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PREDICTING AND MITIGATING CRYSTALLOGRAPHIC DEFECTS IN CARBON NANOTUBES

Abstract

Carbon nanotubes (CNTs) stand out as promising materials for diverse applications, owing to their exceptional properties, including high strength, electrical conductivity, and thermal stability. However, the presence of crystallographic defects in CNTs can significantly influence their properties, causing unpredictable behavior and diminishing overall performance. It becomes imperative to predict and address these defects for the advancement of high-performance CNT-based materials and devices. This paper introduces a methodology that leverages computational models and algorithms in COMSOL and MATLAB to predict and mitigate crystallographic defects in CNTs.he proposed methodology encompasses four primary stages: data collection and preparation, machine learning model development, defect prediction, and defect engineering strategy design. In the initial stage, data on CNT structures with diverse defects—including types, locations, and densities—are gathered through experiments or simulations. The collected data undergoes preprocessing, and pertinent features, such as defect position, shape, and size, are extracted. Moving to the second stage, machine learning algorithms, including decision trees, support vector machines, or neural networks, are constructed in MATLAB to discern patterns associated with various types of defects.This research proposes a comprehensive methodology comprising four key stages: data collection and preparation, machine learning model development, defect prediction, and defect engineering strategy design. In the initial phase, experimental or simulation data capturing diverse defects in carbon nanotube (CNT) structures—varying in types, locations, and densities—are meticulously collected. Following thorough preprocessing, essential features such as defect position, shape, and size are extracted. The subsequent stage involves the development of machine learning algorithms, including decision trees, support vector machines, or neural networks, implemented in MATLAB. These algorithms are trained on the collected data using cross-validation techniques, ensuring both robustness and generalizability. Performance assessment employs metrics such as accuracy, precision, and recall.In the third stage, the trained machine learning algorithms are deployed to predict defects in newly encountered CNT structures. Each prediction is accompanied by a confidence score, offering insights into the likelihood of defect occurrence. This methodology holds promise for advancing defect prediction and engineering strategies in CNT-based materials.In the fourth stage, optimization algorithms are developed in MATLAB to design strategies for defect engineering, such as introducing dopant atoms or applying external stimuli to control defect formation and distribution. The objective function is defined, such as minimizing defect density or maximizing CNT properties. Optimization algorithms, such as genetic algorithms, particle swarm optimization, or simulated annealing, are used to search for optimal solutions.