

## Coarse-grained molecular dynamics simulation of thermal and mechanical behaviors of rocksalt

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### ABSTRACT

Coarse-grained molecular dynamics (CG-MD) is a multiscale method for concurrently coupling atomic subdomain and continuum subdomain in a nano/micro material system. In this study, we first present the theoretical framework of multiscale material modeling. Based on that, we derived two numerical algorithms: force-based coarse-grained molecular dynamics (FB-CG-MD) and stiffness-based coarse-grained molecular dynamics (SB-CG-MD). In the first case, we investigate the effect of mesh sizes on accuracy through the bending of a magnesium oxide (MgO) bar. The interatomic interaction of MgO is described by Coulomb–Buckingham potential. The result obtained by classical MD simulation is considered as the standard solution. From CG-MD simulations, we compare the results of different mesh sizes with the standard solution and the error tells the accuracy of both FB-CG-MD and SB-CG-MD. In the second case, we study the heat conduction problem of an MgO specimen, which is subdivided into two subdomains and each subdomain can be either atomic subdomain or continuum subdomain. One subdomain is controlled at a desired temperature through the use of Upgraded Nosé–Hoover Thermostat, which eliminates unphysical phenomena due to reference frame translation and/or rotation when one uses the original Nosé–Hoover thermostat. The other subdomain is free from temperature control. In the CG-MD model, the temperatures of continuum subdomain and atomic subdomain are determined by nodal velocities and atomic velocities, respectively. Our results show that the thermal energy transfers successfully from atomic subdomain to atomic subdomain, as well as from continuum subdomain to continuum subdomain. It is shown that both FB-CG-MD and SB-CG-MD reduce significantly the number of degrees of freedom in the material system and provide reliable results and improve numerical efficiency.