Abstract Submitted
for the APR21 Meeting of
The American Physical Society

Physics-informed, empirically constrained machine learning for designing Fe-9Cr alloys VYACHESLAV ROMANOV, Department of Energy - US — Materials data analytics can be used to significantly shorten development time of specialized alloys needed for next generation energy applications. Incorporation of the domain knowledge into deep-learning graph structure via fuzzy pre-training and causal process imitation presents a viable approach to developing accurate data-driven models and reliable alloy design tools, with limited datasets. It was demonstrated that the domain knowledge-based empirical constraints not only inhibit overfitting but also allow training more accurate and reliable ML models with improved transparency of the output interpretation. In this study, alloy tensile properties were interpreted with three competing virtual-microstructure models.

Vyacheslav Romanov
Department of Energy - US

Date submitted: 11 Jan 2021 Electronic form version 1.4