

Since the beginning of the new millennium, a significant increase in the manufacturing of new advanced metallic materials like advanced high strength steels, novel aluminium, magnesium or high entropy alloys evident due to the demand from the energy, automotive and aerospace industries. Rising global requirements concerning environmental protection forced the weight-to-property ratio of materials to new heights.

Therefore, scientists applied state-of-the-art research approaches to develop new metallic grades with sophisticated properties that address specific industrial demands. Particular effort was put into the precise control of the microstructure evolution under a combination of many thermo-mechanical operations, as it is one of the most versatile paths to provide the required control of products' final in-use properties. A combination of deformation and varying process conditions (e.g., temperatures, strain rates, strain paths) can be used to initiate and control major groups of phenomena responsible for the microstructure evolution. In metallic materials, these are mainly the texture development associated with, e.g. deformation, phase transformations during heating and cooling and thermally activated phenomena of microstructure restoration in particular static, continuous/discontinuous dynamic and metadynamic recrystallisation's. The latter phenomena were investigated for many decades, both from experimental and numerical points of view, increasing the level of understanding of interactions between processing conditions and microstructural changes. Presently, the increasing computing power and enforced economical aspects make the simulation a powerful examination tool that can provide information about material in an online manner. Computer-aided technology design is more frequently used in the metallic material industry on a daily basis. By reducing the reliance on trial-and-error experimentation, modelling helps lower production costs and shorten development cycles. Additionally, optimising manufacturing processes to achieve desired microstructures efficiently reduces energy consumption and material waste, aligning with the Green Deal policies. In general, these advantages contribute to more sustainable manufacturing practices, aligning with global efforts to minimise environmental impact.

However, commonly used 2D numerical models and experimental techniques often fail to capture the true complexity of modern complex-phase materials and multistage processes.

Information from 2D microstructure results can be deceiving and does not describe the true geometry of microstructural features. In contrast, full-field 3D modelling allows for a comprehensive and closer-to-reality visualisation of microstructures as they evolve, enabling researchers to observe and analyse the interactions between grains and phases in three dimensions at an unprecedented level. Such 3D material investigations require support from advanced experimental techniques and significantly more efficient algorithmic solutions and computational resources that can be executed in an acceptable time.

Therefore, 3D full-field numerical modelling of microstructure evolution in modern metallic materials has to be a cutting-edge approach that merges computational competence with materials science achievements to innovate and optimise material properties and manufacturing processes. Such modelling is pivotal in academic research and industrial applications, providing insights that can transform how materials are designed and used. One of the mentioned essential phenomena allowing the restoration of metallic materials microstructures between large plastic deformations, the static recrystallisation (SRX), was selected as a case study for the current research.

Unfortunately, despite the advantages of full-field methods, the computing time of, e.g., cellular automata models, especially in 3D, is several times longer than that of commonly used simplified phenomenological and even mean-field approaches, which limits their practical applications at the industrial scale. Therefore, a recently proposed machine-learning solution is an attractive concept for overcoming these limitations and speeding up computational efficiency to acceptable levels.

However, developing a reliable convolutional neural network requires the preparation of large data sets of full-field microstructure evolution under various processing conditions for training purposes. To allow that in a reasonable time frame, still computationally efficient CA model is required. The principal investigator (PI) is convinced that the development of the CA model that can utilise the capabilities of the graphical processing units (GPUs) will provide a sufficient amount of 3D data for the NCA model's training purposes.

Unfortunately, mapping conventional CA to the CA model that can take advantage of modern computer architectures, especially graphical units (GPUs), is not trivial and requires a series of fundamental investigations, especially the problem of adapting an enormous number of resources during simulation.

Therefore, the main goal of the present work is to increase the computational efficiency of the cellular automata material evolution models by minimising the computational time through developing a high-performance GPU CA SRX model and further increasing its algorithmic efficiency by the new concept of the neural cellular automata method. Additionally, the solution will be based on integrated physics-based constraints in the CNN to maintain the model's reliability. This will ensure that the model adheres to known physical laws of recrystallisation. The developed model will introduce a new level of accuracy in predicting phenomena occurring under static recrystallization conditions, which is crucial for developing modern processing routes for new materials.