

Abstract Submitted  
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**Development of a Reactive Force Field for Shock-Induced Chemistry in Ti/B Nanocomposite**<sup>1</sup> JASON QUENNEVILLE, Spectral Sciences, Inc. — A ReaxFF reactive force field is under development for describing the physics and chemistry of Ti/B mixtures under shock compression. In this presentation, we will summarize the parameterization of the force field for the reactants and the most stable product of the reaction, TiB<sub>2</sub> in the P6/mmm space group. We will describe the behavior of crystalline TiB<sub>2</sub> under uniaxial and hydrostatic compression and the structure of the crystal with varying void densities as calculated with periodic DFT. In addition, we will compare the results obtained for these properties and others (*e.g.*, lattice constants, elastic constants, bulk modulus) with the newly developed ReaxFF force field. The force field developed in this work for TiB<sub>2</sub> is combined with Ti and B ReaxFF force fields developed previously to yield a force field suitable for describing shock-induced reactions of Ti and B. Preliminary molecular dynamics studies will also be detailed.

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