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The rate dependent response of a bistable chain at finite temperature

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ABSTRACT

We study the rate dependent response of a bistable chain subjected to thermal fluctuations. The study is motivated by the fact that the behavior of this model system is prototypical to a wide range of nonlinear processes in materials physics, biology and chemistry. To account for the stochastic nature of the system response, we formulate a set of governing equations for the evolution of the probability density of meta-stable configurations. Based on this approach, we calculate the behavior for a wide range of parametric values, such as rate, temperature, overall stiffness, and number of elements in the chain. Our results suggest that fundamental characteristics of the response, such as average transition stress and hysteresis, can be captured by a simple law which folds the influence of all these factors into a single non-dimensional quantity. We also show that the applicability of analytical results previously obtained for single-well systems can be extended to systems having multiple wells by proper definition of rate and of the transition stress.

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1. Introduction

The saw-tooth pattern appearing in a (generalized) force–displacement response is the fingerprint of transition processes involving discrete switching events between metastable states. This phenomenon, sometimes termed “discrete phase transformation” (Benichou and Givli, 2013; Manca et al., 2014), is prevalent in small-scale systems and is also a mechanism responsible for a large number of non-linear processes at the macroscale. Examples from materials physics include the behavior of ferromagnetic alloys (Benichou et al., 2013), nano-indentation (Mordehai et al., 2011; Maaß et al., 2012; Wang et al., 2012), nanoslabs of nickel under compression (Pattamatta et al., 2014), uniaxial compression of nanopillars (Jennings et al., 2011; Kunz et al., 2011) and plasticity (Müller and Villaggio, 1977; Puglisi and Truskinovsky, 2002a; Sun and He, 2008; Seelecke et al., 2005). Another important class of materials exhibiting a saw-tooth pattern in force-extension experiments are macromolecular materials, such as DNA (Bosaeus et al., 2012; Gross et al., 2011; King et al., 2013; Raj and Purohit, 2011), spider silk, biopolymers, polysoaps, and artificial elastomers (Benichou and Givli, 2011; Chyan et al., 2004b; Kellermayer et al., 1997; Labeit et al., 2003; Oberhauser, 2001; Oberhauser et al., 2001, 1998; Rief et al., 1997, 1998; Schlierf et al., 2004; Schwaiger et al., 2002; Tskhovrebova et al., 1997; Williams et al., 2003). In proteins for example, this is constituted by elastic

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(entropic) macromolecules reinforced by a finite number of stiff domains, usually in the form of fillers or β-sheets. These domains undergo hard–soft transitions by unfolding into soft (entropic) domains. These discrete switching events give rise to the saw-tooth pattern observed in single molecule force-extension experiments (Benichou and Givli, 2011; Chyan et al., 2004a; Gross et al., 2011; Oberhauser et al., 2002; Rief et al., 1997). Finally, many-particle reversible storage systems, such as lithium-ion batteries (Dreyer et al., 2011, 2010), also exhibit a similar behavior.

A large number of works, some date back to the 1970s (Müller and Villaggio, 1977), have demonstrated that the non-trivial behavior of an elastic chain composed of bistable elements is prototypical for such processes. Most of these works focused on purely static analysis, clarifying issues such as stability and the role of the spinodal region (Puglisi and Truskinovsky, 2000), investigating the effects of interactions beyond the nearest neighbors (Rogers and Truskinovsky, 1997), the behavior in more than one dimension (Kinderlehrer and Ma, 1994; Müller and Villaggio, 1977), and the influence of various types of non-convex springs ranging from Lennard–Jones type potentials (Braides et al., 1999; Truskinovsky, 1996) to tri-parabolic and bi-parabolic approximations of the spring energy (Fedelich and Zanzotto, 1992; Puglisi and Truskinovsky, 2002b).

The dynamic behavior of bistable chains poses a real theoretical challenge, and indeed fewer studies investigated the dynamics of bistable chains. These studies can be roughly divided into two main categories. The first involves modeling inertial dynamics directly (e.g. Balk et al., 2001; Cherkaev et al., 2005; Cohen and Givli, 2014; Efendiev and Truskinovsky, 2010; Slepyan and Troyankina, 1984; Vainchtein, 2010; Qingze and Prashant, 2014). A second approach is to obtain the dynamic response by assuming simplified evolution strategies or kinetic relations (e.g. Givli, 2010; Givli and Bhattacharya, 2009; Puglisi and Truskinovsky, 2002b; Raj and Purohit, 2011).

In nanoscale structures, thermal fluctuations often govern the dynamic response by enabling overcoming energy barriers separating between metastable configurations. Roughly, the response is divided into three regions of rates: at very low rates, the system operates at quasi-equilibrium; at moderate rates thermal noise dominates the behavior, resulting in a stochastic response; and at sufficiently high rates, the system has no time to explore its energy landscape, so stochastic fluctuations become irrelevant and the response is deterministic (Rico et al., 2013). This means that in the passage from low to intermediate and then to high rates the system experiences transitions from deterministic to stochastic and back to deterministic response. In addition, fundamental differences distinguish between these three regions. For example, in the first region (low rates), the system exhibits no hysteresis and transition stresses are lowest. Hysteresis appears in the other two regions, but at intermediate rates it is a consequence of transitions from high-energy to low-energy configurations, while at very high rates it is dominated by a standard damping mechanism.

The rates defining each region may vary significantly, depending on specific features of the energy landscape. Hence, establishing a universal scale that uniquely determines whether a rate is high, low or intermediate is of key importance. Such a scale can also facilitate quantitative predictions of fundamental features, such as hysteresis and transition stress. Addressing this challenge is the main goal of this paper. To this end, we consider the model system of an elastic chain composed of bistable elements connected in series, and study its *rate-dependent* response at finite temperature. Having in mind nanoscale structures and macromolecular materials, the height of energy barriers separating between meta-stable configurations is typically of the order of ten to a few hundreds k_BT, making the system susceptible to thermal noise. In addition, the dynamics of these systems is overdamped, meaning that excess energy associated with switching events completely dissipates into heat.

Experimental investigation of micro-scale structures or macromolecular materials typically involve mechanically induced switching of material domains by techniques such as AFM, optical tweezers, or magnetic tweezers (Brown et al., 2007; Linke and Grutzner, 2008; Oberhauser et al., 2001; Rief et al., 1997; Shulha et al., 2006; Wang et al., 2012). In these experiments, the mechanical load is usually set by moving the experimental stage at some predefined rate. This length constraint introduces mechanical coupling between domains, and dictates a response that is fundamentally different from force-control (dead load/soft device) experiments. In length-control conditions (hard device), energy barriers separating between configurations depend on the overall strain, but also on the overall compliance and on the configuration (number of domains that already switched). On the other hand, in force-control experiments, the energy barriers separating between meta-stable configurations depend on the level of external force but are indifferent to the overall compliance and configuration (Puglisi and Truskinovsky, 2000). Since energy barriers dominate the rate dependent and temperature dependent dissipative behavior of systems susceptible to thermal noise, one must account for the actual loading conditions when analyzing such experiments. The above discussion regarding the difference between force-control and length-control conditions resembles a similar discussion on stretching polymer chains (without domains). It has been shown that different boundary conditions (Helmholtz or Gibbs ensembles) imposed for stretching the polymer lead to different force-extension curves (Keller et al., 2003; Manca et al., 2012b; Sinha and Samuel, 2005). These differences are emphasized when the contour length of the molecule is of the same order of its persistence length, and become indistinguishable at the thermodynamic limit (Winkler, 2010).

Theoretical studies concerning the thermo-mechanical behavior of multi-stable chains susceptible to thermal noise have taken various approaches (e.g. Achenbach and Muller, 1982; Brown et al., 2009; Evans and Ritchie, 1997, 1999; Huo and Müller, 1993; King et al., 2010; Manca et al., 2012a, 2013; Mirny and Shakhnovich, 2001; Muller and Seelecke, 2001; Purohit et al., 2011; Singh et al., 2011; Staple et al., 2009; Su and Purohit, 2009). These works can be roughly divided into three categories: formulation of mathematical models based on two-state theory, a continuum approach based on a Fokker–Planck formulation (Herrmann et al., 2012), and intensive computer based simulations, such as Langevin dynamics (Bonilla

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