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# Phase Transformations and Shape Memory Effects in Finite Length Nanostructures

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## ABSTRACT

We discuss a relatively simple and computationally inexpensive model that has recently been developed to study phase transformations and shape memory effects in finite nanostructures. Our major focus is given to nanowires of finite length and other nanostructures where size effects are pronounced. The main tool used here is based on mesoscopic models developed with the phase-field approach which we and other authors have applied before to study ferroelectrics at the nanoscale. We study the cubic-to-tetragonal transformations in which case the 2D analogue of the model describes the square-to-rectangle phase transformations. The actual model is based on a coupled system of partial differential equations and is solved with a combination of the Chebyshev collocation method and the extended proper orthogonal decomposition. The developed model and its numerical implementation allow us to study properties of nanostructures and several representative examples of mechanical behavior of nanostructures are discussed.

**Keywords:** Low dimensional nanostructures, shape memory alloys, phase transformations, dynamics, coupled nonlinear effects

## 1. INTRODUCTION

In a number of nanostructures, the energy as a function of lattice spacing exhibits two distinct minima that correspond to fcc and bct phases. Such nanostructures may also exhibit shape memory effects which has been confirmed by experimental methodologies. Indeed, it is known that such a situation arises in gold (Au) nanowires, for example. The fact that these nanowires exhibit shape memory effects has also been confirmed computationally with such methodologies as tight-binding and density functional theory (e.g.,[3]). A similar situation holds for ZnO nanowires and many other types of nanowires that show substantial potential for many applications in nano- and bio-nanotechnologies, including Cu, Ni, ZnO, FePd, Al, Ag (e.g.,[7] and references therein).

While many theoretical results up to date have been obtained for infinitely long nanowires, 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. Although there has been mounting evidence towards a positive answer to this question, comprehensive studies of nanowires of finite length are limited due to the fact that the methodologies applied for their studies are computationally expensive. In addition, there are a number of questions that remain open at a large extent, including questions related to temperature-dependent phase stability.

In this contribution, our focus is on the analysis of the nonlinear coupling between mechanical and thermal fields in SMA-based nanowires. We use some generalizations of ideas originally developed for ferroelectric materials to arrive to a model based on a system of coupled partial differential equations.[33,34] The resulting system can be solved efficiently by several different methodologies such as finite volume[29] or finite element methods.[8] In this paper, we apply the Chebyshev collocation method for the solution of the resulting problem, followed by the application of an extended proper orthogonal decomposition as was proposed in.[27,28]

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## 2. EXISTING MODELS AND GINZBURG-LANDAU APPROACHES

Nanowires belong to the class of nanostructures known as low dimensional due to the fact that the motion of electrons inside such structures can be confined spatially. Low dimensional semiconductor nanostructures have many applications in nanotechnology, but they provide serious theoretical and computational challenges when it comes to the prediction of their properties.[6] This especially true when we need to account for finite size effects as it is the case, for example, for finite length nanowires.[18] Coupled effects in nanostructures are also their intrinsic feature that must be accounted for in many areas of applications.[16] One such effect, namely piezoelectric, has been studied for a long time and is known to have importance consequences on bandstructure calculations of low dimensional nanostructures. More recently, the importance of thermal effects has been demostrated in the context of their coupling to electromechanical fields. [19,20]

Shape memory effects at the nanoscale are attracting increasing interest due their importance in MEMS and NEMS applications[24] as well as in other areas, including nanophotonics.[1] In addition to theoretical works, there are a number of experimental studies that provide further details of phase transformations on the nano- and microscopic length scales, primarily based on the transmission electron microscopy (e.g., [25]). Such studies have been carried out for a number of alloys, including NiAl, NiTiCu, CuZnAl and others.

While many coupled effects mentioned above are linear, shape memory effects are strongly nonlinear effects. The importance of nonlinear effects in the context of nanostructures have recently been emphasized in. [17] It was shown that the applicability of linear models is limited for low dimensional nanostructures, in particular quantum dots, and both coupled and nonlinear effects need to be accounted for in the analysis of more realistic structures. Although shape memory effects and associated microstructures have been studied at the nanoscale in various materials such as ferroelectrics, such studies have been very limited for confined nanostructures.[26]

In,[26] a phase-field model was used to study confined ferroelectrics. The authors focused on the equilibrium domain structure only by considering the free energy function as a sum of the Ginzburg-Landau potential, the energy of electrostatic and the energy of elastic interactions. In particular, the Ginzburg-Landau potential in their work was taken as

$$F = \int_V \big[\frac{1}{2}\beta_{ijkl}\frac{\partial \eta_i}{\partial x_k}\frac{\partial \eta_j}{\partial x_l} + f_0(\eta_i)\big]dV. \tag{1}$$

Here the gradient coefficient tensor $\beta_{ijkl}$ is responsible for accounting the interfacial energy and $\eta_i$, $i = 1, 2, 3$ is the three-component order parameter such that the homogeneous state energy density can be approximated by the Landau-Devonshire expansion. For the particular type of transformations from the cubic to tetragonal state in $PbTiO_3$ it was chosen as

$$f_0(\eta_i) = \alpha_1 \sum_{i=1}^{3} \eta_i^2 + \alpha_{12}(\eta_1^2\eta_2^2 + \eta_2^2\eta_3^2 + \eta_3^2\eta_1^2) + \alpha_{11}\sum_{i=1}^{3}\eta_i^4 +$$
$$\alpha_{112}[\eta_1^2(\eta_2^4 + \eta_3^4) + \eta_2^2(\eta_1^4 + \eta_3^4) + \eta_3^2(\eta_1^4 + \eta_2^4)] + \alpha_{123}\eta_1^2\eta_2^2\eta_3^2 + \alpha_{111}\sum_{i=1}^{3}\eta_i^6. \tag{2}$$

Our approach here is different as we ultimately aim at a better understanding of the dynamics of phase transformations. Furthermore, practical challenges of controlling such dynamics made us to concentrate on a somewhat simpler, yet more transparent model for the free energy. In this context, we also note that although further insight into the properties of nanostructures we are interested in can be gained with atomistic approaches (e.g., [21]), the associated with them models are not amenable for control purposes. However, one of the important conclusions of such studies is that they emphasize the importance of microstructures as well as boundary conditions (e.g., in [21] a particular emphasis was given to mechanical boundary conditions). More recent works based of first principles calculations include also the analysis of dynamic coupling between polarization and strain at the nanoscale.[22] A number of works were devoted studying properties of ferroelectrics based on the Landau-Ginzburg-Devonshire theory, including size effects, at the nanoscale. [4,23]

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.[36] However, comprehensive studies of nanowires of finite length are limited due to the fact



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that the methodologies applied for their studies are computationally expensive. In addition, there are a number of questions that remain open at a large extent, including questions related to temperature-dependent phase stability.

In this contribution, we develop a relatively simple and computationally inexpensive model to study phase transformations in finite nanostructures with our major focus given here to nanowires of finite length. In the latter case, the models describing shape memory effects at the mesoscopic level such as those developed in [11,12,14] can be reduced to a 2D case (and in the case of nanowires of infinite length, to the 1D case). We study the cubic-to-tetragonal transformations in which case the 2D analogue of the model describes the square-to-rectangle phase transformations. In particular, our considerations are based on a modification of the coupled system of PDEs for the evolution of displacements $(u_1, u_2)$ and temperature T analyzed previously in.[28,29] In a series of recent papers we developed several efficient methodologies to solve 2D models describing square-to-rectangle phase transformations in materials with memory, in particular the finite volume methodology[29] and a numerical reduction procedure based on the Proper Orthogonal Decomposition (POD). [28] Here we discuss their applications to modelling finite nanostructures. The examples that have been considered include gold (Au), iron-based (FePd), and zinc-based oxide(ZnO) nanowires, but only several representative examples have been included here. Our presentation here builds on and follow our earlier results presented at the Sixth International Conference on Engineering Computational Technology and the Second International Conference on Nanotechnology and accounts for the latest development in the field.

## 3. NONLINEAR COUPLING OF MECHANICAL AND THERMAL FIELDS

To account for the first order phase transformations in ferroelastic materials such as shape memory alloys, time-dependent models of coupled dynamic thermoelasticity must account for a nonconvex highly nonlinear character of the associated free energy function. We start with the following 1D mathematical model: [10,15]

$$\begin{aligned} &\rho\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(k_1\left(\theta-\theta_1\right)\frac{\partial u}{\partial x} - k_2(\frac{\partial u}{\partial x})^3 + \right. \\ &\left. k_3(\frac{\partial u}{\partial x})^5\right) + \nu\frac{\partial}{\partial t}\frac{\partial^2 u}{\partial x^2} - \delta\frac{\partial^4 u}{\partial x^4} + F, \\ &c_v\frac{\partial\theta}{\partial t} = k\frac{\partial^2\theta}{\partial x^2} + k_1\theta\frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + G, \end{aligned} \tag{3}$$

where $u$ is displacement, $\theta$ temperature, $\rho$ density, $k_1$, $k_2$, $k_3$, $c_v$, $\nu$, $\delta$ and $k$ are normalized material-specific constants, $\theta_1$ is the reference temperature for 1D martensitic transformations, and $F$ and $G$ are distributed mechanical and thermal loadings. The interested reader can find efficient numerical procedures for reducing systematically the general 3D model to models such as (3) in.[15]

Although this is only a 1D model for the nonlinear dynamics of ferroelastic materials, it presents a number of challenges in its analysis and numerical implementation due to the coupling between thermal and elastic fields and strong nonlinearities. Furthermore, the inclusion of thermal and mechanical hystereses and the first order martensitic transformations into the model gives additional difficulties. First, we re-write the above system for numerical convenience as follows: [10]

$$\begin{aligned} &c_v\frac{\partial\theta}{\partial t} = k\frac{\partial^2\theta}{\partial x^2} + k_1\theta\epsilon\frac{\partial v}{\partial x} + G, \quad \frac{\partial\epsilon}{\partial t} = \frac{\partial v}{\partial x} \\ &\rho\frac{\partial v}{\partial t} = \frac{\partial}{\partial x}\left(k_1\left(\theta-\theta_1\right)\epsilon - k_2\epsilon^3 + k_3\epsilon^5\right) + \\ &\nu\frac{\partial}{\partial t}\frac{\partial^2 u}{\partial x^2} - \delta\frac{\partial^3\epsilon}{\partial x^3} + F, \end{aligned} \tag{4}$$

where $\epsilon = \partial u/\partial x$ is the strain, and $v = \partial u/\partial t$ is the velocity. Note that this representation is convenient for a reduction of the original PDE-based model to a system of differential-algebraic equations the approach that was initiated in. [14]

More generally, our consideration in this paper is based on the nonlocal model developed in [15] based on the equation of motion

$$\rho\frac{\partial^2\mathbf{u}}{\partial t^2} = \nabla_{\mathbf{x}}\cdot\mathbf{s} + \mathbf{F} \quad \text{with} \quad \mathbf{F} = \rho(\mathbf{f}+\hat{\mathbf{f}}) - \hat{\rho}\mathbf{v}\,, \tag{5}$$



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and the energy balance equation

$$\rho\frac{\partial e}{\partial t} - \mathbf{s}^T : (\nabla \mathbf{v}) + \nabla \cdot \mathbf{q} = g\,, \tag{6}$$

where $\mathbf{u}$ is the displacement vector, $\rho$ is the density of the material, $e$ is the internal energy (per unit mass), $\mathbf{q}$ is the heat flux, $\mathbf{f}$ is a given body force per unit mass, $\hat{\rho}$ and $\hat{\mathbf{f}}$ are nonlocal mass and force residuals respectively (similarly, $g$ accounts for both local and non-local contributions), $\mathbf{v} = \partial\mathbf{u}/\partial t$ is the velocity vector, $\mathbf{s}$ is the stress tensor, $\mathbf{a}^T : \mathbf{b} = \sum_{i,j=1}^{3} a_{ij}b_{ij}$ is the standard notation for the rank 2 tensors $\mathbf{a}$ and $\mathbf{b}$ (further details can be found in [15]). The constitutive relationships that couple stresses, deformation gradients, temperature and heat fluxes have the following general form:

$$\Phi_1(\mathbf{s}, \boldsymbol{\epsilon}) = 0\,, \quad \Phi_2(\mathbf{q}, \theta) = 0\,, \tag{7}$$

where it is implicitly assumed that these relations may involve spatial and temporal derivatives of the functions. Particular forms for $\Phi_1$ and $\Phi_2$ are problem specific. In dealing with phase transformations, the approach adopted in this paper is based on the Landau criterion stating that any isothermal equilibrium configuration of the lattice corresponds to a minimum (global or local) of the free energy function.

In order to characterize both, austenite at high temperature and martensite at low temperature, having in mind the analysis of finite length nanowires and other low dimensional nanostructures, by using a generic expression, the potential energy is constructed on the basis of the modified Ginzburg-Landau free energy function. We follow [32] to get the evolution equations for our case as follows:

$$\frac{\partial^2 u_1}{\partial t^2} = \frac{\partial \sigma_{11}}{\partial x} + \frac{\sigma_{12}}{\partial y} + f_1, \tag{8}$$

$$\frac{\partial^2 u_2}{\partial t^2} = \frac{\partial \sigma_{12}}{\partial x} + \frac{\sigma_{22}}{\partial y} + f_2, \tag{9}$$

$$c_v\frac{\partial T}{\partial t} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + \tag{10}$$

$$a_2 T e_2 \frac{\partial e_2}{\partial t} + g \tag{11}$$

with

$$\sigma_{11} = \frac{\sqrt{2}}{2}\rho\left(a_1 e_1 + a_2(T - T_0)e_2 - a_4 e_2^3 + \right. \tag{12}$$

$$\left. a_6 e_2^5\right) + \frac{d_2}{2}\nabla_x^2 e_2,\ \sigma_{12} = \frac{1}{2}\rho a_3 e_3 = \sigma_{21}, \tag{13}$$

$$\sigma_{22} = \frac{\sqrt{2}}{2}\rho\left(a_1 e_1 - a_2(T - T_0)e_2 + a_4 e_2^3 - \right. \tag{14}$$

$$\left. a_6 e_2^5\right) + \frac{d_2}{2}\nabla_y^2 e_2, \tag{15}$$

where all the notation here are identical to those of. [32]

## 4. CHEBYSHEV COLLOCATION AND PROPER ORTHOGONAL DECOMPOSITION

A similar model has been recently applied in. [2] As we have already mentioned, under appropriate boundary and initial conditions, the models like this can be efficiently solved with several recently developed numerical methodologies, including the Chebyshev collocation procedure, [30] the proper orthogonal decomposition, [28] the genetic algorithm based optimization procedure, [31] and the finite volume methodology, [29] as well as finite element techniques. [9]

For the sake of convenience, the governing equations are re-written in the form of evolution operator equation:

$$\frac{d\mathcal{U}}{dt} = \mathcal{M}(\mathcal{U}), \tag{16}$$



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where $\mathcal{U}$ is the solution and $\mathcal{M}(\mathcal{U})$ is an operator which contains all the spatial derivatives of $\mathcal{U}$. In general, the approximation given by our model will not satisfy Eq.(16), i.e., the residual

$$\mathcal{R} = \frac{d\mathcal{U}^N}{dt} - \mathcal{M}(\mathcal{U}^N) \tag{17}$$

will not vanish everywhere. To determine all the expansion coefficients, the Galerkin method requires the following condition to be satisfied:

$$\int_0^L \left( \frac{d\mathcal{U}^N}{dt} - \mathcal{M}(\mathcal{U}^N) \right) \psi_i(x) dx = 0, \tag{18}$$

where $\psi_i(x)$ are the test functions.

In the Chebyshev collocation methods the trial functions are chosen to satisfy the following conditions:

$$\phi_i(x_j) = \begin{cases} 1, & \text{i = j,} \\ 0, & \text{i} \neq \text{j .} \end{cases} \tag{19}$$

and the test functions are chosen as:

$$\psi_i(x) = \delta(x_i) = \begin{cases} 1, & \text{x=}x_i, \\ 0, & x \neq x_i, \end{cases} \tag{20}$$

where $\{x_i\}$ is a set of chosen discretization points in the computational domain. For the Chebyshev approximation, it is chosen as follows:

$$x_i = L \left( 1 - \cos(\frac{\pi i}{N}) \right) /2, \quad i = 0, 1, \ldots, N, \tag{21}$$

where $L$ is the length of the considered ferroelastic rod.

Following the standard procedure, our equation can be written in a matrix form as:

$$\mathrm{U}_x = \mathrm{DU}. \tag{22}$$

By substituting corresponding approximations of the spatial derivatives, the PDE-based model is converted into a set of Differential-Algebraic Equations (DAEs). The idea of a reduction of the original PDE model to a system of DAEs was first proposed in,[14] followed by a subsequent development of low dimensional models based on the center manifold technique. [15] The application of an efficient time integrator can finally solve the problem in a way similar discussed earlier. [10,28] The described methodology allows us to determine the temperature, stress, strain and displacement of the material at any point of the computational domain at any time. Then, the resultant data can be used for the POD analysis. It is carried out in a way similar to that described in.[27,28]

Having obtained optimal basis functions for the dynamical system, its lower dimensional approximation can be obtained by projecting the full system orthogonally onto the subspace spanned by the chosen basis functions (by the Galerkin projection). The model reduction can be achieved due to the fact that much smaller number of basis functions is needed for the approximation of the full system provided the chosen basis functions are optimal in a sense specified above.

From the above described procedure, we obtain a collection of system states, so that the eigenmode series for the approximation to the system dynamics can be constructed using the extended POD method. First we obtain optimal basis functions for our dynamical system, and then its lower dimensional approximation can be obtained by projecting the full system orthogonally onto the subspace spanned by the chosen basis functions. For the current problem, the phase transformation can take place at different temperatures, by either mechanical or thermal stimulations. There may be no phase transformation if the temperature is sufficiently high. In order to model the dynamics of the ferroelastic material correctly, the empirical eigenfunctions have to take into account the temperature influence. Following, [35] we choose a few (three) representative temperature values to demonstrate the analysis, in particular those for which the system has only martensite phase (low temperature $\theta_1$), metastable austenite and martensite phases (medium temperature $\theta_2$), or only austenite phase (high temperature $\theta_3$), respectively. We denote the collection of snapshots with initial temperatures $\theta_i$ as $\boldsymbol{U}_i$, $i = 1, 2, 3$. If one employs the POD method directly to all the overall snapshots $\boldsymbol{U} = [\boldsymbol{U}_1, \boldsymbol{U}_2, \boldsymbol{U}_3]$ by putting all snapshots together, the characteristics of different blocks will be mixed and dispersed with each other, and that is why we are using the extended POD method to construct the eigenmodes using the snapshots collected in all the blocks. Taking



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all the blocks of snapshots simultaneously into account, the extended POD analysis can be formally represented in the following matrix form:

$$\boldsymbol{U} = \boldsymbol{\phi}\boldsymbol{C}, \tag{23}$$

where

$$\boldsymbol{U} = [\boldsymbol{U}_1\, \boldsymbol{U}_2\, \boldsymbol{U}_3], \qquad \boldsymbol{\phi} = [\boldsymbol{\phi}_1\, \boldsymbol{\phi}_2\, \boldsymbol{\phi}_3] \tag{24}$$

is a collection of snapshots and eigenmodes from each block, while the coefficient matrix is given as follows: [5]

$$\boldsymbol{C} = \begin{bmatrix} \boldsymbol{C}_1 & \boldsymbol{\phi}_1^T\boldsymbol{U}_2 & \boldsymbol{\phi}_1^T\boldsymbol{U}_3 \\ 0 & \boldsymbol{C}_2 & \boldsymbol{\phi}_2^T\boldsymbol{U}_3 \\ 0 & 0 & \boldsymbol{C}_3 \end{bmatrix}, \tag{25}$$

where all the entries in the matrix can be obtained once the blocks of snapshots are provided. For those situations where more snapshot blocks are available, the extended POD can be carried out in a similar manner.

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.[2] 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.[8]

## 5. CONCLUSIONS

Following our recent works, we focused on the development of mesoscopic phase-field-type models for the description of strongly nonlinear coupled thermomechanical effects, such as shape memory effects and phase transformations, in low dimensional nanostructures. We provided details on the implementation of the model with a combination of the Chebyshev collocation method and the extended proper orthogonal decomposition. Several typical examples on the analysis of microstructure evolution in finite nanostructures have been presented. The discussion has been put in the context of other approaches, including those based Landau-Ginzburg-Devonshire theory.

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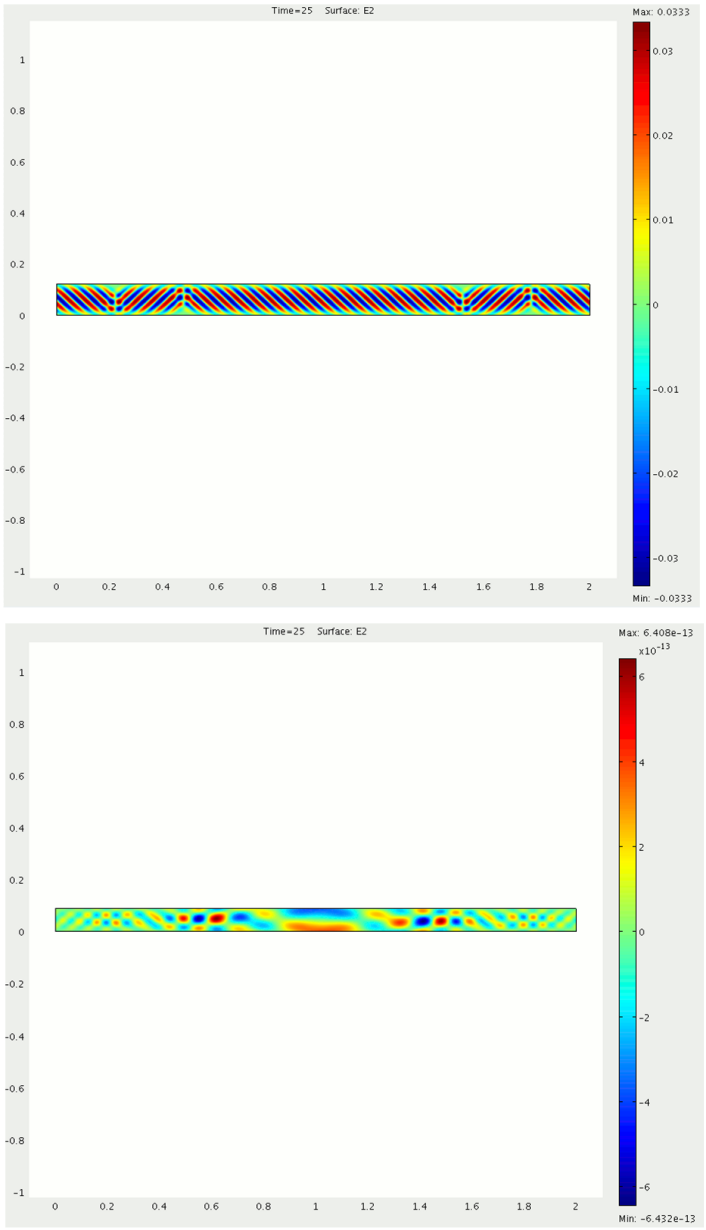


Figure 1. Size dependency of nanowires with increasing diameter-length ratio.


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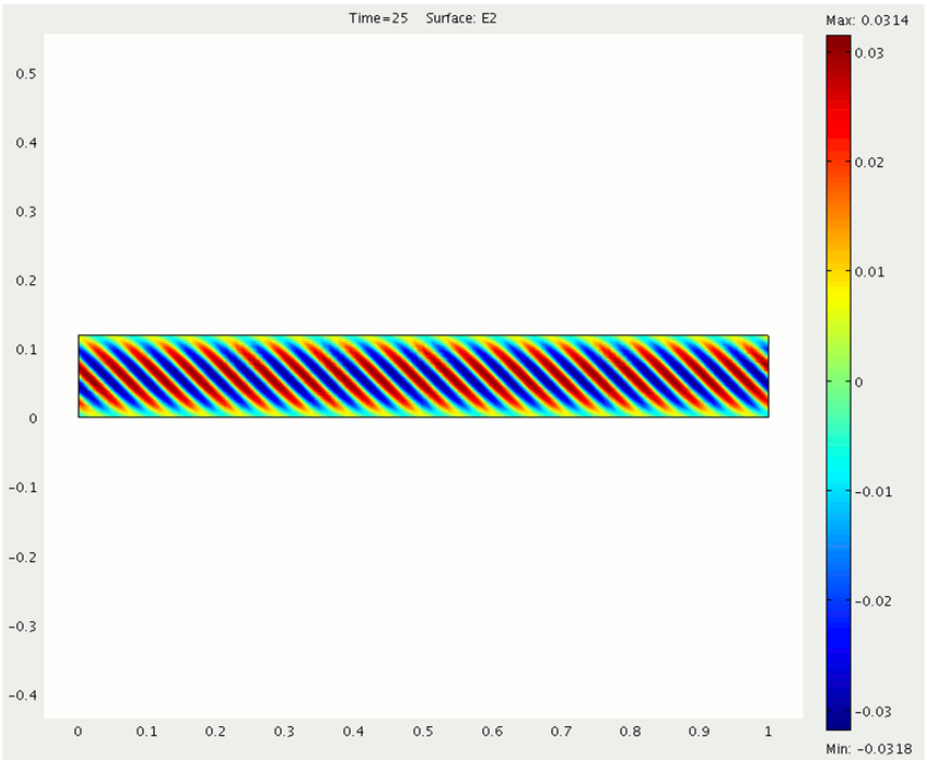


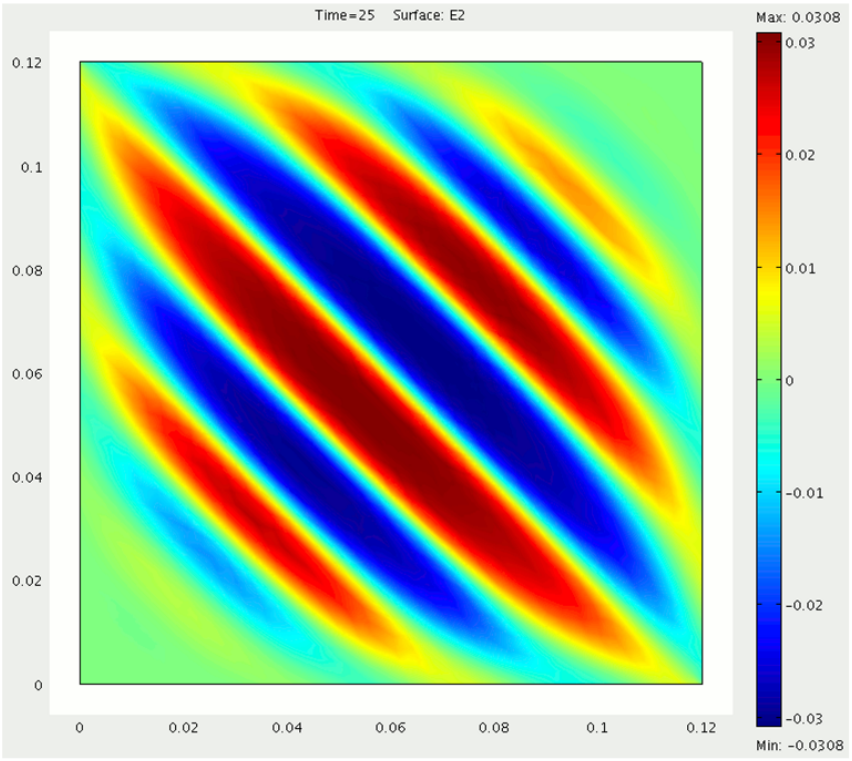


Figure 2. Microstructures in the nanowire of smaller length (left) and in the square nanoplate.



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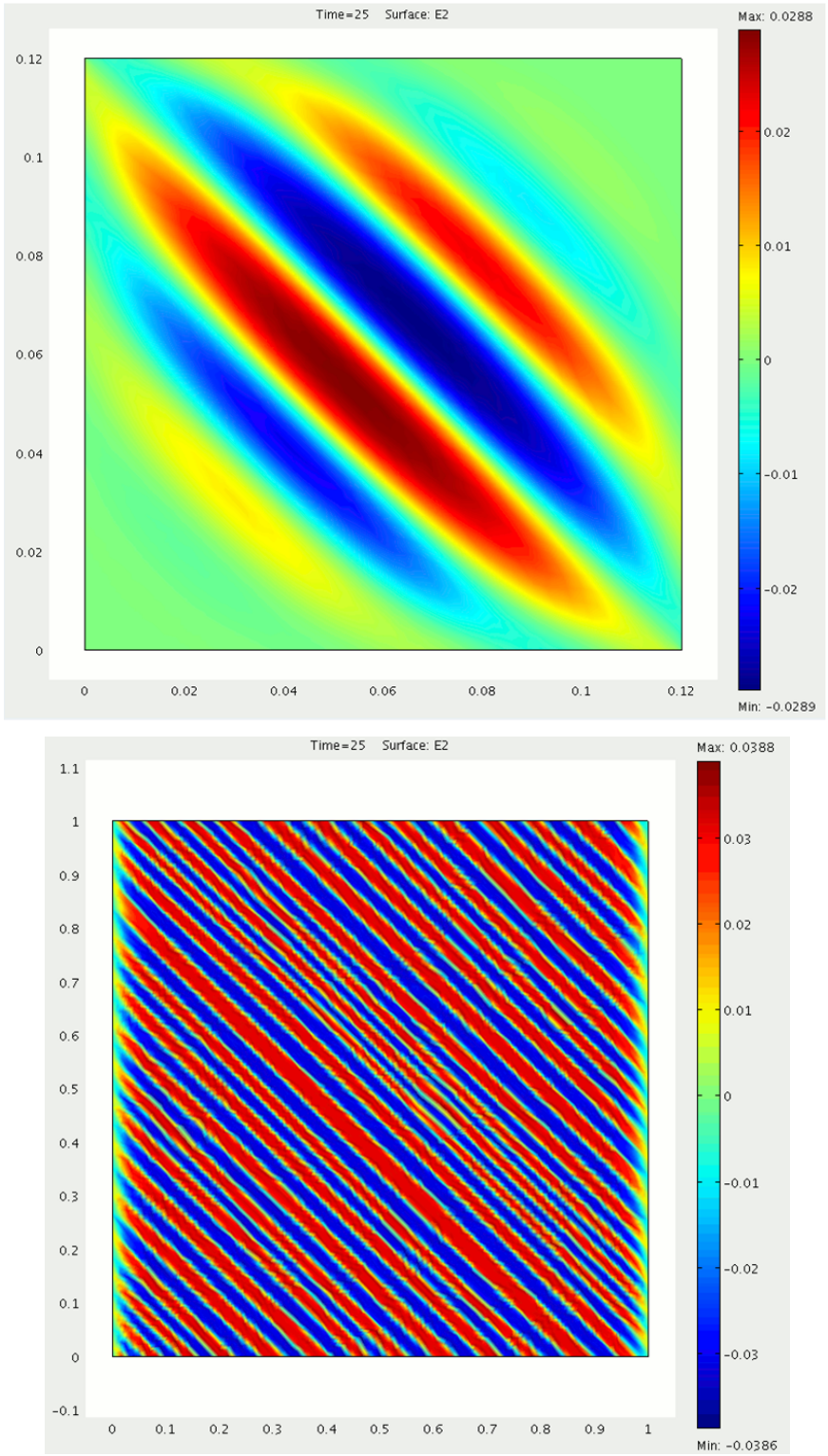


Figure 3. Evolution of microstructure in the square nanoplate.



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