



Thermodynamics of multicomponent, elastic, crystalline solids

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Abstract

The thermodynamic behavior of multicomponent, elastic, crystalline solids is developed, including Euler's equation, the Gibbs equation, the Gibbs–Duhem equation, the conditions to be expected at equilibrium including a new description of stress-deformation behavior, and an extension of the Gibbs phase rule. The predictions of the phase rule are compared with two types of experimental observations including the ten triple points of water.

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1. Introduction

A *simple material* is one such that, for a fixed material particle and a fixed reference configuration, the stress tensor is a functional (function of a function) of the past history of the deformation gradient

$$\mathbf{F} \equiv \text{grad } \mathbf{z} \quad (1)$$

as well as temperature and composition (Truesdell and Noll, 1965, p. 60), where the gradient operation grad is to be performed in the reference configuration. A simple material is called *elastic*, if stress depends only on the current value of \mathbf{F} (Truesdell and Noll, 1965, p. 119).

Non-simple materials fall into three categories: (i) those exhibiting an explicit dependence upon higher-order gradients, (ii) a dependence upon more than one material particle (a non-local theory), or (iii) a dependence upon more than one reference configuration. Rajagopal and Srinivasa (1998) discuss the deformation of inelastic materials in this latter context.

A *solid* has some natural (preferred, stress-free or undistorted) configuration, deformations from which are always experimentally detectable. Consequently, all non-orthogonal transformations from a natural or preferred configuration for a solid can be detected by experiment (Noll, 1958; Truesdell and Noll, 1965, p. 81; Truesdell, 1966, p. 61). For a non-oriented or *isotropic* solid, all orthogonal transformations of the natural or preferred configuration are undetectable experimentally. For an oriented or *anisotropic* solid, some orthogonal transformations are undetectable experimentally (Truesdell and Noll, 1965, p. 82). A

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Nomenclature

\widehat{A}^j	Helmholtz free energy per unit mass	$r_{(A,k)}^\sigma$	rate of production of species A by heterogeneous reaction k
\widetilde{A}^j	Helmholtz free energy per unit volume	R	region occupied by body (because there is no mass transfer at the boundary, we do not distinguish between the region occupied by a body of species A and the region occupied by the multicomponent body, the material particles of which move with the mass-averaged velocity \mathbf{v})
\mathbf{C}	relative right Cauchy–Green strain tensor defined by (8)	S	bounding surface of body
\mathbf{e}	strain tensor defined in Appendix A	\widehat{S}	entropy per unit mass
$\mathbf{e}_{(i)}^{(j)}$	deformed lattice vectors for phase j defined by (2)	t	time
\widehat{E}	sum of internal energy and kinetic energy per unit mass as defined in Eq. (39)	T	temperature
$\mathbf{E}_{(i)}^{(j)}$	unit lattice vectors in natural (equilibrium) configuration for phase j	\mathbf{T}	stress tensor
$\mathbf{E}_{(i)}^{(0)}$	lattice vectors in natural (equilibrium) configuration for the parent phase 0 (as seen in the current frame of reference)	\mathbf{u}	time rate of change of position following a surface point (Slattery, 1999, p. 24); used as displacement in Appendix A
f	degrees of freedom	\widehat{U}	internal energy per unit mass
$\mathbf{f}_{(A)}$	body force per unit mass acting on species A	\mathbf{v}	mass average velocity
\mathbf{f}	body force per unit mass	$\mathbf{v}_{(A)}$	velocity of species A
$\mathbf{F}^{(j)}$	deformation gradient in phase j	\widehat{V}	volume per unit mass
\mathbf{H}	displacement gradient defined in Appendix A	\mathbf{z}	position vector
$\mathbf{H}^{(j)}$	orthogonal transformation for phase j defined by (3)	\mathbf{z}_κ	position of material particle in reference configuration defined by (29)
\mathbf{I}	identity tensor	$Z_{(A)}$	defined by (38)
$I_{(mn)}^{(j)}$	scalar invariants for phase j defined by (7)	\mathbf{Z}_m	defined by (31)
J	number of homogeneous chemical reactions	<i>Greek symbols</i>	
K	number of heterogeneous chemical reactions	ϵ	dimensionless parameters representing the disturbance from equilibrium
M	number of non-zero invariants described by (7)	$\lambda_{(A)}$	Lagrangian multiplier
$M_{(A)}$	molecular weight of species A	λ_e	Lagrangian multiplier
N	number of species	λ_m	Lagrangian multiplier
p	number of phases	$\mu_{(A)}$	chemical potential for species A defined by (16)
$p^{(c)}$	number of crystalline phases	$\mu_{(I,mn)}$	defined by (17)
P	thermodynamic pressure defined by (15)	$\nu_{(A,j)}$	stoichiometric coefficient for species A in homogeneous reaction j : the stoichiometric coefficient is taken to be a negative number for a reactant, positive for a product
Q	number of internal, coherent, solid–solid phase interfaces at which elastic components of stress exist: in the absence of deformation, $Q = 0$		
$r_{(A,j)}$	rate of production of species A by homogeneous reaction j		

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