Emulation of microstructure evolution in FCC metals using machine learning methods based on continuous modeling and experimental data

Fomin E.V.[1,2,@] **and Bryukhanov I.A.**[1]

[1] Institute of Mechanics, Lomonosov Moscow State University, Michurinskiy 1, Moscow, 119192, None

[2] Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk, 454001, Russia

[@] fomin33312@gmail.com

The microstructure of metals and alloys directly influences the strength and mechanical properties of the material and plastic deformation processes [1]. This paper presents the creation of a dataset from the results of numerical simulation and experiment. The first part of the data was obtained using cellular automata [2] and continuum modeling. The second part was obtained from microstructure images of deformed pure aluminum and copper samples.
The resulting dataset was used to train a machine learning emulator for the microstructure evolution process in metals. The emulator consists of convolutional and recurrent layers. To compare the performance of different machine learning emulator architectures, dimensionality reduction methods (UMAP [3]) were used instead of convolutional neural network layers for processing the input data.
The study was supported by grant No 24-71-00078 from the Russian Science Foundation, https://rscf.ru/en/project/24-71-00078/

[1] Mukherjee T, Elmer J W, Wei H L, Lienert T J, Zhange W, Kou S and DebRoy T 2023 *Prog. Mater Sci.* **138** 101153
[2] Fomin E V 2024 *CPMJ* **9**(4) 689–702
[3] McInnes L, Healy J and Melville J 2020 *arXiv:* 1802.03426