# ABSTRACT

A two-dimensional cellular automaton (CA) model has been developed to replicate the process of austenite phase transformation of dual phase steel during heating. The initial microstructure is obtained from earlier static recrystallization (SRX) model containing ferrite and pearlite in recrystallized state. The model is broadly divided into two major categories: (i) austenite nucleation, and (ii) austenite growth. The growth of austenite is mainly controlled by diffusion phenomena, computed in this study by finite difference method. Growth of austenite has been modeled considering cellular automaton transition rules as well as grain boundary curvature. Finally, the kinetics of phase transformation calculated experimentally is compared with the model kinetics and a good agreement is observed.

Further, CA model has been modified in accordance with the experiment which indicates that in case of recrystallized microstructure the austenite nucleate from ferrite-carbide mixture formed within pearlite grains due to competitive growth of cementite. The sturdiness of the CA model is monitored using robustness check. A Morris One-At-a-Time (OAT) global sensitivity analysis has been performed to identify the most impactful input parameters since these type of models are associated with several of them. In this study two model outputs: (i) overall kinetics of austenite phase transformation, and (ii) average austenite grain size, are investigated. The sensitivity analysis revealed that all the input variables have significant impact and hence, all of them are considered during their optimization using Particle Swarm Optimization (PSO) algorithm to obtain best combination of input parameters in order to achieve least error with respect to experimental data.

Next the optimization is carried out to restrict the austenite grain growth which occurs due to heating at higher temperature, based upon the data collected from CA model. Data-driven meta-models are constructed using Evolutionary Neural Network (EvoNN) and Bi-objective Genetic Programming (BioGP) codes. The analyses of the results lead to the fact that heating rate is the most influencing factor and it needs to be large during transformation to obtain a refined microstructure.

In order to get optimum initial microstructure for the CA simulations, the meta-models have been constructed using data obtained from static recrystallization model of dual phase steels using a modified version of EvoNN, which uses a recent *k*-optimality approach in lieu of the conventional Pareto optimality criteria. Four mutually conflicting objectives—(i) overall kinetics, (ii) grain size, (iii) the amount of strain and (iv) the precipitate volume fraction, have been identified as important

and are optimized simultaneously. This approach could successfully optimize all the four objectives together, which is otherwise difficult to achieve using the notion of Pareto optimality criteria.

A simulation based on different heating rate during austenite formation using CA model predicts that the inhomogeneity of carbon in austenite increases with increasing heating rate. Similarly, cold-rolled samples of an automotive grade 0.06 wt.% C steel are annealed at two different heating rates of 1 and 10 °C/s and similar results are obtained. The extent of carbon inhomogeneity is measured using Kernel averaging method for different neighborhood orders (1, 5, 10, 20 and 30). The inhomogeneity of carbon is found maximum when the 10 order of neighborhoods considered for simulated as well as experimental results. The homogeneity of carbon improves with the increasing carbon concentration of steel, as predicted from BioGP, and the carbon mapping plots from auger electron spectroscopy (AES) for medium carbon (0.28 wt.% C) steel experimentally reconfirms this effect. To perform the mechanical testing, a step quenching (SQ) treatment has been designed such that for both heating rates (1 and 10 °C/s), the final microstructure contains similar volume fractions of ferrite and martensite. The dispersion of final martensite in the ferrite matrix upon cooling is affected due to the difference in carbon distribution of prior austenite, as a result of different heating rates employed during heating. Better formability is found for samples prepared by 1 °C/s heating rate but the samples prepared by 10 °C/s heating rate show better combination of strength and ductility as well as strain hardening rate.

Keywords: Cellular Automata, Finite Difference method, Phase transformation, DP steel, Sensitivity analysis, Particle Swarm Optimization, Data-driven modeling, Multi-objective Evolutionary algorithms.