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DESIGN SENSITIVITY ANALYSIS OF LATTICE STRUCTURES USING GENERALIZED LANGEVIN EQUATION

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Abstract

Recently, nanotechnology is an emerging research field which describes modern engineering problems. In many mechanical problems, the nanoscale analysis is nowadays inevitable to elucidate the phenomena of crack propagation, strain localization, and dislocations since these include the microscopic behavior which may not be represented in continuum sense. Therefore, we are continually gaining interest in considering the microscopic level in design. The molecular dynamics (MD) simulation that predicts the microscopic behaviors of materials is a promising tool that describes the complex physical phenomena. However, a huge amount of computation is required for the transient dynamic analysis in atom-based simulations. Since both length scale and time scale used in the MD simulations are very limited by computing power, the MD simulations are impractical in engineering problems. However, it is possible to reduce the computation of MD simulations to the locally confined region of interest considering the effect of surrounding. In such reduced MD models, it is very important to impose the appropriate boundary conditions that could replace the effect of eliminated degrees of freedom (DOFs) and to suppress the spurious wave reflections at the interface between the domain of interest and the outer region.

We present an efficient design sensitivity analysis method of atomic systems. A reduced atomic system is constructed in a locally confined region, utilizing generalized Langevin equation (GLE) for periodic lattice structures. Due to the translational symmetry of lattice structures, the size of time history kernel function that accounts for the boundary effects of the reduced atomic systems could be reduced to a single atom's degrees of freedom. For the problems of highly nonlinear design variables, the finite difference method is impractical for its inefficiency and inaccuracy. Through numerical examples, the derived analytic sensitivity turns out to be accurate and efficient with comparison to the finite difference sensitivity.

KEY WORDS: Design sensitivity Analysis, Generalized Langevin Equation, Time history kernel function, Lattice structures