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Fluctuation relation based continuum model for thermoviscoplasticity in metals



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ABSTRACT

A continuum plasticity model for metals is presented from considerations of non-equilibrium thermodynamics. Of specific interest is the application of a fluctuation relation that subsumes the second law of thermodynamics en route to deriving the evolution equations for the internal state variables. The modelling itself is accomplished in a two-temperature framework that appears naturally by considering the thermodynamic system to be composed of two weakly interacting subsystems, viz. a kinetic vibrational subsystem corresponding to the atomic lattice vibrations and a configurational subsystem of the slower degrees of freedom describing the motion of defects in a plastically deforming metal. An apparently physical nature of the present model derives upon considering the dislocation density, which characterizes the configurational subsystem, as a state variable. Unlike the usual constitutive modelling aided by the second law of thermodynamics that merely provides a guideline to select the admissible (though possibly non-unique) processes, the present formalism strictly determines the process or the evolution equations for the thermodynamic states while including the effect of fluctuations. The continuum model accommodates finite deformation and describes plastic deformation in a yield-free setup. The theory here is essentially limited to face-centered cubic metals modelled with a single dislocation density as the internal variable. Limited numerical simulations are presented with validation against relevant experimental data.

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1. Introduction

The physical processes underlying plastic or viscoplastic deformation in metals are extremely complex and inherently irreversible. Plastic deformation originates from the motion of microscopic defects, primarily the crystallographic slips caused by dislocations. Even though several other mechanisms including twinning, grain boundary sliding, void growth etc. do influence plastic deformation, our present focus will solely be on dislocation motion and evolution as the predominant micro-mechanism driving metal plasticity. In the microscopic scale, the motion of dislocations and their interactions with each other as well as the lattice itself are highly nonlinear and temporally intermittent dynamical flows that render an

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inhomogeneous texture to spatial deformation fields with several characteristic dislocation pattern formations. Still, at the macroscale, the field appears smooth and homogeneous. Motion of dislocations through the lattice requires overcoming an energy barrier with the combined aid of the applied force and thermal fluctuations. The crystal lattice configuration, viz. face-centered cubic (FCC), body-centered cubic (BCC), hexagonal close-packed (HCP), plays an important role in deciding how the thermal activation affects the mechanical response and thus plastic deformations in metals differ depending on the crystal structure.

When driven by an external protocol, a crystalline material with dislocations falls out of equilibrium because of the self energy of dislocations. Langer et al. (2010) argued that a macroscopic system undergoing plastic deformation might be interpreted as being composed of slow configurational degrees of freedom describing infrequent and intermittent atomic rearrangements responsible for the plastic flow and kinetic-vibrational degrees of freedom pertaining to the thermally induced vibrational motion of atoms. Consequently the system may be split into a configuration subsystem and a kinetic-vibration subsystem. The energy of the configurational subsystem, i.e. the self energy of dislocations, along with its own entropy defines a new temperature – the configurational or effective temperature, which must be distinguished from the thermal or kinetic-vibrational temperature. As plastic deformation progresses at the expense of external work, the effective temperature evolves differently from the thermal temperature and establishes a heat current from the configurational subsystem to the other. Consequently a large fraction of the external work that generates dislocations and keeps them in motion, dissipates as heat. This makes evident the highly irreversible and dissipative character of plastic deformation and also suggests the configurational rearrangements to be far from equilibrium.

A desirable, if challenging, goal in continuum mechanics is to develop predictive viscoplasticity models for the complex phenomena of dislocation evolution and motion. The models should be applicable to a wide range of temperature and strain rates as the deformation response of metals depend, to a large extent, on these two parameters. More importantly, several engineering applications of metals at high strain rates, e.g. high speed machining, impact on armor systems, metal forming etc., demand an understanding of the underlying micro-mechanisms of plastic deformation and their exploitation within the predictive model in order to optimize or enhance the design and operations of such systems. Huge research efforts, spanning the last few decades and aimed at developing constitutive models – mostly phenomenological – of plasticity or viscoplasticity, have perhaps not led to a proportionate increment in the physical understanding that might have culminated in a universally acceptable theory. Many such models are posited on the hypothesis of local equilibrium thermodynamics, wherein internal state variables are utilized to characterize the irreversible processes of viscoplasticity. For a historical review of internal state variable theories to model inelastic material behaviours we refer Horstemeyer and Bammann (2010). In parallel, quite a few reported efforts at developing a physically based theory for viscoplastic deformation also do exist (e.g., Zerilli and Armstrong, 1987; Aifantis, 1987; Follansbee and Kocks, 1988; Klepaczko and Rezaig, 1996 to cite a few). However, rather than exploiting the thermodynamic principles, many such models often postulate the constitutive relations in terms of the evolution equations of dislocation densities. These equations explicitly contain terms describing several microscopic phenomena, e.g., dislocation multiplication, annihilation, grain size effect, effect of cell boundaries, twinning, interactions with the lattice and so on. Some of the physically based models also bring in refinements by making a distinction among different types of dislocations – viz. mobile and immobile, statistically stored and geometrically necessary dislocations. Separate evolution equations for different dislocation types are then put forth while accounting for their mutual interactions in some way. While these physical models may certainly conform to the laws of thermodynamics, it should, however, be emphasized that they are often not checked for their thermodynamic consistency.

It is well known that the notions of temperature, heat, energy etc. have their moorings in thermodynamics. However thermodynamics, in its original form, merely provides for a basis encapsulating the principles of equilibrium that a macroscopic system is often believed to follow. Macroscopic work-heat relation is one such example. Founded on Gibbs' ensemble formalism, equilibrium statistical mechanics made it possible to bridge widely separated scales, i.e. micro to macro. For example, it identified the thermodynamic temperature with the vibrational kinetic energy of the constituent particles, associated entropy with the probability distribution of microstates that conform to the specified macroscopic conditions and so on. Unfortunately, away from equilibrium, not only do most of these identifications fail to hold, definitions of quantities such as entropy and temperature also become ambiguous. To be sure, there exists a natural extension of thermodynamics to close-to-equilibrium systems. This extension is based on the local equilibrium hypothesis: the local and instantaneous relations between the thermodynamic quantities in a system out of equilibrium are the same as those for a uniform system in equilibrium. Representing state variables as spatial continuum fields hold only when the length scale over which the continuum fields vary appreciably is much larger than the microscopic length scale. Similarly, the time dependence of the field can be justified when changes occur sufficiently slowly vis-a-vis the macroscopic scale so that at each instant the thermodynamic system underlying each continuum particle gets sufficient time to equilibrate. Because of the usual disparity between macroscopic and microscopic/sub-microscopic scales, many systems do conform to the notion of local equilibrium. There are however several situations where this hypothesis is invalid and the process of viscoplastic deformation of metals might very well be one of them. For a discussion on the local equilibrium hypothesis, its implications and cases where it fails to hold, see Jou et al. (1996). Therefore, a physical understanding of metal plasticity must be based on a confluence of ideas rooted in the geometrical aspects of plastic deformation and a thermodynamic theory applicable in far-from-equilibrium conditions.

Unlike the classical irreversible thermodynamics woven around the local equilibrium hypothesis, there is no natural extension of the equilibrium theory to generic non-equilibrium conditions. There are many schools of contemporary non-

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