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Classical Potential Describes Martensitic Phase Transformations in Titanium[1] THOMAS LENOSKY, RICHARD HENNIG, JOHN WILKINS, Ohio State University, DALLAS TRINKLE, Wright Patterson AFB, SVEN RUDIN, Los Alamos National Laboratory — Titanium is technologically important for aerospace applications and scientifically interesting as it displays martensitic transformations between three crystal structures, hcp, bcc, and omega. We present an efficient classical interatomic potential for Ti that accurately describes all three phases and the structural transformations between them. The potential is of the modified embedded atom form employing cubic splines and incorporating angular bonding terms. The spline parameters are fit to a database of density-functional calculations of energies of different crystalline phases, forces, point defects, and elastic constants. We demonstrate the accuracy of the potential for all three crystalline phases by comparing the phonon spectra with experimental data and density-functional results. Constant stress molecular dynamics simulations determine the Ti phase diagram and thermal expansion as a function of pressure and temperature in good agreement with experimental data. This potential allows for accurate large-scale simulations of Ti under pressure including simulations of shock compression.

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