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Interatomic bond-order potentials for molecular dynamics simulations of materials at extreme conditions ROMAIN PERRIOT, MIKALAI BUDZEVICH, IVAN OLEYNIK, University of South Florida — Molecular dynamics (MD) is a powerful research tool for studying materials at extreme conditions. At the heart of MD are the interatomic potentials, whose quality in describing a variety of chemical effects, including bond-breaking and bond-making, plays a decisive role in delivering meaningful results. We have performed extensive MD simulations of shock compression of covalently bonded materials, such as diamond and silicon, and found that REBO interatomic potential for diamond and EDIP potential for Si have substantial deficiencies at large pressures and temperatures in spite of the fact that the near equilibrium properties of both diamond and silicon are well reproduced. We are addressing this outstanding issue by developing analytic bond-order potentials (BOPs) specifically for the simulation of covalently bonded materials at extreme conditions. These BOPs include explicit analytic expressions for both the σ and π bonds. We will discuss important steps of BOP construction which includes devising a fist-principle database of fundamental materials properties, fitting this database by the orthogonal tight-binding, and devising the analytic BOPs using the direct link between TB and analytic BOPs via the bond orders.

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