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Two-temperature continuum thermomechanics of deforming amorphous solids

Ken Kamrin^{a,*}, Eran Bouchbinder^b^a Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA^b Chemical Physics Department, Weizmann Institute of Science, Rehovot 76100, Israel

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ABSTRACT

There is an ever-growing need for predictive models for the elasto-viscoplastic deformation of solids. Our goal in this paper is to incorporate recently developed out-of-equilibrium statistical concepts into a thermodynamically consistent, finite-deformation, continuum framework for deforming amorphous solids. The basic premise is that the configurational degrees of freedom of the material – the part of the internal energy/entropy that corresponds to mechanically stable microscopic configurations – are characterized by a configurational temperature that might differ from that of the vibrational degrees of freedom, which equilibrate rapidly with an external heat bath. This results in an approximate internal energy decomposition into weakly interacting configurational and vibrational subsystems, which exchange energy following a Fourier-like law, leading to a thermomechanical framework permitting two well-defined temperatures. In this framework, internal variables, that carry information about the state of the material equilibrate with the configurational subsystem, are explicitly associated with energy and entropy of their own, and couple to a viscoplastic flow rule. The coefficients that determine the rate of flow of entropy and heat between different internal systems are proposed to explicitly depend on the rate of irreversible deformation. As an application of this framework, we discuss two constitutive models for the response of glassy materials, a simple phenomenological model and a model related to the concept of Shear-Transformation-Zones as the basis for internal variables. The models account for several salient features of glassy deformation phenomenology. Directions for future investigation are briefly discussed.

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1. Introduction: background and motivation

The elasto-viscoplastic deformation of solids is a complex process that couples widely separate time and length scales. In polycrystalline solids, plastic deformation is mainly mediated by dislocations, which form complex and strongly interacting networks that give rise to a rich macroscopic phenomenology. In disordered solids (e.g. noncrystalline/amorphous solids below their glass temperature and granular materials), which lack long-range structural order, plastic deformation is mediated by localized shear-driven rearrangements involving a small number of basic elements (molecules/atoms/grains). These rearrangements produce inhomogeneous mesoscopic deformation fields that affect their surroundings. In both cases,

* Corresponding author.

E-mail addresses: kkamrin@mit.edu (K. Kamrin), eran.bouchbinder@weizmann.ac.il (E. Bouchbinder).

the small scale dynamics are highly heterogenous, intermittent and seemingly non-deterministic, yet the emergent macroscopic phenomena are quite robust. Developing predictive continuum models that effectively bridge over the widely separate scales remains a major challenge of prime scientific and technological importance.

The most successful methodology for bridging over widely separated scales is equilibrium statistical thermodynamics. However, the viscoplastic deformation of solids is an intrinsically out-of-equilibrium phenomenon, hence standard equilibrium thermodynamics is not directly applicable in this case. Nevertheless, statistical concepts and the most general form of the laws of thermodynamics might still be applicable. Our goal in this paper is to incorporate recently developed out-of-equilibrium statistical concepts into a continuum thermomechanical framework for the large elasto-viscoplastic deformation of amorphous solids. Models for the elasto-viscoplastic deformation of amorphous solids have been quite extensively discussed in recent literature, see for example [Sollich et al. \(1997\)](#), [Falk and Langer \(1998\)](#), [Falk and Langer \(2011\)](#), [Anand and Su \(2005\)](#), [Demetriou et al. \(2006\)](#), [Henann and Anand \(2008\)](#), [Jiang and Dai \(2009\)](#), [Homer and Schuh \(2010\)](#), [Abdeljawad and Haataja \(2010\)](#), and [Li et al. \(2013\)](#).

The basic idea that has emerged in the statistical physics community in the last 15 years or so is that the degrees of freedom of an amorphous/glassy material (i.e. the various contributions to the internal energy and entropy) can be approximately decomposed into two qualitatively different groups ([Cugliandolo et al., 1997](#); [Berthier et al., 2000](#); [Leuzzi, 2009](#); [Cugliandolo, 2011](#)). One group includes the vibrational motions of particles around a mechanically stable configuration (sometimes termed an inherent structure). These motions equilibrate with the thermal reservoir on a microscopic timescale, i.e. the temperature apparent in the vibrational fluctuations quickly evolves to match that of the reservoir. The other group includes the mechanically stable configurations themselves and the slow configurational rearrangements that allow transitions between them. These are mainly driven by external mechanical forces, possibly assisted by thermal fluctuations. It is the configurational degrees of freedom that fall out of internal equilibrium with the vibrational degrees when a glass is formed; and it is these degrees of freedom that undergo structural relaxation when a glass ages and evolve when a glass deforms plastically.

Numerous recent theoretical, numerical and experimental studies have provided quantitative evidence that the configurational degrees of freedom of either an aging or a deforming amorphous/glassy material attain a temperature of their own, which is markedly different from the temperature corresponding to the vibrational fluctuations of the microconstituents. The early works demonstrating the existence of a configurational temperature, usually termed an “effective temperature” in the statistical physics community, were rather exclusively based on deviations from the equilibrium fluctuation–dissipation relation (for a very recent and comprehensive review see [Cugliandolo, 2011](#)). That is, it was shown (mainly using simple models and molecular dynamics simulations) that the long time dynamics of an aging glassy material satisfy a generalized fluctuation–dissipation relation with a temperature that is different from the temperature associated with the vibrational motion of the microconstituents ([Cugliandolo et al., 1997](#); [Cugliandolo, 2011](#)). Of special importance for our present purposes are the colloidal glass experiments of [Maggi et al. \(2010\)](#), which explicitly demonstrate that the effective temperature of a sample slowly evolves toward the thermal (i.e. vibrational) temperature over very long times, and eventually approaches it. This suggests that the two temperatures interact thermodynamically through an equilibration process akin to Fourier's relation to reach a common value. Generalized fluctuation–dissipation relations were also tested for steadily deforming simulated glasses, again demonstrating the existence of a well-defined effective temperature ([Berthier and Barrat, 2002a,b](#)).

Another line of investigation focused on “athermal systems”, i.e. systems where no ordinary thermal (vibrational) fluctuations take place either due to coupling to a zero temperature bath (e.g. in computer simulations) or when the basic elements are too big to experience thermal vibrations. Realistic examples include foams (made of bubbles) and granular materials (made of grains) where the large size of the basic elements induces dissipation that rapidly quenches vibrations. In [Ono et al. \(2002\)](#), Durian's foam model ([Durian, 1995](#)) was studied under slow, steady shear deformation conditions. Five different definitions commonly used to define the ordinary thermal (vibrational) temperature – pressure and energy fluctuation relations, the Green–Kubo relation for the shear viscosity, the Stokes–Einstein relation, and the thermodynamic definition from the rate of change of configurational energy with entropy – were tested and it was discovered that all definitions yielded a similar effective temperature, though the system itself was strictly athermal. Similar ideas were developed and tested for granular materials ([Makse and Kurchan, 2002](#)). Both [Makse and Kurchan \(2002\)](#) and [Ono et al. \(2002\)](#) showed by explicit calculation that the effective temperature is equivalently given by the derivative of the configurational energy with respect to the entropy of configurational states. This implies that the configurational subsystem behaves as a distinct thermodynamic entity, featuring a configurational temperature defined as the derivative of the configurational energy with respect to the configurational entropy, precisely as we formulate in detail below.

Experimental verification of the effective temperature concept is currently limited to systems in which the basic elements are sufficiently large to be directly tracked, such as grains in granular materials and colloidal particles in colloidal glasses ([Song et al., 2005](#); [Wang et al., 2006](#)). We finally note that the literature on the effective (configurational) temperature is immense and cannot be exhaustively reviewed here. The interested reader is referred to [Leuzzi \(2009\)](#) and [Cugliandolo \(2011\)](#) for additional information and relevant references.

Two-temperature thermodynamic frameworks for spatially homogeneous, non-plastically deforming, glassy materials have been investigated by several authors ([Nieuwenhuizen, 1998](#); [Sciortino et al., 1999](#); [Kob et al., 2000](#); [Öttinger, 2006](#)), and extended models coupling the evolution of internal state variables to the new thermodynamic variables have begun to emerge. Applications to amorphous plasticity – recent Shear-Transformation-Zone (STZ) models ([Langer, 2004](#); [Shi et al., 2007](#);

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