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shape memory alloys**

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Fracture and Delamination of Oxide: Fracture and delamination of $1\mu\text{m}$ ($1 \times 10^{-6}\text{ m}$)
 SiO_2 on Si with $1\mu\text{m}$ conical probe tip. Courtesy of Hysitron Inc., Minneapolis, Minnesota, USA

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DIFFUSION KINETICS AND MULTIVARIANT PHASE TRANSFORMATION IN SHAPE MEMORY ALLOYS

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We develop a general modeling framework to analyze the dynamics of multivariant phase transformation in three-dimensional samples of shape memory materials. The model is based on a systematic representation of the Gibbs free energy in stress, temperature and n -dimensional order parameter space. Here n indicates the number of martensitic variants (M). Landau theory has earlier been successfully applied to solve the problem of phase-field evolution in phase transforming solids (see e.g. the works by Artemev *et al.*[1] and Ichitsubo *et al.* [2] and the references therein). In the context of diffusion-less transformation in solid described by the Landau theory of first-order kinetics, the order parameters are the scaled ensemble average of the atomic order variables [3]. The diffusion kinetics based on the time-dependent Ginzburg-Landau equation is thus the homogenized form of the spatio-temporal fluctuation due to atomic reordering. Our main objective in this paper is to study how this diffusion kinetics influences the stress-temperature induced dynamics of phase transformation in microscopic and larger length-scale without attempting to solve a molecular dynamic problem in a coupled manner. Toward this direction we finally arrive at the thermodynamic conservation law whose characteristics is controlled by the phase kinetics.

As a starting point we first address the problem of 3D free energy representation in context of n -variant martensitic transformation. Our free energy model [4] follows the steps similar to those obtained in the works of Levitas and Preston [5,6] to arrive at the invariance and uniqueness properties of the free energy. Also the number of order parameters can be reduced with the help of the symmetry properties across the transformation surfaces. In addition to this we relax some of the conditions involving many unknown material constants, which finally leads to a precise description of austenite-martensite transformation energy barrier and variant-variant interaction energy. In our approach the previously observed non-physical minima of the free energy wells are eliminated. We perform detailed analysis of the proposed free energy model in context of austenite-martensite ($A-M_k$) transformation and variant-variant (M_i-M_j) transformation with sharp interfaces. A link between the evolution of texture using this approach and the classical condition for microstructural compatibility within the framework of continuum deformation theory [7] is discussed. Analytical characterization is then carried out on the existence of diffused interfaces under quasi-static stress-temperature conditions by considering time-independent Ginzburg-Launday equation. Results are compared with those reported by Levitas *et al.* [8] in context of critical nuclei formation in NiAl. Next we turn our attention to the interplay between the diffused states of the variants and the nonlinear thermoelasticity. Relationship between the physical time scale of the atomic reordering process and the time scale at which the parabolicity of the thermodynamic conservation is influenced and completely switched to elliptic problem is analyzed. Numerical simulations on the evolution of microstructure are reported. Method of introducing dislocation mechanism within the present framework will be discussed.

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DIFFUSION KINETICS AND MULTIVARIANT PHASE TRANSFORMATION IN SHAPE MEMORY ALLOYS

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Abstract

In this paper we report a reconstructive approach to modelling the kinetics of martensitic phase transformations in shape memory alloys. A molecular dynamic view of the martensitic phase transition is employed to model the kinetics in a Landau-Ginzburg type microscopic model for finite stress-temperature calculation. A critical analysis on the stability of the numerical model is given. The effect lattice defects and dislocations at the domain walls are considered phenomenologically. Numerical results indicate the possibility of characterizing the model parameters for mechanical fatigue loading under constant temperature.

1. Introduction

Shape Memory Alloys (SMAs) have various applications in transducer devices and in control of dynamical systems. Understanding the effects of dislocations and fatigue on the SMA structural performance becomes essential and such aspects have remained an unexplored area of research till date. It may be noted from a vast literature on SMA modeling that given the availability of numerous phenomenological models, design and analysis involving new SMA structures are found to be extremely difficult task. These phenomenological models vary drastically depending on the number of material constants, conditions at which experiments are done, the effective dimensions and size of the sample, the nature of thermo-mechanical loading and so on. Detailed mathematical understanding of the origin of the SMA microstructure under deformation has been developed over past few decades (see e.g. [1-7]), and computational challenges encountered while applying related theories have been reviewed recently in [8]. However, not much development has taken place till date in which the three-dimensional and the time-dependent dynamics of the real-scale SMA devices could be studied by linking the above theoretical framework to practical engineering applications. The main difficulties encountered to achieve this are mainly numerical and they are in the underlying interdependence of following two aspects: (1) the sequence of energy minimization, at the end of which the global minimum is actually *not attained*, the discrete version of this process is based on *quasi-convexification* of the original non-convex minimization problem, (2) the conditions required to match the spatial discretization with the evolved interfaces dynamically, meaning an efficient implementation of a mesh adaptation scheme within the variational framework (e.g. adaptive finite elements).

While most of the reported mathematical models and their computational treatment for studying the martensitic phase transition in SMAs rely on the various regularizing procedure and the subsequent numerical stabilization procedure of their discrete version, in many situations it is not well understood why certain microstructures are formed and how the related thermodynamic properties can be characterized by practical means. It can be argued that certain information regarding the physics of the problem becomes important but it is not present in the model. Most of the available phenomenological models fall in the above category and they are applicable at macroscopic and mesoscopic scales. A macroscopic model requires the description of the 3D geometry and variational minimization of an appropriate potential involving the thermoelastic energy and the energy due to dynamic self-accommodation of the martensitic variants. Whereas a mesoscopic model, such as the Falk-Kanopka free energy model [9], requires the description of the free energy as a function of the strain invariants of a single crystal and its point group symmetry. The strain field in such model is beyond the resolution of the Bain strain. A more detailed description of the martensitic phase transition requires a microscopic model, such as the model by Levitas and Preston [10], where the invariance of the free energy with respect to the crystallographic point group symmetry is preserved but the discontinuous nature of the deformation across the individual habit planes is introduced. Such information is essential to describe the microstructural evolution. A model similar to those reported in [10-11] and with additional consistency condition on partitioning the chemical energy and the transformation energy in stress-space has been developed by the authors [12]. However, characterization of various thermodynamic quantities in the above microscopic models still requires certain information regarding the transformation path in the sense of statistical average of the atomistic ensemble and ground state quantum-mechanical properties. For such characterization it is important to analyze the atomistic models based on thermal fluctuation [51] and molecular dynamics [52]. In the present paper we analyze the atomistic influence in terms of the Bain transformation path on a Landau-Ginzburg model for finite stress-temperature calculations and evolution of microstructure. The framework thus also couples the necessary features of first-order phase-field models applicable to SMAs (see e.g. [13-15]) with the continuum theory of nonlinear elasticity.

2. A Landau-Ginzburg model of martensitic phase transformation

We approximate the free energy density in the Landau theoretic framework. In such a framework we see a polynomial structure in such a way that the stability of the austenitic phase (A) and j th martensitic variants (M_j), non-minimum diffusion barrier and nucleation can be described in stress-temperature space. The details are given in [12,16]. While extending this approach to multivariant case, several complexities arise because of the inherent nonlinear interplay of the variant-wise contribution. The Gibbs free energy density for N -variant transformation is expressed as

$$\begin{aligned}
G(\sigma, \theta, \eta) = & -\frac{1}{2} \sigma^T \left[\lambda_0 + \sum_{k=1}^N (\lambda_k - \lambda_0) \phi(\eta_k) \right] \sigma - \sigma^T \sum_{k=1}^N \epsilon_{ik} \phi(\eta_k) \\
& - \sigma^T \left[\epsilon_{\theta 0} + \sum_{k=1}^N (\epsilon_{\theta k} - \epsilon_{\theta 0}) \phi(\eta_k) \right] + \sum_{k=1}^N f(\theta, \eta_k) + \sum_{i=1}^{N-1} \sum_{j=i+1}^N \bar{F}_{ij}(\eta_i, \eta_j)
\end{aligned}
\tag{6}$$

where λ is the second-order forth-rank compliance tensor (λ_0 is for A phase), $\epsilon_{\theta k} = \alpha_k(\theta - \theta_e)$, α_0 and α_k are thermal expansion tensor in the A and M_k phase respectively. The fourth term in Eq. (6) represents the chemical part of the free energy including the entropy jumps due to strain and volume fluctuations. $\bar{F}_{ij}(\eta_i, \eta_j)$ is an interaction potential required to preserve the frame-invariance of G with respect to the point group of symmetry and uniqueness of the multivariant PT at a given material point. The description of phase transition is generalized with three sets of ordered states: $\bar{0} = \{0, \dots, \eta_k = 0, \dots, 0\}$, $\bar{1} = \{0, \dots, \eta_k, \dots, 0\}$ and $\bar{\eta}_k = \{0, \dots, \eta_k, \dots, 0\}$. The extremum property of the free energy density requires

$$\frac{\partial G}{\partial \eta_k} = G_0 \eta_k (\eta_k - 1) (\eta_k - \eta_{bk}) = 0, \quad \eta_k = \bar{0}, \bar{1}
\tag{7}$$

$$\frac{\partial^2 G}{\partial \eta_k^2} \leq 0, \quad \eta_k = \bar{0} \quad (A \rightarrow M_k)
\tag{8}$$

$$\frac{\partial^2 G}{\partial \eta_k^2} \leq 0, \quad \eta_k = \bar{1} \quad (M_k \rightarrow A)
\tag{9}$$

The nondimensional transformation barrier across the 0-k surface is given by

$$\eta_{bk} = -6\sigma^T \epsilon_{ik} - \frac{1}{2} \sigma^T (\lambda_k - \lambda_0) \sigma - 6\sigma^T (\epsilon_{\theta k} - \epsilon_{\theta 0}) + 6\Delta G^\theta + G_0/2
\tag{11}$$

The modelling framework discussed so far (see [12,16] for details) describes the phase transformation in terms of the microscopic order parameters ($\eta_k, k=1, \dots, N$). The physical implication is that the statistical ensemble of the order variables (the atomic coordinates and volume of the lattice) is expressed in a spatially homogenized sense where their correlation in the atomistic length scale is approximated by ensemble average. The transformation kinetics can be written in the form of Landau-Ginzburg equation, where the coefficients in the first-order system are related to the ensemble aggregate of the atomistic reordering along the Bain transformation path. Most interestingly, this kinetics plays the main role in controlling the coupling between the microscopic thermodynamic conservation law and the macroscopic momentum balance. In our study, we have analyzed the governing system of partial differential equations (PDEs) obtained from the present model, and these PDEs dynamically switch their characteristics at the onset of transformation spanned over a significantly smaller time-scale

compared to the time scale of the SMA device dynamics. It poses one of the most challenging problems in computational mathematics. It has been suggested in [8] that one way to avoid the inherent oscillation in the computational version of the energy minimization problem is to relax the error-estimates. In our study, the additional difficulty is the fast time scale at which the transformation occurs.

We first write the governing system of partial differential equations as follows. The transformation kinetics is represented by the Landau-Ginzburg equation

$$\frac{\partial \eta_k}{\partial t} = - \sum_{k=1}^N L_{kp} \left[\frac{\partial G}{\partial \eta_p} + \beta_p \nabla \nabla \eta_p \right] + \theta_k \quad (17)$$

where L_{kp} are positive definite kinetic coefficients, β_p are positive definite second rank. The spatial gradient term represents the energy due to nucleating interface. θ_k is the thermal fluctuation satisfying the dissipation-fluctuation theorem. While Eq.(17) governs the evolution process, the macroscopic energy conservation law is governed by the heat conduction equation and the momentum balance equation and they are nonlinearly coupled. A detailed formulation of the resulting initial boundary value problem can be found in [16].

3. Atomistic scale influence on the microscopic model parameters

The kinetics in Eq. (17) is a general description of the first-order kinetics. Therefore it is essential to analyze various properties of this equation. For such analysis, let us consider the molecular dynamic model in [17] which accounts for both the atomic coordinate as well as the volume fluctuation of the lattice. The Hamiltonian of the ensemble can be expressed as

$$H = \frac{1}{V} \int_V \left[\frac{1}{2} \sum_i m_i \dot{s}_i^T (h^T h) \dot{s}_i + \frac{1}{2} m' Tr(h^T h) + \Phi(r_{ij}) + p \det(h) \right] dV \quad (20)$$

where $r_i = \mathbf{h} \mathbf{s}_i$ denotes the position vector of the i th atom in the ensemble with \mathbf{s} as the atomic coordinate with respect to the lattice and the three components of the lattice vector in the columns of \mathbf{h} . In Eq. (20), the first two terms represent the momentum, the third term represents the potential involving the electron density and the core-core repulsion, and the last term represents the work done due to pressure. The equations of motion of the atom are given by

$$\ddot{s}_i = - \sum_{j \neq i} m_i^{-1} \frac{1}{r_{ij}} \frac{d\Phi(r_{ij})}{dr_{ij}} (s_i - s_j) - (h^T h)^{-1} \left[\frac{d}{d\tau} (h^T h) \right] s_i \quad (21)$$

$$\ddot{h} = m'^{-1} (\sigma - p) \det(h) (h^T)^{-1} \quad (22)$$

where τ denotes the time in the atomistic scale. Integrating Eq. (21) over the characteristic time T_0 and with the help of Eq. (22) in (21), we obtain the kinetics equation in (17) without the surface energy term. It is seen that

$$L \approx \tau_0 \sum_{i \neq j} \frac{1}{m_i r_{ij}^2} (s_{0i} - s_{0j}) \quad (23)$$

where s_0 represents the coordinate of the atom in the parent phase. The vector of the order parameter η in the present model is given by

$$\dot{\eta} = \left\langle \frac{1}{\tau_0} \int_{\tau}^{\tau + \tau_0} \dot{s}_i d\tau \right\rangle$$

(24)

Further, we make the following observations: (1) the form of the Gibbs free energy in Eq. (6) arises from the various terms in Eq. (21) and (2) the kinetics in Eq. (17) is essentially the microscopic representation of the Bain transformation path in the correlation length scales of the strain fluctuation and the volume fluctuation and the entropy jumps in the non-equilibrium thermodynamics are due to both of these fluctuations [18].

4. Effect of loading rates on the kinetics

In order to develop numerical integration scheme for the present type of non-smooth boundary value problem one requires a variational statement and stable numerical integration scheme. Here we report several numerical results describing the kinetics in one-dimension and study the effects of strain rate and force due to nucleation at the domain wall on the stress-strain curve.

In experimental studies of SMAs, one often sees additional inelastic effects under fatigue loading [19]. Such effects are attributed to lattice defect, dislocation and slips at the grain boundaries. Noting the term $\partial \Phi / \partial r_{ij}$ Eq. (21), it follows that the growth of lattice defect and dislocation at the domain wall alters the electron densities with time scale same as that of the loading cycle. Assuming that such details are not included in the atomic potential, as is in the experimental situation, we modify the free energy scaling parameter G_0 in Eq. (7) as

$$G_0 = \frac{1}{2} \tilde{G}_0 \left(1 + c_1 e^{-c_2 n_f} \right) \quad (25)$$

where n_f if the number of fatigue cycles, c_1 and c_2 are constants which can be estimated from the changes in strain-train hysteresis curves. The one-dimensional kinetics is given by

$$\dot{\eta} + L_{11} \beta_1 \frac{\partial^2 \eta}{\partial x^2} + L_{11} G_0 \eta (\eta - 1) (\eta - \eta_b) = 0 \quad (26)$$

For simplicity of the analysis here we drop the spatial derivative and include its effect in the stress in case of nucleation at the domain wall, i.e.

$$\sigma_{xx} \leftarrow \left(\sigma_{xx} + \beta_1 \frac{\partial \eta}{\partial x} \right) \approx \left(\sigma_{xx} + \beta_1 \tau_0 \frac{\dot{\eta}}{l_c} \sqrt{\frac{\theta}{\theta_{cr}}} \right) \quad (27)$$

where l_c is the correlation length for volume fluctuation. For a chosen time stepping $t^{i+1} - t^i = \Delta t \gg \tau_0$, we have the following cubic polynomial in η^{i+1} :

$$(L_{11} G_0 \Delta t)(\eta^{i+1})^3 - [L_{11} G_0 \Delta t (1 + \eta_b(\sigma_{xx}^i))] (\eta^{i+1})^2 + (L_{11} G_0 \Delta t \eta_b(\sigma_{xx}^i) + 1) (\eta^{i+1}) - \eta^i = 0$$

which accounts for the branching of the transformation path. Extending the above procedure to the multivariant situation in higher dimensions, evolution of the phases can be tracked following the transformation path that satisfies Eqs. (8)-(9).

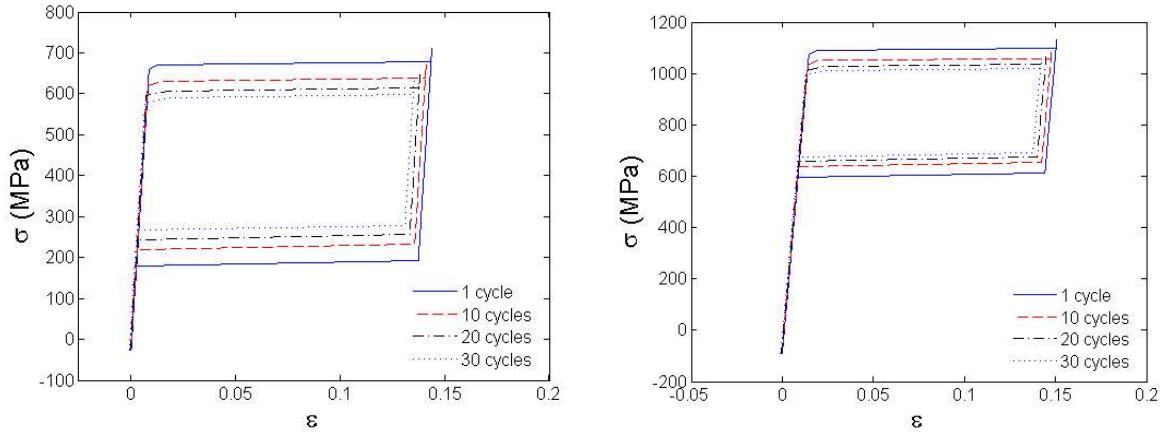


Fig. 1. Changes in the stress-strain curve over the number of fatigue cycles at constant temperature (a) $\theta = 320\text{ K}$ (b) $\theta = 360\text{ K}$.

Based on the one-dimensional analysis of the kinetics discussed above the strain controlled numerical tests are performed. The effects of fatigue cycles on the hysteresis under constant temperature are shown in Figs. 1(a) and (b). Material properties of Ni-Al are used. The simulations resemble those observed in tests under fatigue loading.

In the above two examples the effect of nucleating interface is neglected, i.e. $\beta_1 = 0$. Fig. 2 shows the effect of stress due to nucleating surface. The present analysis indicates that the effect of the terms $L_{11} \Delta t$ for given values of characteristic time τ_0 and correlation length l_c is significant. It may be noted from Eq. (23) that L_{11} is again dependent on the number of atoms undergoing reordering and hence a function of the correlation length.

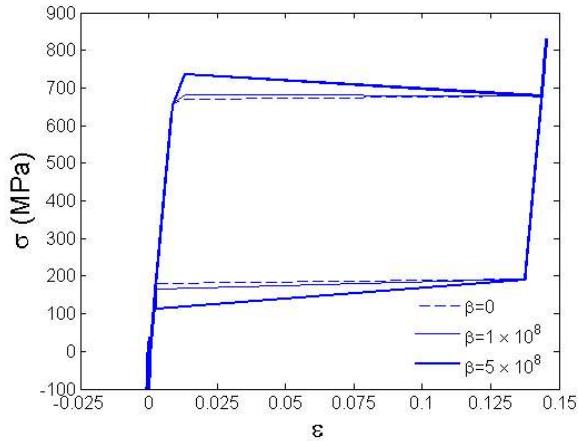


Fig. 2. Changes in the stress-strain curve for various nucleation stiffness factor $\beta = \beta_1$ at constant temperature $\theta = 320 K$.

5. Conclusions

The analysis presented in this paper establishes a reconstructive approach to deal with the dynamics of martensitic phase transitions for practical computation. A phenomenological description of lattice defects and dislocations at the domain walls is employed and numerical results demonstrate one the possibility of characterizing the model properties under mechanical fatigue loadings. By extending the present one-dimensional analysis to higher dimensions for the branches of the transformation paths, an accurate and stable numerical scheme for microstructure evolution can be designed.

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Editor's Preface

This volume contains two-page abstracts of the 698 papers presented at the "16th European Conference of Fracture," (ECF16) held in Alexandroupolis, Greece, July 3-7, 2006. The accompanying CD attached at the back cover of the book contains the full length papers.

The abstracts of the fifteen plenary lectures are included in the beginning of the book. The remaining 683 abstracts are arranged in 25 tracks and 35 special symposia/sessions with 303 and 380 abstracts, respectively. The papers of the tracks have been contributed from open call, while the papers of the symposia/sessions have been solicited by the respective organizers. Both tracks and symposia/sessions fall into two categories, namely, fracture of nanomaterials and structures and engineering materials and structures with 88 and 595 papers, respectively.

Started in 1976, the European Conference of Fracture (ECF) takes place every two years in a European country. Its scope is to promote world-wide cooperation among scientists and engineers concerned with fracture and fatigue of solids. ECF16 was under the auspices of the European Structural Integrity Society (ESIS) and was sponsored by the American Society of Testing and Materials, the British Society for Stain Measurement, the Society of Experimental Mechanics, the Italian Society for Experimental Mechanics, and the Japanese Society of Mechanical Engineers. ECF16 focused in all aspects of structural integrity with the objective of improving the safety and performance of engineering structures, components, systems and their associated materials. Emphasis was given to the failure of nanostructured materials and nanostructures and micro and nanoelectromechanical systems (MEMS and NEMS). The technical program of ECF16 was the product of hard work and devotion of more than 150 world leading experts to whom I am greatly indebted. The success of ECF16 relied solely on the dedication and titanic work of the members of the Scientific Advisory Board, the pillars of ECF16. As chairman of ECF16 I am honored to have them on the Board and have worked closely with them for a successful conference.

Fracture mechanics analysis has been successful for many years in the prevention of failures of engineering materials and structures. It is based on the realistic assumption that all materials contain crack-like defects from which failure initiates. New technological developments, however, raise new challenges for fracture mechanics research and development. Quasi-brittle materials including concrete, cement pastes, rock, soil, etc. are being extensively used in engineering applications. Layered materials and especially thin film/substrate systems are becoming important in small volume systems used in micro and nanoelectromechanical systems (MEMS and NEMS). Nanostructured materials are being introduced in our every day life. In all these problems fracture mechanics plays a major role for the prediction of failure and safe design of materials and structures. Failure of materials and structures at the micro and nano scale levels are adequately addressed at ECF16 with 93 papers referred to in this area.

More than nine hundred participants attended ECF16, while more than eight hundred fifty papers were presented, far more than any other ECF over a thirty year period. The participants of ECF16 came from 49 countries. Roughly speaking 66% came from Europe, 17% from the Americas, 8% from the Far East and 9% from other countries. I am happy and proud to have welcomed in Alexandroupolis well-known experts who came to discuss problems related to the analysis and prevention of failure in structures. The tranquility and peacefulness of this small town provided an ideal environment for a group of scientists and engineers to gather and interact on a personal basis. Presentation of technical papers alone is not enough for effective scientific communication. It is the healthy exchange of ideas and scientific knowledge, formal and informal discussions, together with the plenary and contributed papers that make a fruitful and successful meeting. Informal discussions, personal acquaintance and friendship play an important role.

I am proud to have hosted ECF16 in the beautiful town of Alexandroupolis, site of the Democritus University of Thrace and I am pleased to have welcomed colleagues, friends, and old and new acquaintances.

I very sincerely thank the authors who have contributed to this volume, the symposia/sessions organizers for their hard work and dedication and the referees who reviewed the quality of the submitted contributions. Our sponsors' support, give in various forms, is gratefully acknowledged. The tireless effort of the members of the Organizing Committee as well as of other numerous individuals, and people behind the scenes is appreciated. I am deeply indebted to the senior students of the Department of Electrical and Computer Engineering of the Democritus University of Thrace Messrs. N. Tsiantoulas and S. Siallis for their hard work and dedication in the preparation of the ECF16 website in a timely and efficient manner and the organization of the conference, and for their efforts in helping me compile this volume. Finally, a special word of thanks goes to Mrs. Nathalie Jacobs of Springer for the nice appearance of this book and her kind and continuous collaboration and support.

January 2006

Xanthi, Greece

Emmanuel E. Gdoutos

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Fracture of Nano and Engineering Materials and Structures

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Edited by

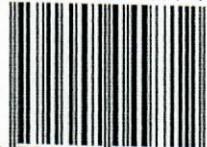
E.E. Gdoutos

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The volume contains the latest research work of renowned experts in the area of failure of engineering materials and structures and is useful for the student, the engineer and the researcher who wants to get an integrated picture of the recent developments in the area of fracture mechanics and fatigue.

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