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Physics-guided, 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. The focus of this study was on developing iron-based alloys that can withstand higher temperature and higher mechanical stress to facilitate accelerated improvement in efficiency and reliability of the power plants. Incorporation of the domain knowledge into deep learning graph structure, initialization and optimization processes, and informed cross-validation presents a viable approach to developing accurate data-driven models and reliable alloy design tools, with limited datasets. The key idea is to digitize empirical domain knowledge, build the graph based on causality relationships, and use machine learning (ML) methodology to identify promising alloy compositions, rank factors affecting their performance, and optimize the processing parameters for specific applications. It was demonstrated that imposition of the domain knowledge and empirical constraints prevents overfitting and allows building more accurate and reliable ML models with improved transparency of the output interpretation.

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