Abstract Submitted
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A Multiphase, Multicomponent Model for Combustion in the Titanium-Boron System[1] SUSHIL KUMAR, JOHN B. BDZIL, MOSHE MATALON, D. SCOTT STEWART, Mechanical Science and Engineering, University of Illiinois, Urbana, IL 61801 — Modeling combustion by reaction diffusion processes in initially, separated pure compounds in the condensed phase of metals, their oxides and intermetallics, is an important area of research in material science. We present a one-dimensional combustion model of the Titanium-Boron system, which is thermodynamically consistent. A simplified stoichiometric reaction mechanism is used in which liquid Titanium and liquid Boron reacts to form Titanium diBoride. An analytical form, suggested by Fried and Howard [1], is used to represent the equilibrium equation of state (EOS) for the solid and liquid phases of all three substances. This EOS produces results that gives and excellent fit to the known experimental data for the pure chemical phases. A multicomponent mixture EOS is created to account for the phase transitions and reaction between the individual species. We use numerical simulations to examine the results from conservation equations at constant pressure and compare them to experiments.

[1] Fried, Laurence E., and W. Michael Howard. "Explicit Gibbs Free Energy Equation of State Applied to the Carbon Phase Diagram." Physical Review B 61.13 (2000): 8734-743.

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D. Scott Stewart
Mechanical Science and Engineering,
University of Illiinois, Urbana, IL 61801

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