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Probabilistic Analysis and Design of HCP Nanowires: an Efficient Surrogate Based Molecular Dynamics Simulation Approach

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We investigate the dependency of strain rate, temperature and size on yield strength of hexagonal close packed (HCP) nanowires based on large-scale molecular dynamics (MD) simulation. A variance-based analysis has been proposed to quantify relative sensitivity of the three controlling factors on the yield strength of the material. One of the major drawbacks of conventional MD simulation based studies is that the simulations are computationally very intensive and economically expensive. Large scale molecular dynamics simulation needs supercomputing access and the larger the number of atoms, the longer it takes time and computational resources. For this reason it becomes practically impossible to perform a robust and comprehensive analysis that requires multiple simulations such as sensitivity analysis, uncertainty quantification and optimization. We propose a novel surrogate based molecular dynamics (SBMD) simulation approach that enables us to carry out thousands of virtual simulations for different combinations of the controlling factors in a computationally efficient way by performing only few MD simulations. Following the SBMD simulation approach an efficient optimum design scheme has been developed to predict optimized size of the nanowire to maximize the yield strength. Subsequently the effect of inevitable uncertainty associated with the controlling factors has been quantified using Monte Carlo simulation. Though we have confined our analyses in this article for Magnesium nanowires only, the proposed approach can be extended to other materials for computationally intensive nano-scale investigation involving multiple factors of influence.

Key words: hcp-nanowire; Yield strength; Surrogate; Monte Carlo simulation; Uncertainty; Sensitivity; Optimum design