomly placed on the lattice and no additional new nuclei are created. For the case of a constant nucleation rate, a fixed number of nuclei are randomly placed on the lattice after each MCS. If a new nucleus is placed in a grain which already has been recrystallised, that nucleus is removed. During the evolution of the microstructure an un-recrystallised site can change orientations to either another un-recrystallised orientation (grain growth) or to a recrystallised orientation (recrystallisation). Un-recrystallised sites are allowed to reorient to recrystallised orientations when the un-recrystallised site is adjacent to a recrystallised neighbour site. Recrystallised orientations are allowed to reorient to other recrystallised orientations. The present model assumes an isotropic distribution of grain boundary energy. Figure 1 shows the flow chart of the MC algorithm for simulation of recrystallisation.

*D Kinetics of recrystallisation*

The recrystallisation phenomena is characterized by the sigmoidal time dependence of the recrystallised volume fraction, $F$, described by Jhonson, Mehl, Avrami and Kolmogorov (JMAK) equation [13] as follows:

$$F = 1-\exp(-At^p) \tag{16}$$

where t is elapsed time, $A$ and $p$ are constants. $A$ is a function of the nucleation rate and the JMAK exponent $p$ is a function of both nucleation and growth rates. The value of $p$ is $3$ in two dimensions for constant nucleation rate [2]. Equation 16 can be written as:

$$\ln\left[\ln\left(\frac{1}{1-F}\right)\right] = \ln(A) + p\ln(t) \tag{17}$$

Equation 17 yields a straight line of slope equal to the JMAK exponent $p$ when the left-hand side is plotted as a function of $ln(t)$.

*E. Computational procedure*

In the simulation of grain growth, the grain structure was initialized with a two dimensional square lattice of 400X400 size and a grain orientation $Q$ (=50) has been assigned to each lattice site in a random manner. To simulate static recrystallisation, the starting microstructure was obtained from normal grain growth simulation The grain orientation has been assigned values in the range from 1 to $Q_u$ to each un-recrystallised lattice site and recrystallised lattice sites were assigned an orientation in the range $Q_u$+1 to $Q$ (=100) in a random manner. Static recrystallisation studies have been performed for initial grain sizes of 40 micron for different strains of 2, 3, 4 and 5 at a typical operating temperature of 900°C. Simulations were performed at a fixed nucleation rate of 0.2 per MCS, corresponding to 1 nucleus added at every 5 MCS. The grain size was calculated as $d = \sqrt{A}$, where $A$ is the number of lattice sites associated with a particular grain. The time domain iteration was carried out for 20000 MCS.

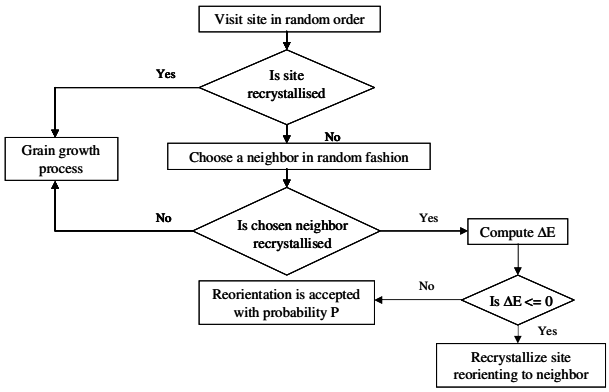
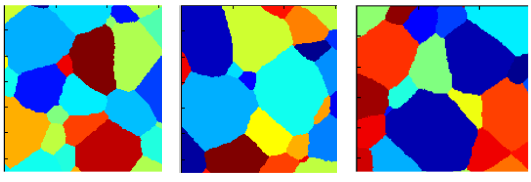



Fig.1.Flow chart describing the simulation of recrystallisation

The MC algorithm has been implemented in an in-house developed ANSI $C^{++}$ code under Linux platform which has been seamlessly integrated with a commercial numerical and graphics package for visualization. The code has been used to predict the grain growth evolution and two dimensional microstructural maps for C-Mn steel at different temperatures. The effect of strain at a typical operating temperature on the recrystallisation and growth kinetics has also been computed and validated for TRIP steel. In order to facilitate faster computation, the simulation code was implemented in the National grid computing initiative of C-DAC, GARUDA. Earlier the MC code was implemented in an in-house workstation (2.0 GHz, 2 GB RAM) in a sequential mode. The GARUDA based computation has significantly alleviated the computational efficiency with the reduction of CPU time and consequently faster convergence of the algorithm was achieved.

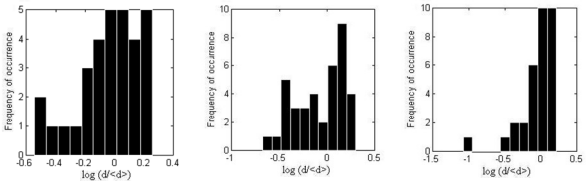
## III. RESULTS AND DISCUSSIONS

Figure 2 shows the simulated microstructural maps after 10000 MCS at different discrete temperatures i.e. 1273 K, 1373 K and 1473 K respectively. Figure 3 describes grain size distribution at different temperatures a) 1273 K, b) 1373 K and c} 1473 K at a given MCS of 10000. Figures 4-5 show temporal evolution of grain size as a function of MCS and physical time respectively at different temperatures. The functionality between physical time and MCS has been elaborately described in the earlier published literature [14] which has not been reproduced. It may be observed from these



(a) (b) (c)

Fig.2: The simulated microstructure after 10000 MCS at different temperatures a) 1273 K, b) 1373 K, c) 1473 K




(a) (b) (c)

Fig. 3: Grain size distribution at different temperatures a) 1273 K, b) 1373 K c) 1473 K at 10000 MCS

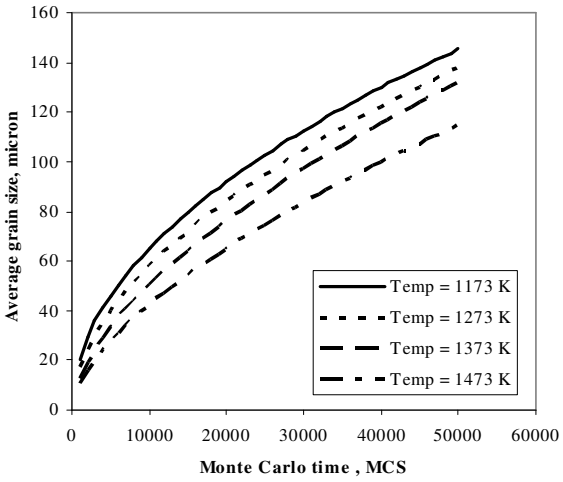



Fig. 4: Average grain size variation with Monte Carlo time step at different temperatures

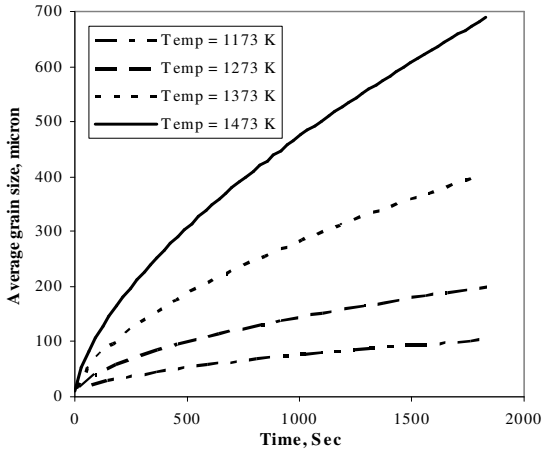



Fig.5: Average grain size variation with physical time at different temperatures

figures that the evolution process follows power growth kinetics [1, 4]. The value of growth exponent, *n* has been estimated to be in the range 0.50-0.62 for corresponding temperature range of 1173 K - 1473K pertains to C-Mn steel. Figure 6 shows the validation of current MC prediction with Yoshie model [10]. In order to verify the predictive capability of the present model, all the pertinent model parameters used

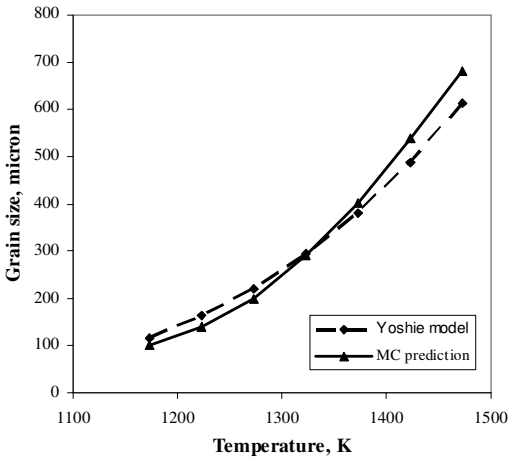



Fig. 6: Validation of MC grain growth prediction with Yoshie model [10]

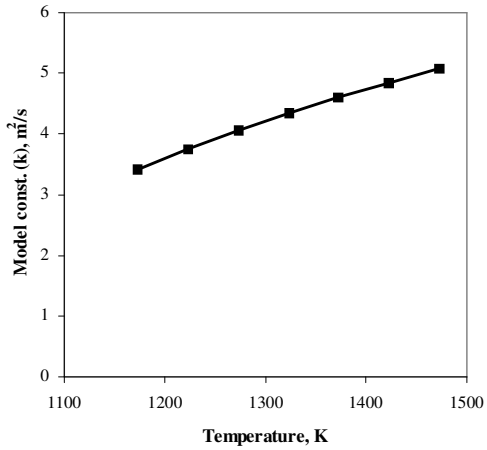



Fig. 7: Variation of grain growth model constant (k) as a function of temperature

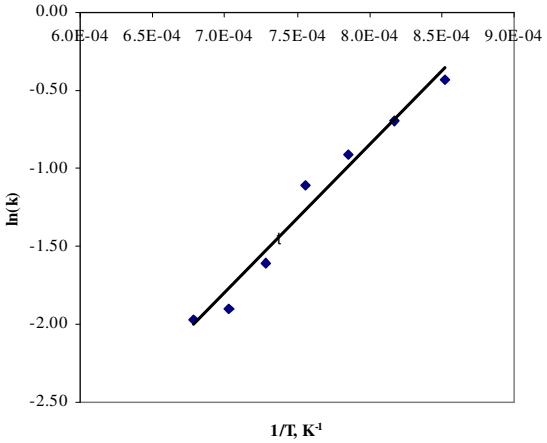



Fig. 8: Logarithmic variation of model constant (k) as a

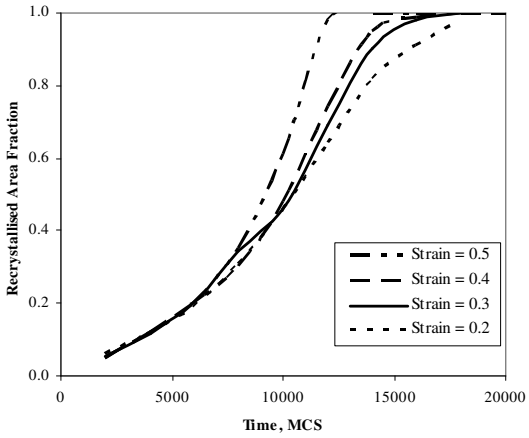



Fig. 9: The recrystallised area fraction, F, as a function of MCS

in the simulation has been kept similar to the Yoshie model as reported in the earlier work [14]. It may be observed that current MC calculations are in good agreement with the Yoshie model prediction for C-Mn steel. Figure 7 shows variation of model constant ($k$) as a function of temperature. It has been found that $k$ increases with increasing temperature which is consistent with respect to Arrhenius temperature dependence functionality. Figure 8 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 78945 J, which is found to be in close agreement with the value cited in the literature for similar grade of steel [15, 16] .

Figure 9 shows the computed volume fraction of static recrystallisation at different strains as a function of MCS. It may be observed from these figures that the evolution process follows typical JMAK kinetics [13]. Figure 10 shows the recrystallised area fraction, F, as a function of physical time for different strains. The MC prediction has been validated

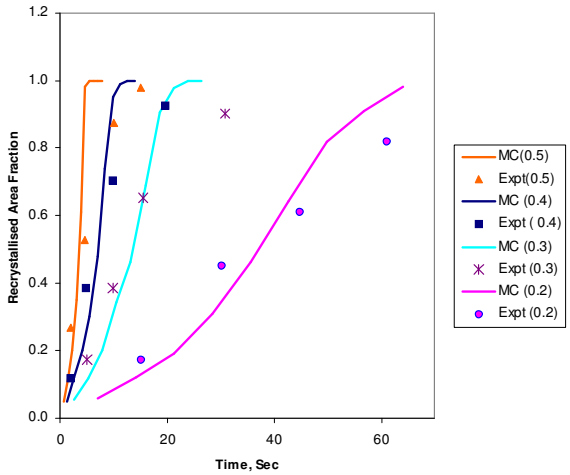



Fig. 10: The recrystallised area fraction, F, as a function of physical time at different strains for the TRIP steel

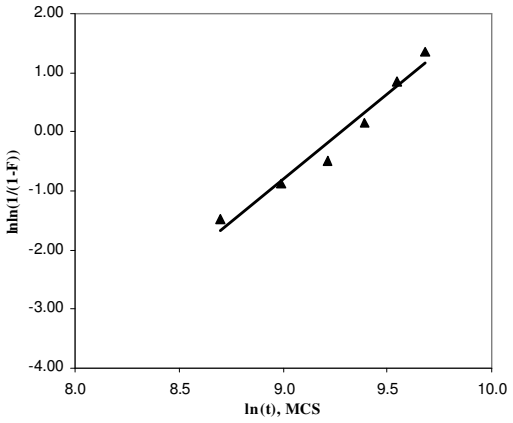



Fig 11: Graphical representation of Eq. 17 for the strain = 0.3

with the published literature data for TRIP steel [17]. The continuous lines represent the MC prediction and the markers represent the experimental data. It may be observed that the experimental data matches relatively well at the lower strains. The slope of the curve in Fig. 11 is the Avrami exponent, and readily calculated to be 2.88. This value is in close agreement with the published data [2] demonstrating the efficacy of present MC simulation. Figure 12 shows a comparison of the recrystallised area fraction calculated from Avrami equation, experimental data and the present MC model. The broken lines represent the Avrami model prediction. It may be observed that the MC prediction is in good agreement with Avrami kinetics. Figure 13 shows the simulated recrystallised mean grain size as a function of strain. The growth rate of recrystallised grains is faster at higher strain values which is phenomenologically consistent in terms of deformation mechanism. The percentage of static recrystallisation increases with the increased strain. The temporal evolution of microstructure at different MCS for the strain of 0.2 has been

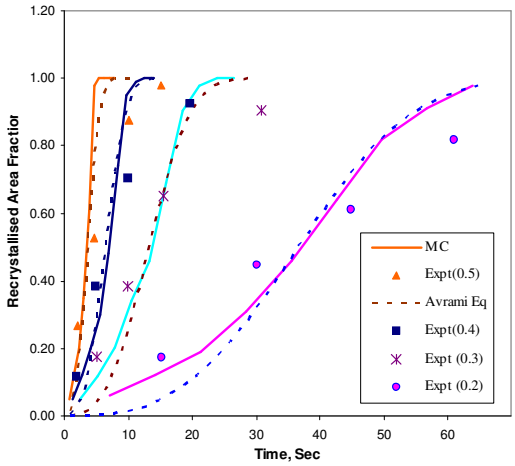



Fig. 12: The recrystallised area fraction, F, as a function of physical time at different strains for the TRIP steel

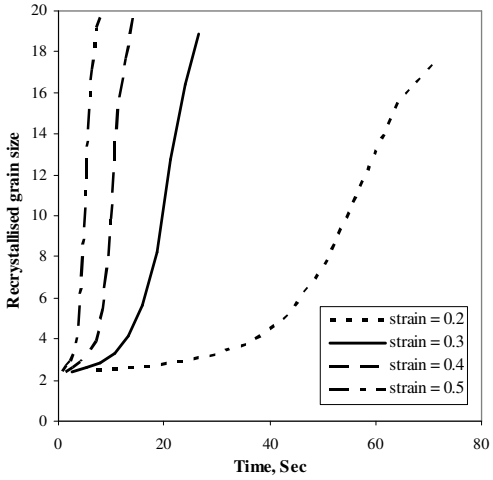
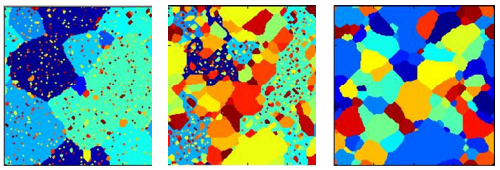



Fig. 13: The recrystallised grain size as a function of physical time for different strains fro the TRIP steel [17]



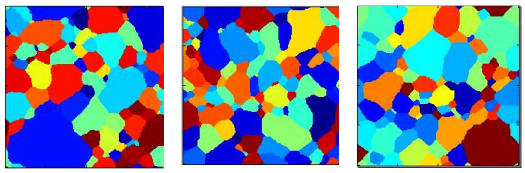
(a) (b) (c)

Fig.14: The simulated microstructure during static recrystallisation at different MCS for strain = 0.2 a) 6000 K, b) 14000 K, c) 20000 K

depicted in Fig.14. It may be observed that at initial stages, the recrystallised grains grow in isolation. As time proceeds impingement of the growing grains begins to occur. Finally, at later stages the recrystallised grains are surrounded, almost entirely, by other neighbour recrystallised grains. At this stage, recrystallization proceeds only in the small fraction of yet un-recrystallised material and the predominant growth process switches to grain growth. During the period of isolated growth the recrystallised grains remain circular and have approximately the same radius. The boundaries are somewhat irregular, and small regions of un-recrystallised matrix are sometimes trapped behind the recrystallised grains. However, as the boundary continues to advance, the trapped regions are recrystallised and are incorporated within the surrounding grain. Figure 15 shows the evolution of microstructure for different strains of 0.3, 0.4 and 0.5 at a typical temperature of 900 °C.

## IV. CONCLUSIONS

The temporal evolution and topology of grain growth pertaining to C-Mn steel has been simulated using MC method. In this simulation framework, the effect of temperature on the grain growth behaviour has been studied. Two important model parameters, namely, the grain growth exponent ($n$) and material constant ($k$) have been estimated to predict the grain size. The average grain size variation as a



(a) (b) (c)

Fig.15: The simulated microstructure during static recrystallisation at 20000 MCS for different strains a) 0.3, b) 0.4, c) 0.5

function of MCS as well as physical time has also been computed and the effect of temperature on the growth kinetics has been studied. Further investigation was carried out to study the effect of different strains at a typical operating temperature on the kinetics of static recrystallisation. This has been accomplished using a dislocation-strain interaction model, which is seamlessly integrated with the present MC simulation paradigm. The simulated microstructure, kinetics of recrystallisation and recrystallised grain size has been predicted under different strains and validated succesfully. It is concluded that the MC simulation is a powerful tool to capture mesoscopic phenomena in metal forming operation using high-end computational resources. The salient features of the typical cluster of the GARUDA grid which has been utilized to expedite the computation are as follows: (1) Resource: POWERS; AIX Intel Xeon; RHEL 5.1, (2) Nodes X CPU = 40X8 = 320, (3) Computational power in Giga flops: 4044.

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