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Multi-scale Modeling of Thermal-Electromechanical Response of Piezoelectric Thin Film LIMING XIONG, The George Washington University, JAMES LEE, The George Washington University, YOUPING CHEN, The George Washington University, YAJIE LEI — This study aims at understanding and improving the properties of the piezoelectric thin films through numerical simulation. On the basis of first principle calculation, empirical inter-atomic potential is obtained by fitting to the lattice parameters, energy surface and phonon dispersion relation. Both traditional MD simulation and a new atomistic multi-scale field theory are employed to simulate the material behavior of piezoelectric thin films under thermal, electrical and mechanical loading. Results are well agreed with each other between MD simulation and the newly developed field theory. Meanwhile, it is found out that the newly developed field theory is more efficient in studying nonequilibrium phenomenon, high temperature and high pressure working conditions for thin films. Size effects, thermal conductivity, failure process and material behavior in harsh environments for the thin films are investigated, which provide us with scientific information for the design and optimization of industrial application.

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