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DEVELOPING MESOSCOPIC MODELS DESCRIBING PHASE TRANSFORMATIONS IN FINITE NANOWIRES AND NANOPLATES

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Abstract. Microstructures in finite nanostructures such as nanowires and nanoplates are studied with mesoscopic models. Results of computational experiments for nanowires with different diameter-to-length ratio and for finite nanoplates are presented.

1 INTRODUCTION

It has been known for some time that in gold (Au) nanowires, the energy as a function of lattice spacing exhibits two distinct minima that correspond to fcc and bct phases. The fact that these nanowires exhibit shape memory effects has also been confirmed computationally with such methodologies as tight-binding and density functional theory. A similar situation holds for many other nanowires that show substantial potential for many applications in nano- and bio-nanotechnologies, including Cu, Ni, ZnO, FePd, Al, Ag, etc.

While many results up to date have been obtained for infinitely long nanowires (as well as for infinitely large nanoplates), including those obtained with ab initio calculations, the question has remained on whether phase transformations is a generic effect for the same material-type nanowires of finite length. Recently, there has been mounting evidence towards a positive answer to this question. However, comprehensive studies of finite nanowires and nanoplates are limited due to the fact that the methodologies applied for their studies are computationally expensive.

In this contribution, we present a relatively simple and computationally inexpensive model to study phase transformations in finite nanostructures with our major focus given here to finite nanowires and nanoplates. Based on our previous results, the models describing shape memory effects at the mesoscopic level for the case of square-to-rectangle transformations can be reduced to a two-dimensional case.

2 LANDAU MODELS IN THE ANALYSIS OF NANOSTRUCTURES

A better understanding of such complex multiscale phenomena as phase transformation in crystal materials often requires a molecular resolution. This leads to computationally costly procedures. At the same time, many problems involving phase transformations can be dealt with efficiently by developing mesoscopic models which can be viewed as coarse grained with respect to the full molecular dynamic modeling.

In what follow, we are interested in microstructures of finite length nanowires, as well as finite size nanoplates, where the shape memory effect and martensitic phase transformations are observed. Although phase transformations in bulk are now much better understood, many new challenges appear already for thin films[1], and more so at the nanoscale. This is particularly true for nanostructures with geometric constraints, e.g. nanowires of finite length. We focus on two types of phase transformations: cubic-to-tetragonal and square-to-rectangle. All examples that follow are given for the latter case, while the former case is viewed as its three-dimensional generalization[2].

In order to characterize both, austenite at high temperature and martensite at low temperature, by using a generic expression, the potential energy is constructed on the basis of the modified Ginzburg-Landau free energy function. We follow[3] to get the evolution equations for our case as follows:

$$\frac{\partial^2 u_1}{\partial t^2} = \frac{\partial \sigma_{11}}{\partial x} + \frac{\sigma_{12}}{\partial y} + f_1, \quad \frac{\partial^2 u_2}{\partial t^2} = \frac{\partial \sigma_{12}}{\partial x} + \frac{\sigma_{22}}{\partial y} + f_2, \tag{1}$$

$$c_v \frac{\partial T}{\partial t} = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + a_2 T e_2 \frac{\partial e_2}{\partial t} + g \tag{2}$$

with

$$\sigma_{11} = \frac{\sqrt{2}}{2} \rho (a_1 e_1 + a_2 (T - T_0) e_2 - a_4 e_2^3 + a_6 e_2^5) + \frac{d_2}{2} \nabla_x^2 e_2, \ \sigma_{12} = \frac{1}{2} \rho a_3 e_3 = \sigma_{21}, \tag{3}$$

$$\sigma_{22} = \frac{\sqrt{2}}{2} \rho (a_1 e_1 - a_2 (T - T_0) e_2 + a_4 e_2^3 - a_6 e_2^5) + \frac{d_2}{2} \nabla_y^2 e_2, \tag{4}$$

where all the notation here are identical to those of[3]. A similar model has been recently applied in[4]. Under appropriate boundary and initial conditions, the above model can be efficiently solved with recently developed numerical methodologies, including the Chebyshev collocation procedure[5], the proper orthogonal decomposition[6], the genetic algorithm based optimization procedure[7], and the finite volume methodology[8], as well as finite element techniques[1].

3 RESULTS

A number of examples for nanostructures of different geometry and materials have been analyzed with the above model, and in what follows we present only a few representative calculations carried out for iron-based (FePd) nanostructures. Values of parameters for FePd can be found in[4]. In Fig. 1 we observe the formation of microstructures in two nanowires with increasing diameter-to-length ratio (same length, increasing diameter). With decreasing length of the nanowire, the microstructure acquires a more regular pattern as seen in Fig. 2 (left). In all these three cases $K_g = 1 \times 10^{-4}$. The analysis of the evolution of the microstructure for a square nanoplate is given in Fig. 2 (right) and Fig. 3. In this case, $K_g = 5 \times 10^{-5}$. All the results here have been obtained for $\theta_0 = 265K$ and presented for $\theta = 250K$. A typical number of degree of freedom in these finite element calculations is on the order of 100,000. Results on critical diameters of finite length nanowires will be presented elsewhere. Finally, we note that some initial three-dimensional modelling results with mesoscopic models were presented in[2].

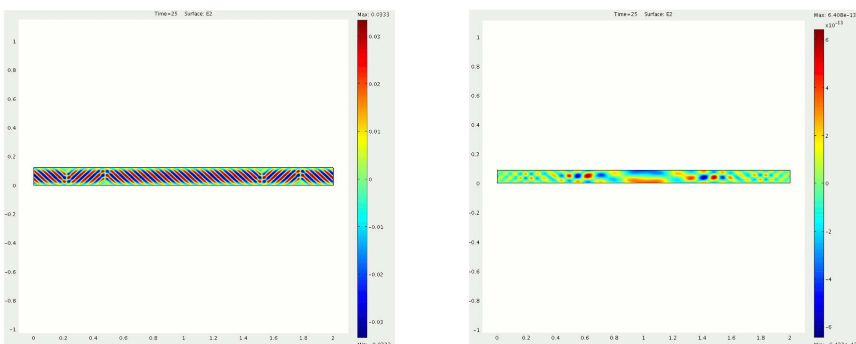

Figure 1: Size dependency of nanowires with increasing diameter-length ratio.

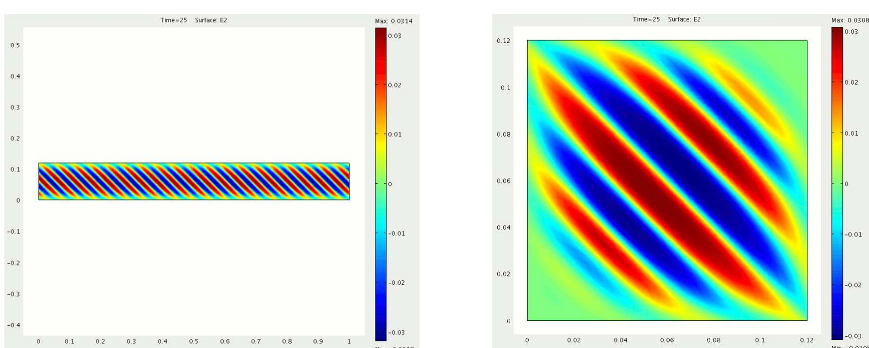

Figure 2: Microstructures in the nanowire of smaller length (left) and in the square nanoplate.

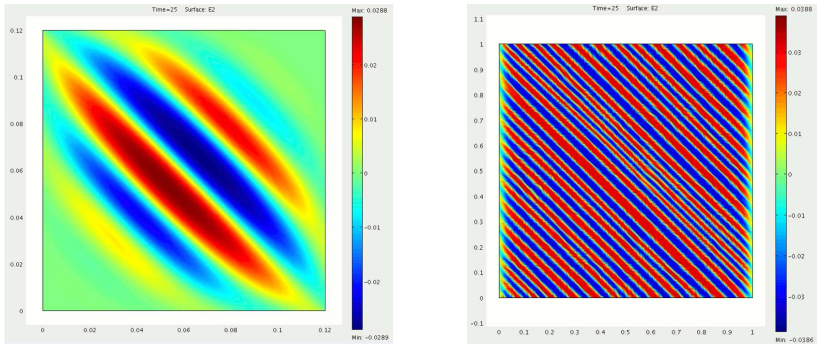

Figure 3: Evolution of microstructure in the square nanoplate.

4 Conclusions

We have presented results on the analysis of microstructure evolution in finite nanostructures with mesoscopic models, focusing on finite nanowires and nanoplates.

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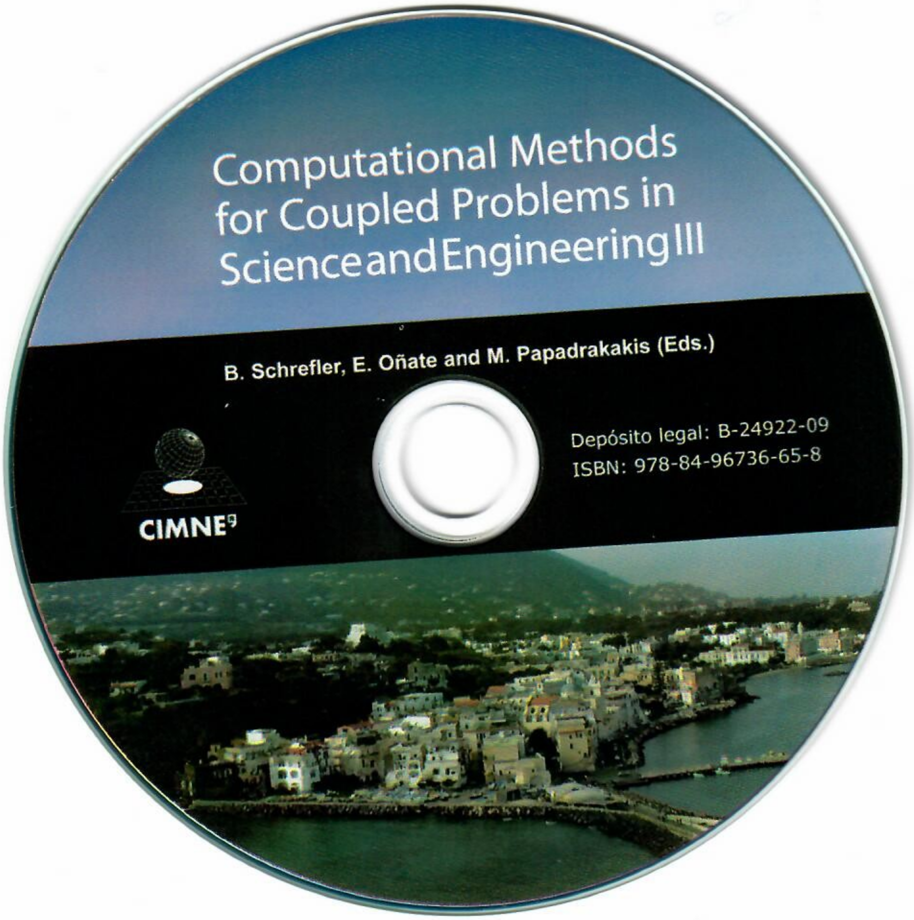
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