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► **To cite this version:**

Luca Bellino, Giuseppe Florio, Stefano Giordano, Giuseppe Puglisi. NON LOCAL AND THERMAL EFFECTS IN A BI-STABLE LATTICE. 25th International Congress of Theoretical and Applied Mechanics (25th ICTAM), Aug 2021, Milan, Italy. hal-03450773

**HAL Id: hal-03450773**

**<https://hal.science/hal-03450773>**

Submitted on 26 Nov 2021

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## NON LOCAL AND THERMAL EFFECTS IN NANOWIRES PHASE TRANSITION

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**Summary** Interface energy and thermal effects are comparable when micro dimensional scales are considered, leading to a temperature dependent phase transition strategy that, from a macroscopic point of view, often leads to the presence of a stress-peak characterizing the nucleation stress and the size of the first phase from the propagation ones. To account for these phenomena, in a Statistical Mechanics framework, we consider next to nearest neighbor (NNN) interactions on a chain of bi-stable elements, and we obtain fully analytical result describing the aforementioned effects on the thermo-mechanical response of the system. Moreover, we validate our model by comparing it with the temperature dependent phase transition behavior experimentally observed on memory shape nanowires.

Effective, microstructure based models have been shown to be able to describe the thermo-mechanical response of different materials undergoing phase transitions (*e.g.* new bio-inspired materials [1] or shape memory alloys, SMA [2]). Here, by extending [3, 4], we consider a prototypical example constituted by a chain of elements with bistable potentials, describing a material with two distinct phases (i.e. folded–unfolded configuration in a macromolecule or austenitic and martensitic phases in SMA [2]). As in the continuous analogue of higher order gradient theories [5], here we describe the important role of interfacial energy by considering NNN interactions (see Figure 1). The zero temperature behavior of this system was described in [6, 3, 4]. Here we consider the role of temperature analyzing the behavior of the bistable chain with non local NNN interactions in the framework of equilibrium Statistical Mechanics [7, 8, 9].

The energy function –dimensionalized with respect to  $lk$ , where  $k$  is the stiffness and  $l$  the reference length in the first phase– for a chain of  $n$  bistable oscillators is (see Figure 1a)

$$\varphi(\{S_j\}, \{\varepsilon_j\}) = \varphi_{NN} + \varphi_{NNN} = \frac{1}{2} \sum_{j=1}^n \left[ (\varepsilon_j + \varepsilon_0)^2 \frac{(1 - S_j)}{2} + (\zeta(\varepsilon_j - \varepsilon_0)^2 + 2\eta) \frac{(1 + S_j)}{2} \right] + \frac{1}{2} \sum_{j=1}^{n-1} \alpha (\varepsilon_j + \varepsilon_{j+1})^2, \quad (1)$$

where  $\varepsilon_j$  is the strain of  $j$ -th domain,  $\pm\varepsilon_0$  is the reference strain of the two configurations, respectively. Here  $\zeta$  is the relative stiffness between the two wells,  $\eta$  is the relative transition energy and  $\alpha < 0$  (ferromagnetic interaction) is the reference stiffness of the NNN harmonic springs. We have also introduced the “spin” variable  $S_j$  that can assume the value  $\pm 1$  depending on the phase of the bi-stable oscillator, as shown in figure 1b.

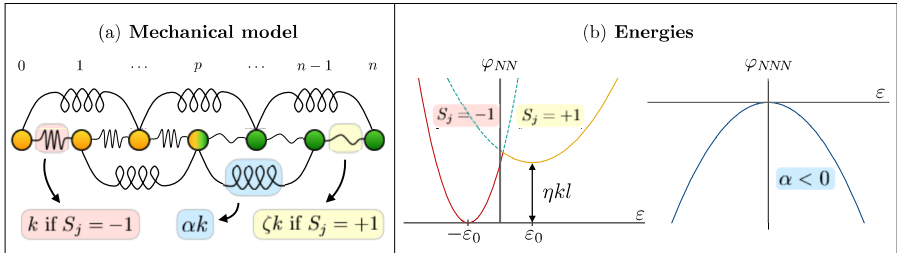


Figure 1: (a) Scheme of the chain with bistable units and NNN interactions. (b) NN and NNN energies.

To obtain fully analytical results, the NNN interaction is introduced in a perturbative framework (*i.e.*  $|\alpha| \ll 1$ ) and the two parabolas modeling the NN energy terms are extended beyond the spinodal point [10, 8, 9] (see Fig 1b). We study the system in thermal equilibrium in the regimes of both soft (Gibbs ensemble) and hard (Helmholtz ensemble) devices, when a constant force  $\sigma$  or a fixed displacement  $\delta$  are applied, respectively [11]. In the former case we obtain the expressions for the stress strain relation and the expectation values of both number of interfaces and nucleated phase fraction:

$$\langle \tilde{\varepsilon} \rangle = (1 - 4\alpha) \left[ 2\varepsilon_0 \langle \chi \rangle_{\mathcal{G}} + (\sigma - \varepsilon_0) \right], \quad \langle \chi \rangle_{\mathcal{G}} = \frac{\sum_{p=0}^n \sum_{i=0}^{n-1} \mathcal{W}_{p,i} \chi e^{\Gamma_{p,i}(\sigma)}}}{\sum_{p=0}^n \sum_{i=0}^{n-1} \mathcal{W}_{p,i} e^{\Gamma_{p,i}(\sigma)}}, \quad \langle i \rangle_{\mathcal{G}} = \frac{\sum_{p=0}^n \sum_{i=0}^{n-1} \mathcal{W}_{p,i} i e^{\Gamma_{p,i}(\sigma)}}{\sum_{p=0}^n \sum_{i=0}^{n-1} \mathcal{W}_{p,i} e^{\Gamma_{p,i}(\sigma)}}, \quad (2)$$

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where  $p$  is the number of elements in phase 2,  $i$  is the number of interfaces and  $\beta = \frac{1}{k_B T}$ , with  $k_B$  the Boltzmann constant and  $T$  the absolute temperature ( $\zeta = 1$  for simplicity of the expression),  $\mathcal{W}_{p,i}$  is a combinatorial counting coefficient and  $\Gamma_{p,i}(\sigma)$  is a characteristic function for the Gibbs ensemble (see [11] for details).

On the other hand, at fixed displacement  $\delta$ , we obtain

$$\langle \sigma \rangle = \frac{[\varepsilon - (1 - 4\alpha)(2\langle \chi \rangle_{\mathcal{H}} - 1)\varepsilon_0]}{(1 - \frac{4\alpha}{n}(n - 1))}, \quad \langle \chi \rangle_{\mathcal{H}} = \frac{\sum_{p=0}^n \sum_{i=0}^{n-1} \mathcal{W}_{p,i} \chi e^{\Omega_{p,i}(\delta)}}{\sum_{p=0}^n \sum_{i=0}^{n-1} \mathcal{W}_{p,i} e^{\Omega_{p,i}(\delta)}}, \quad \langle i \rangle_{\mathcal{H}} = \frac{\sum_{p=0}^n \sum_{i=0}^{n-1} \mathcal{W}_{p,i} i e^{\Omega_{p,i}(\delta)}}{\sum_{p=0}^n \sum_{i=0}^{n-1} \mathcal{W}_{p,i} e^{\Omega_{p,i}(\delta)}}, \quad (3)$$

where  $\Omega_{p,i}(\delta)$  is a characteristic function for the Helmholtz ensemble (see [11] for details).

In figure 2 we show the theoretical results obtained with our model (Fig. (a)) and the comparisons with the experimental data of Molecular Dynamic simulations performed by Lu at al [12] (Fig. (b)) and Wu [13] (Fig. (c)). In the first row of figure 2, can be observed that as the discreteness of the system increases, the nucleation (peak) stress becomes higher with respect to propagation one. On the other hand, as the temperature increases the stress peak decreases while the regime is opposite for increasing interfacial energy, showing a direct competition between the two energies during the transition process. In the second row of figure 2 we present the comparison of our analytical results with two different molecular dynamic simulations, obtaining an excellent agreement among the data.

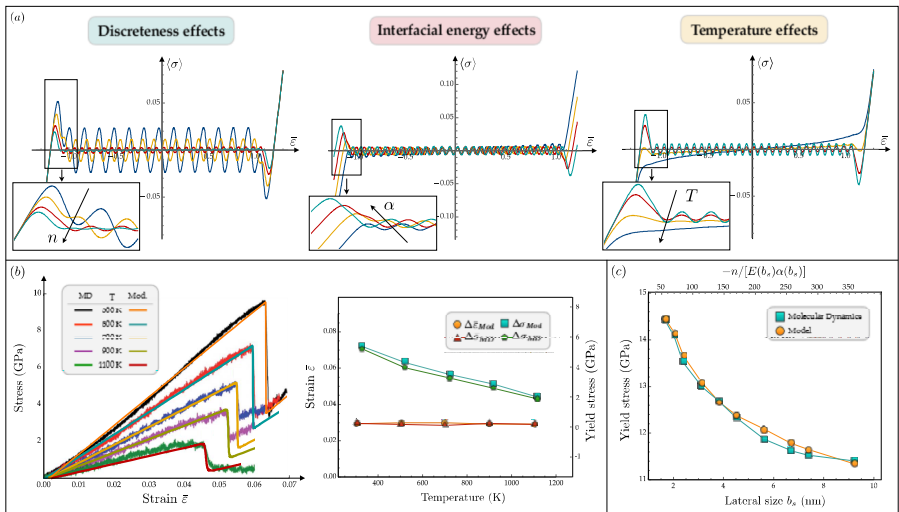


Figure 2: First row: theoretical results showing the effects of the discreteness of the system, of the interfacial energy and of the temperature in the case of applied displacement. Bottom row: comparison with the Molecular Dynamic simulations of memory shape nanowires of Lu et al. in figure (b) [12] and of Wu in (c) [13].

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