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**Sensitivity of Force Fields on Mechanical Properties of Metals Predicted by Atomistic Simulations** SEYED MOEIN RASSOULINEJAD-MOUSAVI, YUWEN ZHANG, Department of Mechanical and Aerospace Engineering, University of Missouri, Columbia, Missouri 65211, USA — Increasing number of micro/nanoscale studies for scientific and engineering applications, leads to huge deployment of atomistic simulations such as molecular dynamics and Monte-Carlo simulation. Many complains from users in the simulation community arises for obtaining wrong results notwithstanding of correct simulation procedure and conditions. Improper choice of force field, known as interatomic potential is the likely causes. For the sake of users' assurance, convenience and time saving, several interatomic potentials are evaluated by molecular dynamics. Elastic properties of multiple FCC and BCC pure metallic species are obtained by LAMMPS, using different interatomic potentials designed for pure species and their alloys at different temperatures. The potentials created based on the Embedded Atom Method (EAM), Modified EAM (MEAM) and ReaX force fields, adopted from available open databases. Independent elastic stiffness constants of cubic single crystals for different metals are obtained. The results are compared with the experimental ones available in the literature and deviations for each force field are provided at each temperature. Using current work, users of these force fields can easily judge on the one they are going to designate for their problem.

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