

Abstract Submitted
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Interatomic bond-order potentials for atomistic simulations of materials at extreme conditions YONGXUE YU, IVAN OLEYNIK, Univ. of South Florida — Molecular dynamics simulations provide an excellent opportunity to address fundamental physics and chemistry of materials at extreme conditions. However, the results of MD modeling can only be as reliable as the ability of the interatomic potentials to properly describe a variety of chemical effects including bond-breaking and bond-making. Our recent MD simulations of shock compression of covalently bonded materials such as diamond and silicon using REBO interatomic potential for diamond and EDIP potential for Si showed that the properties of C and Si systems at large pressures and temperatures are not well described in spite of the fact that the near equilibrium properties of both diamond and silicon are well reproduced. We present new results on development of analytic bond-order potentials (BOPs) for covalently bonded materials at extreme conditions. These BOPs are derived using the powerful concepts of moments of density of states, Green's function and Lanczos recursion, applied within the two-center, orthogonal tight-binding bond representation of electronic structure. Importantly, they include explicit analytic expressions for both the σ and π bonds. We will describe details of BOP construction including devising a first-principle database of fundamental materials properties, its fitting by the tight-binding (TB) model, and devising the analytic BOPs using the direct link between TB and analytic BOPs via the bond orders. Validation of analytic BOPs by comparison with first-principles high-pressure data will also be discussed.

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