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A fitting empirical potential for NiTi alloy and its application. GUOWU REN, TIEGANG TANG, Institute of Fluid Physics, Chinese Academy of Engineering Physics, Mianyang, 621999, HUSEYIN SEHITOGLU, Department of Mechanical Science and Engineering,University of Illinois at Urbana-Champaign,Urbana, Illinois 61801 — Due to its superelastic behavior, NiTi shape memory alloy receives considerable attentions over a wide range of industrial and commercial applications. Limited to its complex structural transformation and multiple variants, semiempirical potentials for performing large-scale molecular dynamics simulations to investigate the atomistic mechanical process, are very few. In this work, we construct a new interatomic potential for the NiTi alloy by fitting to experimental or ab initio data. The fitting potential correctly predicts the lattice parameter, structural stability, equation of state for cubic B2(austenite) and monoclinic B19'(martensite) phases. In particular the elastic properties(three elastic constants for B2 and thirteen ones for B19') are in satisfactory agreement with the experiments or ab initio calculations. Furthermore, we apply this potential to conduct the molecular dynamics simulations of the mechanical behavior for NiTi alloy and the results capture its reversible transformation.

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