THERMODYNAMICALLY SELF-CONSISTENT MODEL FOR A MATERIAL THAT UNDERGOES SOLID-LIQUID-GAS PHASE TRANSITIONS WITH CHEMICAL REACTIONS

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ABSTRACT

We describe the results in [1,2] concerning a thermomechanical model for an energetic material that uses two independent state variables to represent the phase transformation and the extent of chemical reaction. The presented model is thermodynamically self-consistent and can describe a material that undergoes phase transitions from solid to liquid to gas with exothermic chemical reaction. In various limits, the material is a classical elastic solid, a Newtonian viscous liquid, and a compressible gas.

INTRODUCTION

Modeling the phase change from solid to liquid to gas involves positing of balance laws additional to the basic continuum laws of mechanics. Gurtin [3] has argued for a separate balance of configurational forces acting near the boundaries separating pure phases in the volumetric bulk. The argument for such configurational forces is similar to those used to explain classical surface tension forces. Those forces do work, and thus the work related to the configurational forces must be accounted for in the overall energy balance. Representative of three distinctly pure phases, the order parameters of phase field variables are assigned φ = 0, 1, and 2 for solid, liquid and gas phases of a material.

The second law of thermodynamics (the Clausius-Duhem inequality) restricts the form of the constitutive theory so that the rate processes are entropy increasing. In particular, the energy equation becomes so rich as to account for many additive terms of the Helmholtz free energy as posed before the second law restriction. Various parts associated with the energies are $\psi = \psi_{\text{thermal}} + \psi_{\text{reaction}} + \psi_{\text{phase}} + \psi_{\text{gradient}} + \psi_{\text{elastic}} + \psi_{\text{plastic}}$. This explicit partitioning of the Helmholtz free energy is a key aspect of the model in this work.

Because the framework in which the model is derived is general, the present formulation can be extended to include additional constitutive features of a material [4].

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