

# Theory, Modeling and Experiments of Nano-structured Surfaces by Plasma Ions

N.M. Ghoniem<sup>1</sup>, Daniel Walgrae<sup>2</sup>, Christopher Matthes<sup>2</sup>

<sup>1</sup>Mechanical & Aerospace Engineering Department, UCLA, Los Angeles, CA 91344

<sup>2</sup>Instituto de Fisica Interdisciplinar y Sistemas Complejos (CSIC-UIB),  
E-07122 Palma de Mallorca, Spain

A theoretical framework for the evolution of solid surfaces bombarded with plasma ions is presented. The continuum model is based on the original developments of Sigmund[1], Bradley and Harper (BH)[2], and Makeev[3]. Recognizing that near surface energy deposition can produce sputtering events downstream rather than at the point of ion impact, the theory takes into account the interplay between the curvature-dependent sputtering and additional surface relaxation processes, for example as a result of surface diffusion. Taking Sigmund's conclusions that the surface height evolution rate is proportional to its curvature normal to the ion beam,  $\kappa$ , BH balance the roughening rate by surface relaxation rate that is proportional to the second spatial derivative of  $\kappa$ . Thus, the evolution equation for the surface height is [4]:  $h_{,t} = S\kappa + B\kappa_{,ss}$ , where the subscripts denote time (t) derivative and arc length (s) derivatives. The BH equation is usually replaced by a small slope approximation,  $\kappa \approx \Delta h$ , where  $\Delta$  is the Euclidian Laplacian. The coefficients S and B are for the rate of roughening by sputtering (includes angular dependence of the sputtering coefficient), and the surface diffusion smoothing rate (includes surface diffusion coefficient), respectively. We present linear, non-linear and numerical simulations of the equations governing surface patterning under ion or plasma bombardment. We also show experimental results on the influence of pre-existing surface texture on pattern-forming instabilities. Experiments show that low-energy (150 eV) Ar ion energy deposition in the near surface layer result in the amorphization of W at room temperature to a depth of 5-10 nm. The surfaces of nano rods become rippled as a result of an ion-induced roughening instability, with an observed wave-length of 300 nm. Because of the low sample temperature and incident ion energy, the origin of surface ripples does not appear to be related to thermal surface diffusion nor near surface collision cascades.

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[4] Jonah Erlebacher, Michael J Aziz, Eric Chason, Michael B Sinclair, and Jerrold A Floro. “Nonlinear amplitude evolution during spontaneous patterning of ion-bombarded si (001). *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films*, 18(1):115–120, 2000.

## **Predicting interface dislocation structure and energy using anisotropic elasticity theory**

N. Abdolrahim<sup>1</sup>, A. J. Vattré<sup>2</sup>, K. Kolluri<sup>1</sup>, M. J. Demkowicz<sup>1</sup>

<sup>1</sup>Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge MA, 02139

<sup>2</sup>CEA, DAM, DIF, F-91297 Arpajon, France

Frank-Bilby theory generates multiple candidate misfit dislocation structures for an interface with given crystallography. Additional conditions are required to determine which of these structures is the unique structure exhibited by a real interface. We compute the strain energies of all candidate structures generated by Frank-Bilby theory and predict that the one with lowest energy is the correct solution. Our calculation is based on anisotropic linear elasticity theory and uses Burgers vectors consistent with prescribed far-field displacement gradients. We compare our predictions with MD simulations of several fcc/bcc interfaces using disregistry analysis and discuss the potential impact of our findings on engineering of designer interfaces.

## **Thin film buckling on substrate: effect of pressure and plasticity**

Jérôme Colin, A. Ruffini, Christophe Coupeau, Alain Cimetière, Jean Grilhé

Institut P', Université de Poitiers, ENSMA, SP2MI-Téléport 2, F86962 Futuroscope-  
Chasseneuil cedex, France

The thin film buckling on substrate has been theoretically investigated at the mesoscopic scale in the framework of the Foppl-von Karman (FvK) theory of thin plates and, at the microscopic scale, through atomistic simulations.

The first problem to be considered is the buckling of a stressed thin film when an overpressure is considered onto the upper free surface of the film. It is found from an analytical description using the FvK formalism that an overpressure may be responsible for the partial re-deposition of the buckle or its complete re-deposition through the snap through phenomenon. A shape diagram of the film is finally displayed in the stress-applied pressure plane.

In a second part, atomistic simulations of the thin film buckling are presented and the formation of dislocations in the film/substrate interface after the film has buckled is discussed. The formation of the buckle and the dislocation emergence at the buckle edges has been then analytical described using the linear elasticity theory. A stability diagram for the film is provided with respect to the buckling and dislocation emission phenomena.

# **A microstructural phase field approach to shock-induced martensitic transitions in iron**

Aurélien Vattré, Christophe Denoual

CEA, DAM, DIF, F91297 Arpajon, France

A thermodynamically consistent phase field approach for multivariant transformations for shock wave propagation is developed at large strains. Thermodynamic potential includes the description of complex energy landscapes based on reaction pathways and the second law of thermodynamics is used to determine the driving force for change in transformational strain gradients. Kinetic relations lead to the time-dependent Ginzburg-Landau equations with nonlinear, anisotropic and different elastic properties of phases. The morphological features of the bcc–hcp–bcc transformations in iron are investigated and the importance of the plastic deformations in the shock-induced structural transitions is discussed in details.

## Phase Field Modeling of Widmanstätten structures

Maeva Cottura, Benoît Appolaire, Yann Le Bouar, Alphonse Finel

ONERA-CNRS, Laboratoire d'Etude des Microstructures, 29 avenue de la division  
Leclerc, 92320 Chatillon, France

Widmanstätten microstructures have long been studied in physical metallurgy. Numerous experimental observations have evidenced the growth of colonies composed of parallel lamellae, sharing a same crystalline orientation, starting most often from grain boundaries of the mother phase to the grain interior. Such microstructures, resulting from a diffusion-controlled process at high temperatures, have been observed in many metallic alloys such as steels, Cu-Zn or Ti-based alloys. Despite a large number of studies devoted to this microstructure, the understanding of Widmanstätten structures remains incomplete, in particular their growth kinetics featuring a stationary rate under isothermal conditions, as opposed to the usual kinetics observed in diffusion-controlled phase transformations.

Following the first calculations performed by [*M. Fleck, C. Hüter, D. Pilipenko, R. Spatschek, E.A. Brener, Phil. Mag. 90 (2010) 265*], a phase field model has been developed to investigate the role of anisotropic elasticity on the diffusion-controlled growth of acicular precipitates featuring stationary growth rates.

In a first step, the consequences of the elastic driving forces on the microstructure evolution will be discussed for different anisotropies, corresponding to different materials where Widmanstätten structures are observed. In a second step, the model extended to account for a viscoplastic activity will be used to study in what respect plasticity may change the conclusions drawn previously.

## **2D phase-field simulation of grain size distribution in ceramics**

Diego Gómez-García, Bibi Malmal Moshtaghioun, Francisco Luis Cumbreña Hernández,  
Arturo Domínguez Rodríguez

Department of Condensed Matter Physics, University of Seville, P. O. Box 1065, 41080  
Seville, SPAIN

Grain size distribution is a landmark for the analysis of mechanical response of sintered ceramics. It is particularly remarkable to determine the parameters controlling the stationary grain size distribution of a collective of grain powders during sintering. This research work describes a phase-field simulation of the evolution of grain size distribution under external fields (mechanical or electrical forces). A model for the stationary grain size distribution is proposed and it is assessed from the simulation runs. A comparison with different ceramic systems is outlined and discussed in detail.

This research work is funded by the Spanish Ministry of Economy through the project MAT2012-38205-C02-01.

# **A Phase-field model for Displacive Phase Transformations in Elastically Anisotropic and Inhomogeneous Polycrystals**

Tae Wook Heo<sup>1</sup>, Long-Qing Chen<sup>2</sup>

<sup>1</sup>Condensed Matter and Materials Division, Lawrence Livermore National Laboratory,  
Livermore, California 94550, USA

<sup>2</sup>Department of Materials Science and Engineering, The Pennsylvania State University,  
University Park, Pennsylvania 16802, USA

Displacive phase transformations are common in a wide spectrum of materials ranging from metals to ceramics when a material is subject to temperature variation and/or mechanical deformation. In this presentation, we present a phase-field model for displacive phase transformations in polycrystalline materials incorporating inhomogeneous elasticity. The relaxation of misfit strain between parent and transformed product phases or among different structural variants of transformed product phases near grain boundaries is taken into account. It is applied to the *fcc* to *bcc* martensitic transformation described by a Bain strain in a polycrystalline Fe-31at.%Ni metallic alloy. The focus is on the effect of grain boundaries on the displacive transformation behavior and microstructure evolution. Employing simple bicrystals, the effects of grain boundary characteristics such as the degree and range of the misfit strain relaxation at the grain boundary and grain boundary curvature on the phase behaviors near a grain boundary are examined for both a flat or a curved grain boundary. The model is then applied to polycrystals containing multiple grains. The effects of misfit strain relaxation at grain boundaries, elastic anisotropy, grain texture, and applied stress on the kinetics and the microstructures of displacive transformations are discussed. The predicted microstructures near grain boundaries are compared to the experimental observations in literature.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 12-ERD-053.

# Multi-scale Modeling of Irradiation-Induced Morphology Evolution

Dr. Scott A. Norris

Southern Methodist University

Ion beam irradiation is an essential basic tool in many industries, used widely for chemical doping and surface processing. For over 50 years, spontaneously-forming ripple-like structures have been occasionally observed during this process, but the observation in 1999 of highly-ordered, hexagonal arrays of nanoscale dots on irradiated GaSb has sparked an intense renewed interest in ion-induced surface modification. It has been hoped that this process could form the basis of a "bottom-up" process to cheaply and rapidly manufacture arrays of nanostructures, or induce surface coatings with tunable opto-electronic properties. However, despite many years of accumulated study of ion irradiation, and thorough knowledge of the generic ingredients for ordered structures, a definitive explanation for their origin in this system has remained elusive.

In this talk I will describe a multi-scale approach to this problem: a means by which statistical information extracted from an ensemble of single-ion impact simulations – lasting only picoseconds – can be incorporated into a continuum-level partial differential equation on the surface evolution that occurs over seconds. The result is a generic framework relating surface normal velocity to the moments of the function describing the single-ion impacts (the "crater function"). After describing the general result, and application to a simple system with reasonable success, we will discuss extensions underway:

- \* to rapidly explore a large parametric space of materials and conditions
- \* to also inform a continuum description of the significant stress imparted into the film
- \* to describe multi-component materials, which exhibit a greater variety of patterns
- \* to describe the related regime of Ion-Beam Assisted Deposition (IBAD)

The latter extension is of particular future interest, as the fundamental nature of the phase-separation instability is modified by the IBAD process, which additionally provides a means of transferring compositional patterns from the thin film into the bulk, as the patterned surface is continually covered up by new material.