A Gibbs formulation for continuum modeling of multicomponent materials with phase change and chemistry

D. Scott Stewart

University of Illinois, Mechanical Science and Engineering, University of Illinois, Urbana, IL 61801
and
Explosive Technology Consulting Services, Niceville, Florida, 32578

Energetic material condensed phase constituents come into contact, chemically react and simultaneously undergo phase change. Phase change in a given molecular material is often considered separately from chemical reaction. Continuum phase field models often use a indicator function to change the phase in different regions according to an evolutionary (Ginzburg-Landau) equation. But chemical kinetic descriptions of change (according to physical chemistry formulations) count species or component concentrations and derive kinetic evolution equations based on component mass transport. We argue the latter is fundamental and that all components, designated by both phase and chemical characters are treated as distinct chemical species. We pose a self-consistent continuum, thermo-mechanical model based on specified Gibbs potentials for all relevant species/components that are present in a single material. Therefore a single stress tensor, and a single temperature is assumed for the material for all relevant component-species, for all equilibrium potentials, interaction energies and material properties. We discuss recent examples, drawn from modeling both propellants and explosives, where we have applied the Gibbs formulation to model behavior of complex reactive materials.