

# Non-classical mechanics and thermodynamics for continuum modelling of solids

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## Abstract

This thesis dwells upon several aspects of continuum mechanics and thermodynamics to model elastic and inelastic response of solids. Broadly, the work presented may be categorized into two parts— one focusing on the development of generalized continuum description in the context of elastic materials and the other on the thermodynamics of dissipative processes whilst considering, in some detail, the physics of deformation too.

The first part begins with the proposal for a state-based micropolar peridynamic theory for linear elastic solids. The main motivation is to introduce additional micro-rotational degrees of freedom to each material point and thus naturally bring in the physically relevant material length scale parameters into peridynamics. Non-ordinary type modelling via constitutive correspondence is adopted here to define the micropolar peridynamic material. Along with a general three dimensional model, homogenized one dimensional Timoshenko type beam models for both the proposed micropolar and the standard non-polar peridynamic variants are derived. The efficacy of the proposed models in analyzing continua with length scale effects is established via numerical simulations of a few beam and plane-stress problems. Continuing with our effort in developing homogenized reduced dimensional models, a state-based peridynamic formulation for linear elastic shells is presented next. The emphasis is on introducing, perhaps for the first time, a general surface based peridynamic model to represent the deformation characteristics of structures that have one geometric dimension much smaller than the other two. A new notion of curved bonds is exploited to model force transfer between the peridynamic particles describing the shell. Starting with the three dimensional force and deformation states, appropriate surface based force, moment and several deformation states are arrived at. Upon application on the curved bonds, such states yield the necessary force and deformation vectors governing the motion of the shell. The peridynamic shell theory is numerically assessed against simulations on static deformation of spherical and cylindrical shells and those on flat plates.

As a transition to the second part of the thesis, our next work shares features of the first part (micropolarity and homogenization) as well as the second (equation with viscous force, i.e., dissipative process). Starting with a micropolar formulation, known to account for nonlocal microstructural effects at the continuum level, a generalized Langevin equation (GLE) for a particle, describing the predominant motion of a localized region through a single displacement degree-of-freedom, is derived. The GLE features a memory dependent multiplicative or internal noise, which appears upon recognising that the micro-rotation variables possess randomness owing to an uncertainty principle. Unlike its classical version, the new GLE qualitatively reproduces the experimentally measured fluctuations in the steady-state mean square displacement of scattering centers in a polyvinyl alcohol slab.

In the second part of the thesis, a series of physically motivated models for dislocation mediated thermoviscoplastic deformation and micro-void mediated ductile damage in metals are proposed. The methodology of modelling brittle damage also constitutes another part of discussion. The models are, in essence, posited in the framework of internal-variables theory of thermodynamics, wherein effective dislocation densities, void volume fractions etc., which assume the role of internal variables, track permanent changes in the internal structure of metals undergoing plastic deformation and damage. The thermodynamic formulation involves a two-temperature description of viscoplasticity and damage that appears naturally if one considers the thermodynamic system to be composed of two weakly interacting subsystems, namely, a kinetic- vibrational subsystem of the vibrating atomic lattices and a configurational subsystem of the slower degrees-of-freedom of defect motion. While most of the models are proposed satisfying the thermodynamic requirements asserted by the second law, one specific interest, however, has been to explore the possible application of a fluctuation relation that subsumes the second law of thermodynamics en route to deriving the evolution equations for the internal variables. Full-fledged three-dimensional continuum formulations, valid for the finite deformation regime, are also set forth. Several numerical exercises, including impact dynamic simulations, are carried out and validated against experimental data.