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Density Functional Theory and Finite Deformation Elastic and Thermoelastic Constitutive Relationships ZHIBO WU, SATHYA HANAGUD — This paper addresses the problem of obtaining the complete constitutive relationships for solids under conditions of finite deformations from first principles by the use of the density functional theory, phonon thermal energy contributions, electron thermal energy contributions and foundations of continuum mechanics of finite deformation elasticity and thermoelasticity. In the work, to date, the invariance requirements concerning the crystal symmetry under specific rotations and objectivity is not addressed. This means if the deformed coordinates x $\rightarrow$QF then U(F) = U(QF) for every Q in the spatial orthogonal group. (The deformation gradient is denoted by F.) First, this implies that U= U(C) =U(F^TF) where C = F^TF is the stretch or the Cauchy-Green deformation tensor. Next, the crystal symmetry is characterized by the material or solid symmetry group G_M . Then U(C) = U (QC) for all Q$\in G_M$ .This then requires the use of structural tensors introduced by Boehler. Thus, to satisfy the principle of objectivity the energy obtained from DFT by straining the lattice should be expressed as functions of the invariants of the stretch tensor C and the structural tensors applicable to the specific crystal symmetry group. Then, the second Piola-Kirchhoff stress tensor S = F^{-1}T = $2\partial U/\partial C$. T is the first Piola- Kirchhoff stress tensor. For thermoelasticity the free energy is then obtained.

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