DYNAMICS AND NONLINEAR CONTROL OF OSCILLATIONS IN A COMPLEX CRYSTALLINE LATTICE

E.L. Aero, B.R. Andrievsky, A.L. Fradkov, S.A. Vakulenko *

* *Institute for Problems of Mechanical Engineering of RAS,*
61 Bolshoy Ave. V.O., St.Petersburg, 199178, Russia
e-mails: aero@microm.ipme.ru; alf@control.ipme.ru

Abstract: A highly nonlinear system of acoustic and optical oscillations in a complex crystalline lattice consisting of two sublattices is analyzed. The system is obtained as a generalization of the linear Carman–Born–Kun Huang theory. Large displacements of atoms up to structure stability loss and restructuring are admitted. It is shown that the system has nontrivial solutions describing movements of fronts, emergence of periodic structures and defects. Strong interaction of acoustic and optical modes of oscillations for media without center of symmetry, energy exchange between modes and excitation of the optical mode by means of torque applied to the ends of the lattice (rod) are examined. Control algorithm based on speed-gradient method is proposed. Simulation results demonstrate that application of control may allow to eliminate or reduce influence of initial conditions

Keywords: Energy control, Speed gradient, Complex lattice, Nonlinear oscillations, Shock waves

1. INTRODUCTION

Properties of complex oscillatory systems such as atomic lattices are determined by interaction of large number of degrees of freedom. Studying such properties as structure and phase transitions, formation of defects, shock waves and others requires consideration of strongly nonlinear phenomena. Some nonlinear effects may arise spontaneously and can be studied based on free oscillations theory. However, purposeful changes of the crystal state demand for development of the methods of controlling its properties, particularly, control of its nonlinear oscillations.

In the first part of the paper (Secs. 2–4) appropriate models of complex crystalline lattice are developed and their nonlinear dynamics are analyzed. In the second part (Sec. 5) application of nonlinear control methods to analysis of complex crystalline lattice is made.

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2. MODELING INTERACTION OF ACOUSTIC AND OPTICAL MODES

In (Aero, 2002) the following system of equations describing interaction of acoustic and optical modes in a nonlinear continuum model of crystal without center of symmetry is proposed:

$$\rho \ddot{U}_i = c_{ikj} u_{k,j} + \lambda_{ikjm} U_{k,jm};$$
$$(.)_{k,j} \to \partial(.)_k/\partial x_j;\ (.)_{k,jn} \to \partial^2(.)_k/\partial x_j \partial x_n \quad (1)$$
$$\mu \ddot{u}_i = -\frac{\partial \Phi}{\partial u_i} - c_{kij} u_{k,j} + \kappa_{ikjm} u_{k,jm}. \quad (2)$$

Here $U_i(x_1, x_2, x_3, t)$, $u_i(x_1, x_2, x_3, t)$ are unknown functions describing components of displacements due to acoustic and optical modes in crystal, correspondingly. The vector $U_i(x_j, t)$ represents displacement of the center of inertia of each elementary cell (pair of atoms), while the vector $u_i(x_j, t)$ represents mutual displacement for pair of atoms within the elementary cell of relative displacement of sublattices. Hereafter the following standard notations are used: repeated indices assume summation, upper dot stands for the time derivative, spatial derivatives are denoted by means of comma in the indices as it is shown in (1). The coefficients c_{ijk}, $\bar{c}_{ijk}$, κ_{ikjm}, λ_{ikjm} are the components of the tensors describing elastic properties of the lattice. They possess a certain symmetry under permutation of indices, (Aero, 2002). The nonlinearities in the system are specified by the scalar energy function $\Phi(u_i)$, describing interaction of atoms in an elementary cell. It also reflects internal translational symmetry in a complex lattice – relative displacement of sublattices for a period or for an integer number of periods does not imply change of the complex lattice structure. In a more general case the function $\Phi(u_i)$ may be replaced by another vector periodic function of the argument u. Note that using approximation $\Phi \approx u_i u_i$, Eqs. (1), (2) are transformed into a continuum analog of the well known linear Carman–Born–Kun Huang model, (Born and Huang Kun, 1998). In the case of media with center of symmetry the second spatial derivatives appear instead of the first ones in both equations, see (Aero, 2002).

The system (1), (2) possesses the conservation law with the following energy integral:

$$E = \int_\Omega \Big(\frac{1}{2}\big(\rho \dot{U}_i \dot{U}_i + \mu \dot{u}_i \dot{u}_i + \lambda_{ikjm} U_{k,j} U_{i,m} + \kappa_{ikjm} u_{k,j} u_{i,m}\big) + c_{ikj} u_k U_{i,j} + \bar{c}_{ikj} u_k u_{i,j} + \Phi\Big) d^3x. \quad (3)$$

In the expression (3) the symmetries under permutation of indices for material tensors are taken into account.

The existence of a single integral of motion is not sufficient for describing general solutions behavior when $t \to \infty$. However, it becomes possible after introducing dissipative terms in Eqs. (1), (2) proportional to the first time derivatives. Since the system energy is bounded from below for small values of the coupling c between modes, it is possible to justify existence and uniqueness of the system solutions for all $t > 0$ and their convergence to the stationary solutions of Eqs. (1), (2).

3. EQUILIBRIUM SOLUTIONS OF THE ONE-MODE SYSTEM

It seems not possible to describe all the equilibrium solution in general case. At first only equilibrium solutions for the one-mode system (1), (2) will be considered. Such solutions are determined from the equations

$$c\phi_x + \lambda U_{xx} = 0, \quad -\Phi'(\phi) - cU_x + \kappa\phi_{xx} = 0. \quad (4)$$

The system will be studied on the interval $(0, l)$ with zero Dirichlet boundary conditions at the ends of the interval. Eliminating U by means of the first equation we obtain

$$\kappa\phi_{xx} = \Phi'(\phi) + A(\phi) - c^2\lambda^{-1}\phi, \quad \phi(0) = \phi(l) = 0, \quad (5)$$

where A is linear averaging operator

$$A = c^2 \lambda^{-1} l^{-1} \int_0^l \phi \, dx.$$

Below only the most interesting and physically natural case $\Phi' = -a \sin\phi$ with $a > 0$ will be studied. For $c = 0$ the problem (5) is well studied (Molotkov and Vakulenko, 1988). For every a it has a finite number of equilibria $N(a)$, depending on a. For small values of a only the trivial equilibrium exists. When a grows, new nontrivial equilibrium solutions emerge, bifurcating from the zero solution for some $a = a_n$. The first solution has the form of arch and does not have any roots. The second one has only one root, the third one has two roots, etc. For $a \in \big(a_n, a_{n+1}\big)$ there exist $2n + 1$ solutions: one trivial and $2n$ nontrivial ones of the form $\pm\phi_k(x)$, $k = 0, 1, \dots, n-1$, where every ϕ_k has exactly k zeros. According to the result of (Born and Huang Kun, 1998), all the nonzero equilibria are hyberbolic, i.e. the corresponding operator of the linearized system does not possess zero eigenvalue. The bifurcation values a_n are easy to calculate: for $l = \pi$ they are equal to n^2.

It is easy to show by means of standard perturbation theory that the above results concerning the number of solutions hold for small c. Obviously, the results do not hold for sufficiently large c, since the energy of the system is not bounded from below. It can be interpreted from physics point of view as an instability arising from interaction of optical and acoustic modes. The bifurcation points $a_n(c)$ can be easily calculated for small c. Assuming $\lambda = \pi$, $\kappa = 1$ without loss of generality, we obtain

$$a_n(c) = n^2 + c^2\lambda^{-1}\left(-1 + 2\Big(\frac{1-(-1)^n}{\pi n}\Big)^2\right)$$

Let us turn to analysis of the case $x \in \big(-\infty, \infty\big)$ and consider the existence problem for the travelling solutions of shock wave type.

4. SOME DYNAMIC PROBLEMS

Let us study some special solutions to the problem. Let only one component of u and only one component

(x or y) of U be distinct from zero and all the solutions depend on only one coordinate $x = x_1$ and on time t.

After adding dissipative terms containing first time derivatives Eqs. (1), (2) take the following form:

$$\rho\ddot{U} + \rho_1\dot{U} = cu_{,x} + \lambda U_{,xx},$$
$$u_{,x} = \partial u/\partial x,\ U_{,xx} = \partial^2 U/\partial x^2 \qquad (6)$$
$$\mu\ddot{u} + \mu_1\dot{u} = -a\sin u - cU_{,x} + \kappa u_{,xx}. \qquad (7)$$

If $\rho_1 = \mu_1 = 0$ then the system (6), (7) possesses the conservation law with the following energy integral:

$$E = \int_\Omega \Big(\frac{1}{2}(\rho\dot{U}^2 + \mu\dot{u}^2 + \lambda U_{,x}^2 + \kappa u_{,x}^2) + cUu_{,x} + a(1-\cos u)\Big) d^3x. \qquad (8)$$

If $c = 0$ then the system into to independent equations: the equation for optical mode turn into a nonlinear wave equation while dynamics of acoustical mode are described by a linear equation.

4.1 Shock waves as 1D kinks

Consider a kink-like solution of the system (6), (7) defined on the whole real axis: $x \in (-\infty, \infty)$. Such a solution (shock wave) according to (Maslov and Omelyanov, 1981), has two distinct limits u_+ and u_- for $x \to \infty$. It tends to its limits with an exponential rate. Such properties are typical for many nonlinear hyperbolic and parabolic equations, (Molotkov and Vakulenko, 1988). Besides, in the absence of the dissipative terms there is usually a whole family of kink solutions, depending on their propagation rate V. In the presence of dissipation for typical simple bistable (unlike periodic ones) nonlinearities the propagation rate V may take values only from some discrete set.

If $c\tilde{\varepsilon}$ is small, it is possible to construct asymptotic solutions describing perturbed solutions of such a type by means of a standard procedure, (Maslov and Omelyanov, 1981; Molotkov and Vakulenko, 1988). Let a solution be represented by the asymptotic series

$$\phi = \sigma^0(z) + \epsilon\sigma^1(z,\tau) + \ldots,\quad z = x - Vt - q(\tau), \qquad (9)$$
$$U = \epsilon U^0(z) + \epsilon^2 U^1(z,t) + \ldots,\quad \tau = \epsilon^2 t \qquad (10)$$

where the leading term $\sigma^0 = \sigma(x - Vt)$ is a kink solution of Eq. (7) with $\varepsilon = 0$, $q = 0$. The function U^0 is determined from the equation

$$(\rho V^2 - \lambda)U^0_{,zz} - V\rho_1 U^0_{,z} = \sigma^0_{,z}. \qquad (11)$$

It is easy to show that Eq. (11) has a bounded solution which time derivative exponentially decreases when $z \to \infty$ and has the following form

$$U^0_{,z}(z) = \exp(az)\int_{+\infty}^{z} \exp(-as)\sigma^0(s)\,ds. \qquad (12)$$

The kink coordinate is determined by a function $q(\tau)$, satisfying equation

$$\mu M\frac{d^2q}{d\tau^2} + \mu_1 M\frac{dq}{d\tau} = \int_{-\infty}^{\infty} U^0_{,z}\sigma^0_{,z}\,dz, \qquad (13)$$

where M is a "mass" of a kink which is equal to $\int_{-\infty}^{\infty} U^0_{,z}\sigma^0_{,z}\,dz$. In the beginning the kink moves with a varying speed depending on parameters ρ_1, ρ, λ, μ_1, V. In the limit $t \to \infty$ the speed of the kink approaches its steady-state value.

4.2 Free nonlinear oscillations

Consider the initial-boundary problem for Eqs. (6), (7) on the bounded interval $0 \le x \le h$ with the initial conditions

$$U(\chi,0) = U^0(\chi),\ \ u(\chi,0) = u^0(\chi),$$
$$\partial U/\partial\tau(\chi,0) = V(\chi), \qquad (14)$$
$$\partial u/\partial\tau(\chi,0) = \nu(\chi),\quad \chi = x/h, \qquad (15)$$

and the boundary conditions

$$(A_1U + B_1\partial U/\partial\chi)(0,t) = F_1(t),$$
$$(a_1U + b_1\partial u/\partial\chi)(0,t) = f_1(t),$$
$$(A_2U + B_2\partial U/\partial\chi)(0,t) = F_2(t),$$
$$(a_2U + b_2\partial u/\partial\chi)(0,t) = f_2(t), \qquad (16)$$

In Fig. 1 the numerical solution of the system (6), (7) is shown for the case when at the initial time $t = 0$ a triangular distribution of the acoustic displacements $U(\chi)$ (dashed line), zero optical displacements $u(\chi)$ (dashed line) and zero velocities of both variables. Zero values of both functions are also given in the ends of the interval $(0,1)$. In fact, in the initial time instant $t = 0$ the deformations ($2\varepsilon = U_{,x}$) are given that have opposite signs in the left and right parts (domains) of the interval. Sharp boundary between domains is interpreted as a defect. The evolution of the deformations for several values of the finite time $t = T_1$ is shown with solid lines.

Simulations demonstrate strong interaction of the oscillation modes. An inherent structure $u(\chi)$ emerges in the form of two domains of opposite signs (bold solid line). It means appearance of the two phases with different values of the order parameter $+u$ and $-u$.

A strong dependence of the system motion on initial conditions and, certainly, on the coefficients of the equations is observed. To eliminate dependence on initial conditions an approach of control theory is applied in the next section.

5. CONTROL OF NONLINEAR OSCILLATIONS

Application of the control methods allows to eliminate dependence of solutions on initial conditions.

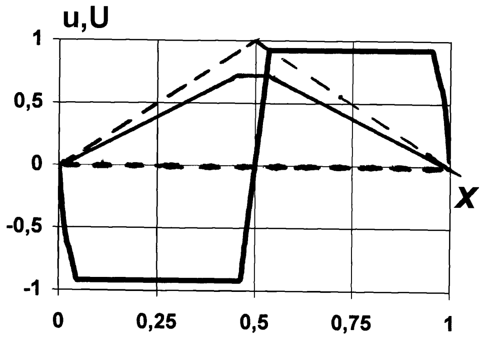

Fig. 1. Free evolution of optical and acoustic modes.

Besides, it allows to create purposeful energy exchange between modes leading to the rebuilding of the lattice structure and to phase transitions. The control goal may correspond to either excitation or to suppression of specific oscillation modes. Let us study the possibility of the optical mode excitation by means of changing the torque applied to the ends of the rod (undimensional lattice) according to a feedback mechanism. To design appropriate feedback the speed-gradient method, (Fradkov, 1979; Fradkov and Pogromsky, 1998) will be employed.

5.1 Speed-gradient method

A number of feedback design methods are based on reduction of the current value of some goal (objective) function $Q\big(x(t),t\big)$. The current value $Q\big(x(t),t\big)$ may reflect the distance between the current state $x(t)$ and the current point of the goal trajectory $x_*(t)$, such as $Q(x,t) = \big|x - x_*(t)\big|^2$, or the distance between the current state and the goal surface $h(x) = 0$, such as $Q(x) = \big|h(x)\big|^2$, or the value of some characteristic of the system dynamics that is desirable to diminish. For continuous-time systems the value $Q(x)$ does not depend directly on control u and decreasing the value of the speed $\dot{Q}(x) = \partial Q/\partial x F(x,u)$ can be posed as immediate control goal instead of decreasing $Q(x)$. This is the basic idea of the speed-gradient (SG) method, proposed by Fradkov (1979), where a change in the control u occurs along the gradient in u of the speed $\dot{Q}(x)$. The general SG algorithm has the form

$$u = -\Psi\big(\nabla_u \dot{Q}(x,u)\big) \tag{17}$$

where $\Psi(z)$ is vector-function forming acute angle with its argument z. For affine controlled systems $\dot{x} = f(x) + g(x)u$ algorithm (17) is simplified to:

$$u = -\Psi\big(g(x)^T \nabla Q(x)\big) \tag{18}$$

Special cases of (17) are the proportional SG-algorithm

$$u = -\Gamma \nabla_u \dot{Q}(x,u), \tag{19}$$

where Γ is a positive-definite matrix, and the relay SG-algorithm

$$u = -\Gamma \operatorname{sign}\Big(\nabla_u \dot{Q}(x,u)\Big). \tag{20}$$

Another version of the SG-algorithm is its differential form

$$u = -\Gamma \nabla_u \dot{Q}(x,u). \tag{21}$$

Justification of the SG-method is based on a Lyapunov function V decreasing along trajectories of the closed-loop system. The Lyapunov function is constructed from the goal function: $V(x) = Q(x)$ for finite form algorithms and $V(x,u) = Q(x) + 0.5(u - u_*)^T\Gamma^{-1}(u - u_*)$ for differential form algorithm (21), where u_* is the desired (ideal) value of the control vector.

5.2 Control law design

Suppose that the bending torque applied to the ends of the rod is considered as the control action. It is assumed that the torque applied to the left end is balanced by the torque applied to the right end, i.e. compression force is identically zero. Then the boundary conditions 16 read $F_1 = F_2 = 0$, $f_1(t) = -f_2(t) = f$, where f is the control variable. Let the control goal be formulated as increase of the optical mode energy E. According to the speed-gradient method the goal function Q should be introduced such that achievement of the control goal corresponds to maximization of the goal function. In this case the kinetic component K of the energy can be chosen as the goal function, i.e $Q = K$, where

$$K = (hs/2)\sum_{i=1}^{n} \dot{u}_i^2. \tag{22}$$

According to the speed-gradient method, the asymptotic maximization of the functional (22) can be achieved by choice of the controlling action which sign coincides with the sign of the speed-gradient (gradient of the speed of changing Q along the solutions of the system)

$$f = -R\Big(\nabla f \dot{Q}(x,f)\Big) \tag{23}$$

where x is the state vector (function) of the controlled system (6), (7), f is the vector of controlling variables, R is a vector-function forming an acute angle with its argument, e.g. multiplying by a positive factor or taking sign of each component of the vector argument.

For the sake of simplicity the problem is discretized by means of replacing the first and second derivatives in the system equations (6), (7) and in the expression for the energy (3) by their finite differences as follows: $(u_{i+1}-u_i)/h$; $(u_{i+1}-u_i)/T$; $(u_{i+1}-2u_i+u_{i-1})/h^2$; $(u_{i+1} - 2u_i + u_{i-1})/T^2$.

Direct calculation yields the following form of the speed-gradient function:

$$\psi = \big(1/h\big)\big(\dot{u}_1/a_1 - \dot{u}_n/a_n\big) \tag{24}$$

Therefore the control algorithm for excitation of the optical mode may have e.g. the "relay" form

$$f = \gamma \operatorname{sign}\big(\dot{u_1}/a_1 - \dot{u}_n/a_n\big) \tag{25}$$

Numerical results are obtained for the oscillations excitation in the discrete version of the system consisting of $n = 50$ atoms. The following constants in the equations are chosen: $\rho = 0.9$, $\rho_1 = 0$, $\mu = 2.5$, $\mu_1 = 1$, $c = 5$, $a = 1.5$, $\lambda = \kappa = 1$, $A_1 = A_2 = 1$, $a_1 = a_2 = 1$, $B_1 = B_2 = b_1 = b_2 = 0$.

The control algorithm $f = 0.5\,\mathrm{sign}\left(\dot{u}_1/a_1 - \dot{u}_n/a_2\right)$ is used. In Fig. 2 the shapes of the acoustic mode $U(\chi)$ and the optical mode $u(\chi)$ are shown for time $t = 15$. In the initial time $t = 0$ both functions are equal to zero. The evolution of the energy of the modes is shown in Fig. 3. It is seen that the effect of control leads to a strong excitation of the optical mode.

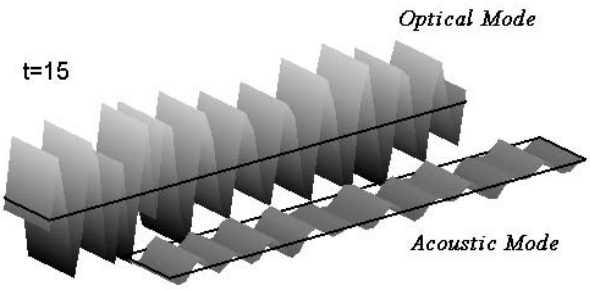

Fig. 2. Controlled excitation of optical mode.

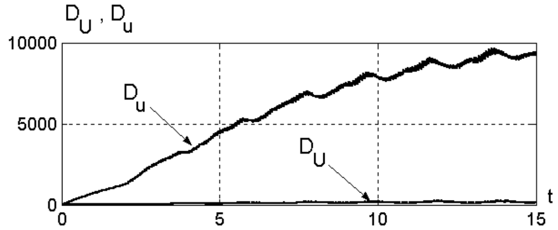

Fig. 3. Evolution of energy of the modes in the controlled system.

An important question in crystalline lattices dynamics is sencitivity to changes of initial conditions. A number of simulations have been performed to examine dependence of limit energy of modes on the initial conditions. Figure 4 shows the results for two different triangular functions $U(\chi)$ like in Fig. 1. At the initial time $t = 0$ zero optical displacements $u(\chi)$, $U(\chi)|_{\chi=0.5} = 1$ (line *a*) and $U(\chi)|_{\chi=0.5} = 10$ (line *b*) are taken. Initial velocities of both variables are zeroized. It is seen that changes of initial displacement in order of magnitude leads in $3 \div 5\%$ changes of limit energy of each mode.

6. NONFEEDBACK CONTROL

For study of microscopic systems the problem of physical realization of control arises. The main difficulty is to implement the feedback exploiting measurements of microscopic phase variables deflections. To solve an analogous problem in the area of molecular and quantum control (Brown and Kocarev, 2000;

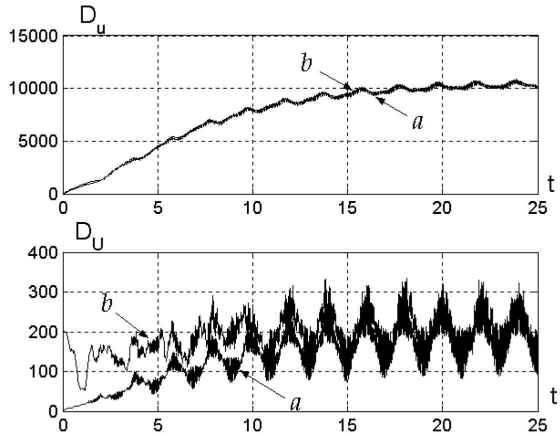

Fig. 4. Dependence of energy of the modes on the initial conditions in the controlled system.

Laser control, 2001; Fradkov, 2003) the idea of using program (feedforward, nonfeedback) control was proposed. In our case the idea is to first calculate controlling action $f(t)$ as a function of time during simulation of the system with feedback algorithm (25). Then the precalculated function $f(t)$ is applied to the physical system during experiment. At the second stage neither measurements nor feedback is used.

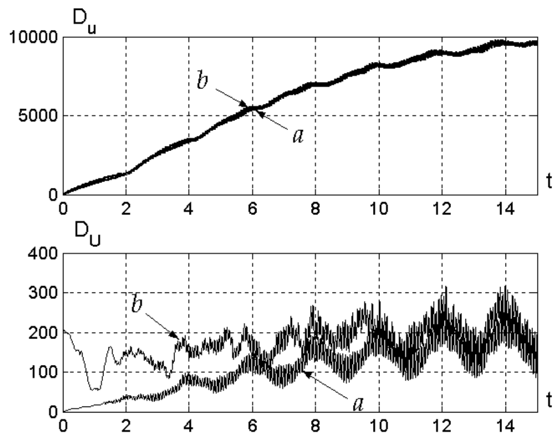

Fig. 5. Dependence of energy of the modes on the initial conditions in the nonfeedback system.

To analyse efficiency of such an approach the simulation of the system with nonfeedback control action was performed. The results are shown in Fig. 5. Initial conditions were chosen same as for feedback control, both for calculation of program control $f(t)$ and for its testing. It is seen that nonfeedback control designed using the proposed method the result is quantitatively the same as with feedback algorithm (25) (cf. Fig. 4).

7. CONCLUSIONS

A new nonlinear dynamical theory of crystalline bodies has been proposed describing movements of fronts, emergence of periodic structures and defects, energy exchange between modes. It also allows to describe other complex phenomena such as cardinal rebuilding of the body structure, including phase transitions of martencite type and others. The role of the order parameter is played by the inherent displacement $u(x, y, z)$ depending on coordinates.

An important result of the paper is demonstration of the possibility of purposeful excitation of the optical mode by means of torque applied to the ends of the lattice (rod) in a broad range of initial conditions on the steady-state oscillations. It means that application of control may allow to eliminate or reduce influence of initial conditions.

Another conclusion is based on the well-known fact that static strains (deformations) influence phase state of smart materials. It implies that application of control of energy exchange between macroscopic deformation and microscopic degrees of freedom may allow to control dynamics of phase transitions and, particularly, effect of the memory shape which is characteristic for smart materials.

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