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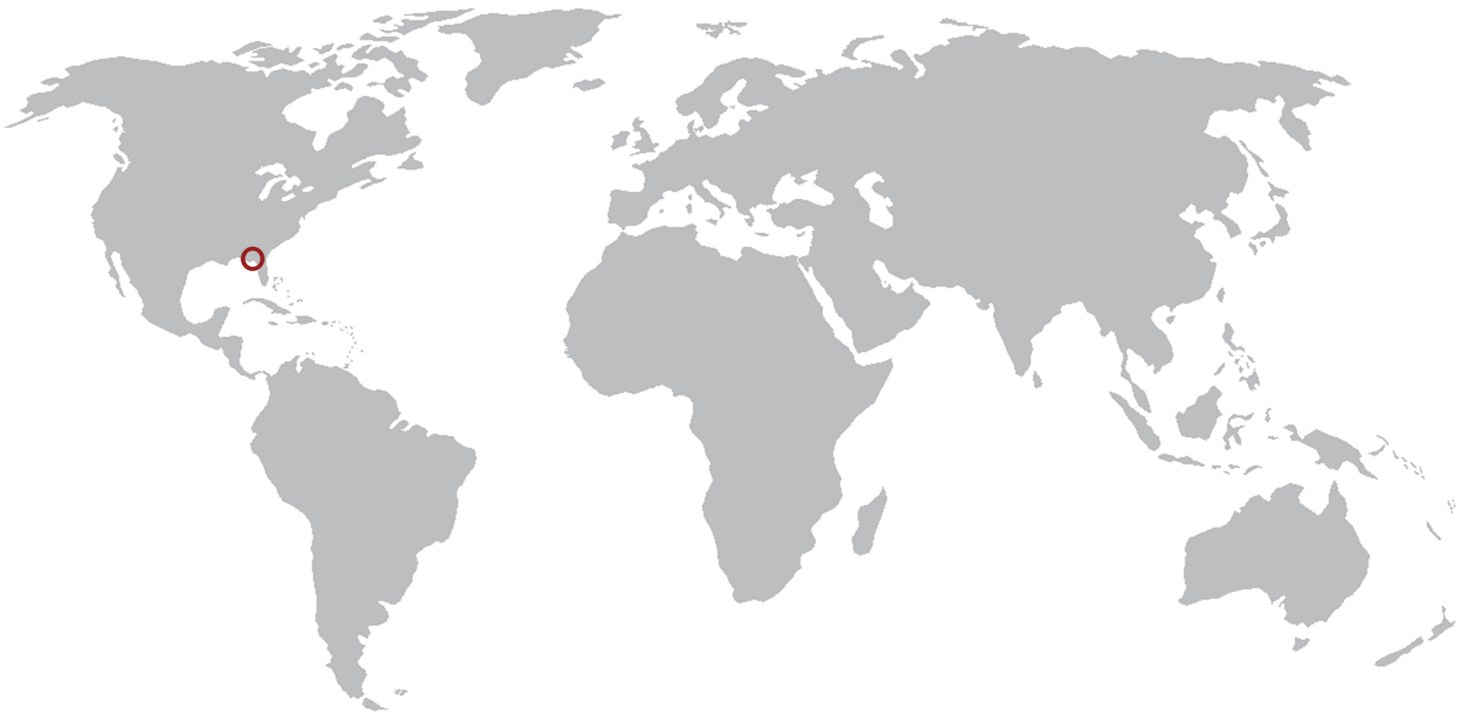
MMM 2008

Fourth International Conference

MULTISCALE MATERIALS MODELING

OCTOBER 27-31, 2008 ▪ TALLAHASSEE, FLORIDA, USA

Tackling Materials Complexities via Computational Science



Hosted by the Department of Scientific Computing and Florida State University

DEPARTMENT OF Scientific COMPUTING

FLORIDA STATE UNIVERSITY 1851 VIRES ARTES MORES

Proceedings of

MMM 2008

Fourth International Conference

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Anter El-Azab
Editor

Organized and Hosted by
The Department of Scientific Computing and
Florida State University

DEPARTMENT OF Scientific COMPUTING

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Forward

The field of multiscale modeling of materials promotes the development of predictive materials research tools that can be used to understand the structure and properties of materials at all scales and help us process materials with novel properties. By its very nature, this field transcends the boundaries between materials science, mechanics, and physics and chemistry of materials. The increasing interest in this field by mathematicians and computational scientists is creating opportunities for solving computational problems in the field with unprecedented levels of rigor and accuracy. Because it is a part of the wider field of materials science, multiscale materials research is intimately linked with experiments and, together, these methodologies serve the dual role of enhancing our fundamental understanding of materials and enabling materials design for improved performance.

The increasing role of multiscale modeling in materials research motivated the materials science community to start the Multiscale Materials Modeling (MMM) Conference series in 2002, with the goal of promoting new concepts in the field and fostering technical exchange within the community. Three successful conferences in this series have been already held:

- The First International Conference on Multiscale Materials Modeling (MMM-2002) at Queen Mary University of London, UK, June 17-20, 2002,
- Second International Conference on Multiscale Materials Modeling (MMM-2004) at the University of California in Los Angeles, USA, October 11-15, 2004, and
- Third International Conference on Multiscale Materials Modeling (MMM-2006) at the University of Freiburg, Germany, September 18-22, 2006.

The Fourth International Conference on Multiscale Materials Modeling (MMM-2008) held at Florida State University comes at a time when the wider computational science field is shaping up and the synergy between the materials modeling community and computational scientists and mathematicians is becoming significant. The overarching theme of the MMM-2008 conference is thus chosen to be "*Tackling Materials Complexities via Computational Science*," a theme that highlights the connection between multiscale materials modeling and the wider computational science field and also reflects the level of maturity that the field of multiscale materials research has come to. The conference covers topics ranging from basic multiscale modeling principles all the way to computational materials design. Nine symposia have been organized, which span the following topical areas:

- Mathematical basis for multiscale modeling of materials
- Statistical frameworks for multiscale materials modeling
- Mechanics of materials across time and length scales
- Multiscale modeling of microstructure evolution in materials
- Defects in materials
- Computational materials design based on multiscale and multi-level modeling principles

- Multiscale modeling of radiation effects in materials and materials response under extreme conditions
- Multiscale modeling of bio and soft matter systems

The first five topical areas are intended to cover the theoretical and computational basis for multiscale modeling of materials. The sixth topical area is intended to demonstrate the technological importance and industrial potential of multiscale materials modeling techniques, and to stimulate academia-laboratory-industrial interactions. The last two topical areas highly overlap with the earlier ones, yet they bring to the conference distinct materials phenomena and modeling problems and approaches with unique multiscale modeling aspects.

This conference would not have been possible without the help of many individuals both at Florida State University and around the world. Of those, I would like to thank the organizing team of MMM-2006, especially Professor Peter Gumbsch, for sharing their experience and much organizational material with us. I also thank all members of the International Advisory Board for their support and insight during the early organizational phase of the conference, and the members of the International Organizing Committee for the hard work in pulling the conference symposia together and for putting up with the many organization-related requests. Thanks are due to Professor Max Gunzburger, Chairman of the Department of Scientific Computing (formerly School of Computational Science) and to Florida State University for making available financial, logistical and administrative support without which the MMM-2008 would not have been possible. The following local organizing team members have devoted significant effort and time to MMM-2008 organization: Bill Burgess, Anne Johnson, Michele Locke, Jim Wilgenbusch, Christopher Cprek and Michael McDonald. Thanks are also due to my students Srujan Rokkam, Steve Henke, Jie Deng, Santosh Dubey, Mamdouh Mohamed and Jennifer Murray for helping with various organizational tasks. Special thanks are due to Bill Burgess and Srujan Rokkam for their hard work on the preparation of the proceedings volume and conference program.

I would like to thank the MMM-2008 sponsors: Lawrence Livermore National Laboratory (Dr. Tomas Diaz de la Rubia), Oak Ridge National Laboratory (Dr. Steve Zinkle) and Army Research Office (Drs. Bruce LaMattina and A.M. Rajendran) for the generous financial support, and thank TMS (Dr. Todd Osman) for the sponsorship of MMM-2008 and for advertising the conference through the TMS website and other TMS forums.

I would also like to thank all plenary speakers and panelists for accepting our invitation to give plenary lectures and/or serve on the conference panels. Lastly, I would like to thank the session chairs for managing the conference sessions.

Anter El-Azab
Conference Chair

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Contents

Plenary Talks

Plenary Talks

Architecture in nanospace

Sir Harold Kroto

Nobel Prize for Chemistry 1996, Francis Eppes Professor
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ABSTRACT

As Chemistry and Physics at one borderline and Chemistry and Biology at the other begin to become indistinguishable, multidisciplinary research is leading to the fascinating "new" overarching field of Nanoscience and Nanotechnology (N&N). Ingenious strategies for the creation of molecules with complex exactly-specified structures and as well as function are being developed - basically molecules that "do things" are now being made. In fact N&N is not new but appears to be the "Frontier Chemistry of the 21st Century." When the molecule C60 Buckminsterfullerene and its elongated cousins the carbon nanotubes or Buckytubes were discovered, it suddenly became clear that our understanding of the factors governing the bottom-up assembly of atomic and molecular structures involving carbon and other atoms was quite naïve, especially with regard to dynamic construction events at nanometer dimensions.

New experimental approaches which focused on the way atoms cluster together have led to the production of novel nanostructures and a general refocusing of research interests on ways of controlling so-called "bottom-up self-assembly." This new approach is leading to novel advanced materials with new applications. Fascinating fundamental insights into formation mechanisms have been revealed and nanoscale devices, which parallel devices in standard engineering, are now being created. On the horizon are possible applications ranging from civil engineering to advanced molecular electronics so promising to transform the socio-economics of everyday life. These fundamental advances suggest that supercomputers in our pockets (as well as our heads) and buildings which can easily withstand powerful hurricanes and earthquakes are possible. However if these breakthroughs are to be realised in practice a paradigm shift in synthetic chemical techniques will be necessary so we can create, at will, really large molecules with accurately defined structures at the atomic level. This presents one of the greatest technical challenges for chemists. It is also worth pondering implications of the fact that the C60 molecule, which is almost exactly one nanometer in diameter, was discovered during an experiment aimed at understanding earlier astronomy results which had uncovered puzzling facts about the molecular constituents of dusty interstellar clouds which are up to 100 light years in size - indeed some 1028 or a thousand million, million, million, million times larger than C60!

To illustrate some of the key issues, material from the Vega Science Trust website (http://www.vega.org.uk) which makes TV/Internet programmes to improve the general level science understanding as well as the Global Educational Outreach website (http://www.geoset.info) which is a cache of SET educational material for teachers, will be used.

Nanomechanics and the study of human disease states

Professor Subra Suresh

Dean of Engineering, Ford Professor of Engineering
Massachusetts Institute of Technology, Cambridge MA 02139-4307 USA

ABSTRACT

This lecture will deal with select topics at the intersections of nanotechnology, engineering, biology and human health. For this purpose, molecular changes induced by external factors or biochemical processes occurring naturally in the human body will be considered with a variety of state-of-the-art experimental and computational tools. The alterations to nanoscale responses of the whole cell, cell membrane and cytoskeleton will be explored using a variety of multi-scale probes and analyses. Attention will be focused on examples derived from applications of nanotechnology tools to the study of Plasmodium falciparum and Plasmodium vivax malaria, several types of hereditary hemolytic disorders, and metastatic invasion of tumor. Case studies of targeted gene inactivation methods to probe specific molecular effects at the intersections of nanotechnology, engineering, biology and human health will also be presented. Multi-scale computational simulations will be presented with the aim of elucidating shape thermodynamics of healthy and pathological states of biological cells. Potential applications of these results for disease diagnostics, therapeutics and drug efficacy assays will also be explored.

Multiscale Modeling of the Mechanical Behavior of Structural Materials in Nuclear Energy Systems

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ABSTRACT

The multiscale modeling methodology is now a cornerstone in world programs aimed at designing radiation-resistant structural materials in the harsh environments of Nuclear Energy Systems. The strategy is based on a hierarchy of models connected sequentially at appropriate interfaces of length and time scales, and utilizes concepts of "separation of scales." Basic defect properties, such as the energetics of point defect formation and migration, and lattice resistance to dislocation slip, are determined by ab initio methods, and are parameterized and utilized in upper length-scale methods. Molecular dynamics simulations reveal specific outcomes of reactions between defects (e.g. dislocations and point defect clusters), or the structure of displacement damage caused by energetic particle collisions. The collective behavior of mobile point defect cluster ensembles is determined by Kinetic Monte Carlo simulations, where the degrees of freedom are reduced to those pertinent to the defects themselves and not all participating atoms. Plastic deformation and fracture phenomena at the micron length scale are fundamentally determined through 3-dimensional Dislocation dynamics simulations. We outline here this strategy, and show how it is used to understand and design radiation-resistant materials. Examples of modeling the low-temperature embrittlement and fracture of ferritic/ martensitic steels and the shift in the Ductile-to-Brittle-Transition-Temperature (DBTT) by neutron irradiation will be given. At the component length scale, we discuss the development of microstructure-based constitutive models that can be incorporated into crystal plasticity. A global-local approach for coupling large-scale global Finite Element Modeling (FEM) to crystal plasticity analysis of local deformation at critical regions of fusion structures will also be shown.

1. Introduction

The environment in which structural materials in nuclear energy systems operate is undoubtedly harsh, and may be regarded as one of the severest ever known to man. These materials must operate reliably for extended periods of times without maintenance or repair. They must withstand the assaults of high particle and heat fluxes, as well as significant thermal and mechanical forces. Moreover, the most significant dilemma here is that actual operational conditions cannot be experimentally established in isolated laboratories, with all of the synergistic considerations of neutron spectrum, radiation dose, heat and particle flux, and large component size. Because of these considerations, research efforts are increasingly reliant on carefully-designed experiments and theoretical concepts to design and develop reliable structural

materials. Empirical approaches have not been optimum in the development of radiation-resistant materials. Fortunately, the tremendous progress achieved during the past decade in the area of multiscale modeling is beginning to enable rational development of radiation-resistant structural materials. We will first outline here the physical limitations imposed on structural materials in the nuclear environment, highlighting some of the key problems. The multiscale modeling approach to the solution of some of these research problems is then discussed, with particular reference to progress made in modeling fundamental physics questions at several length scales.

2. Physical Limits on Structural Materials in the Nuclear Environment

A wide range of structural materials has been considered over the past 25-30 years for nuclear energy applications [1]. This list includes conventional materials (e.g. austenitic stainless steel), low-activation structural materials (ferritic/martensitic steels, V-4Cr-4Ti, and SiC/SiC composites), oxide dispersion strengthened (ODS) ferritic steels, conventional high temperature refractory alloys (Nb, Ta, Cr, Mo, W alloys), titanium alloys, Ni-based super alloys, ordered intermetallics (TiAl, Fe_3Al, etc.), high-strength, high-conductivity copper alloys, and various composite materials (C/C, metal-matrix composites, etc.). Strong emphasis has been recently placed on the development of three reduced-activation structural materials: ferritic/martensitic steels containing 8-12% Cr, vanadium base alloys (e.g. V-4Cr-4Ti), and SiC/SiC composites, and reduced-activation Oxide Dispersion Strengthened (ODS) ferritic steels. Additional alloys of interest for fusion energy applications include copper alloys (CuCrZr, Cu-NiBe, dispersion-strengthened copper), tantalum-base alloys (e.g. Ta-8W-2Hf), niobium alloys (Nb-1Zr), molybdenum, and tungsten alloys. In the following, we briefly discuss the most limiting properties of these materials, and outline the role of multiscale modeling in addressing these limitations.

2.1. Low-Temperature Limits

The lower temperature limits for structural materials are strongly influenced by radiation effects. For body-centered cubic (BCC) materials such as ferritic-martensitic steels and the refractory alloys, radiation hardening at low temperatures can lead to a large increase in the Ductile-To-Brittle-Transition-Temperature (DBTT) [2]. For SiC/SiC composites, the main concerns at low temperatures are radiation-induced amorphization (with an accompanying volumetric swelling of ~11%) and radiation-induced degradation of thermal conductivity. The radiation hardening in BCC alloys at low temperatures ($0.3T_m$) is generally pronounced, even for doses as low as 1 dpa. The amount of radiation hardening typically decreases rapidly with irradiation temperature above $0.3\ T_m$, and radiation-induced increase in the DBTT may be anticipated to be acceptable at temperatures above $0.3T_m$. The brittle behavior occurs when the temperature dependent yield strength exceeds the cleavage stress. Numerous studies have been performed to determine the radiation hardening and embrittlement behavior of ferritic-martensitic steels. The hardening and DBTT shift are dependent on the detailed composition of the alloy. For example, the radiation resistance of Fe-9Cr-2WVTa alloys appears to be superior (less radiation hardening) to that of Fe-9Cr-1MoVNb. The radiation hardening and DBTT shift appear to approach saturation values following low temperature irradiation to doses above 1-5 dpa, although additional high-dose studies are needed to confirm this apparent saturation behavior. At higher doses under fusion conditions, the effects of helium bubble accumulation on radiation hardening and DBTT need to

be addressed. Experimental observations revealed brittle behavior (K_{IC}~ 30 MPa $m^{1/2}$) in V-(4-5)%Cr-(4-5) %Ti specimens irradiated and tested at temperatures below 400 ^{O}C. Therefore, 400 ^{O}C may be adopted as the minimum operating temperature for V-(4-5)%Cr-(4-5)%Ti alloys in fusion reactor structural applications [1]. Very little information is available on the mechanical properties of irradiated W alloys. Tensile elongation of ~ 0% have been obtained for W irradiated at relatively low temperatures of 400 and 500 ^{O}C and fluence of 0.5-1.5×10^{26} n/m^2 (~2 dpa in tungsten). Severe embrittlement (DBTT > 900 ^{O}C) was observed in un-notched bend bars of W and W-10% Re irradiated at 300 ^{O}C to a fluence of 0.5×10^{26} n/m^2. The minimum operating temperature which avoids severe radiation hardening embrittlement is expected to be 900± 100 ^{O}C.

2.2. High-Temperature Limits

The upper temperature limits are dictated by four different mechanisms: Thermal creep, high temperature helium embrittlement, void swelling, and chemical compatibility. Void swelling is not anticipated to be significant in ferritic-martensitic steel or V-Cr-Ti alloys up to damage levels in excess of 100 dpa, although swelling data with fusion-relevant He:dpa generation rates are needed to confirm this expectation and to determine the lifetime dose associated with void swelling. The existing fission reactor database on high temperature (Mo, W, Ta) refractory alloys [3] indicates low swelling (~2%) for doses up to 10 dpa or higher. Void swelling is considered to be of particular importance for SiC and also Cu alloys [1]. An adequate experimental database exists for thermal creep of ferritic-martensitic steels and the high temperature (Mo, W, Nb, Ta) refractory alloys. Oxide-dispersion-strengthened ferritic steels offer significantly higher thermal creep resistance compared to ferritic-martensitic steels, with a steady-state creep rate at 800 ^{O}C as low as 3×10^{-10} s^{-1} for an applied stress of 140 MPa. The V-4Cr-4Ti creep data suggest that the upper temperature limit lies between 700 and 750 ^{O}C. The predicted thermal creep temperature limit for advanced crystalline SiC-based fibers is above 1000 ^{O}C.

In fusion energy systems, helium generation rates are substantially higher than in fission reactors. Helium embrittlement may cause a reduction in the upper temperature limit, but sufficient data under fusion-relevant conditions are not available for any of the candidate materials. Due to a high density of matrix sinks, ferritic/martensitic steel appears to be very resistant to helium embrittlement. An analysis of helium diffusion kinetics in vanadium alloys predicted that helium embrittlement would be significant at temperatures above 700 ^{O}C. The lower temperature limits for the refractory alloys and ferritic/ martensitic steel are based on fracture toughness embrittlement associated with low temperature neutron irradiation. The minimum operating temperature for SiC/SiC composites is based on radiation-induced thermal conductivity degradation, whereas the minimum temperature limit

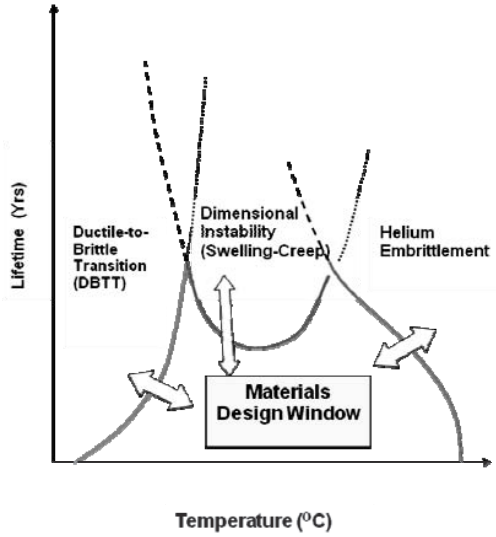

Figure (1): Operational Design window for structural materials in nuclear energy systems.

for CuNiBe is simply chosen to be near room temperature. The low temperature fracture toughness radiation embrittlement is not sufficiently severe to preclude using copper alloys near room temperature, although there will be a significant reduction in strain hardening capacity as measured by the uniform elongation in a tensile test. The high temperature limit is based on thermal creep for all of the materials except SiC and CuNiBe. Due to a lack of long-term (10,000 h), low-stress creep data for several of the alloy systems, a Stage II creep deformation limit of 1% in 1000 h for an applied stress of 150 MPa was used as an arbitrary criterion for determining the upper temperature limit associated with thermal creep. Further creep data are needed to establish the temperature limits for longer times and lower stresses in several of the candidate materials. The limits on lifetime of structural materials in a nuclear energy system are schematically illustrated in Figure (1).

3. The Multiscale Modeling Approach to the Design of Radiation-Resistant Materials

Design of advanced structural materials for applications in Gen-IV fission reactors and in fusion energy systems is being aided by progress in multiscale modeling efforts [5]. We discuss here the specific approach that is being pursued in the development of physically-based constitutive models of plasticity and fracture. Conventional models so far have considered separately irradiation effects on microstructure evolution, and post irradiation mechanical testing. The aim was usually to determine the increase in the yield strength caused by irradiation. This was rather reasonable because in post-irradiation experiments the yield stress is usually the maximum possible stress. The basic physical picture of this has been investigated in a series of experimental, theoretical and modeling studies. Experimental studies have demonstrated that during irradiation the pre-existing dislocations get decorated by Self-Interstitial Atom (SIA) clusters [5]. It has been shown theoretically and by atomistic modeling that this decoration is caused by glissile SIA clusters/dislocation loops produced in collision cascades. Consideration of this microstructural feature led to the so called cascade induced source hardening (CISH) model [6], which has been used to explain the increase in yield stress and the yield drop by the blocking effects of decoration to pre-existing dislocations. Both of these effects have been shown to arise from the fact that these dislocations cannot move and activate usual Frank-Reed sources, which raises the yield stress of the system under deformation (radiation hardening), and in the limit leads to plastic instability through activation of a few sources operating under very high stress.

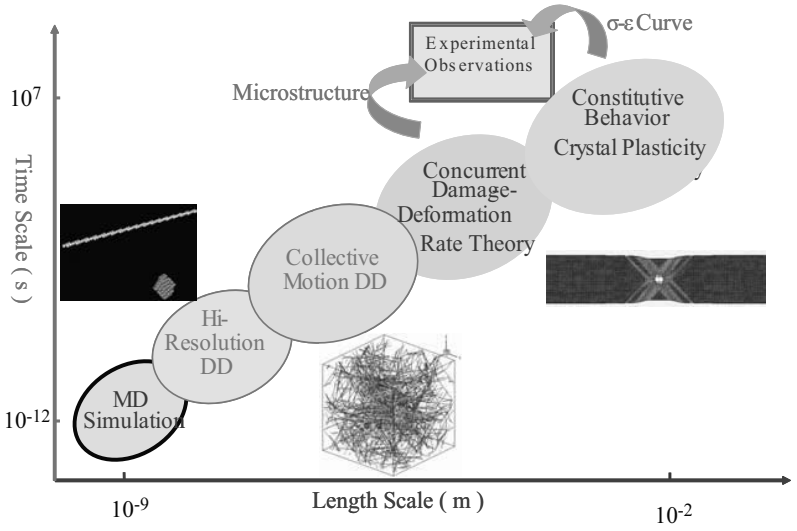

Figure (2): The multiscale modeling approach for deformation & fracture of structural materials in nuclear

The new data obtained in in-reactor experiments have showed that dislocation decoration plays even more important role than it was expected in CISH model [7]. Thus, the fact that the yield stress and the following plastic flow stress depends on the pre-yield irradiation dose is, in principle, consistent with the CISH. The pre-deformation dose defines the level of decoration and if the decoration is still not well developed, the dislocation can move and multiply. However, such a moving dislocation drags the decoration with it, and also sweeps defects on its way. This increases the resistance for dislocation motion, which now depends on strain and damage rates - the lower is the first and the higher is the second, the more damage is accumulated in the system, resulting in hardening of the bulk. This can explain the increase of the flow stress observed in in-reactor experiments [7]. However a quantitative description needs to take into account a number of mechanisms such as dislocation drag of the decoration, interaction of this with already accumulated radiation defects, transformation into hardening effects, the effect of dislocation dynamics on microstructure evolution, and the description of time and dose dependence of the flow stress. To tackle these issues and enable materials design, a combined multi-scale approach is being developed, as shown in Figure (2). The approach is based on (1) analytical combination of rate theory and continuum dislocation dynamics, (2) large scale three-dimensional dislocation dynamics, and (3) large scale atomistic modeling using molecular dynamics (MD) and molecular statics (MS). Each technique has its own range of the particular problems to consider and the crucial issue it that there is a strong overlap and feedback between all them.

In the multiscale approach outlined here, the dynamics of dislocations in the environment of constantly produced defects is studied at the atomic-level with Molecular Dynamics (MD) simulations [8,9]. Dislocation-defect reactions modifying dislocation properties/structure are taken into account. Dislocation-obstacle interactions are described with the atomic-scale accuracy taking into account change in both dislocations and obstacles. Properties of decorated dislocations are very different from undecorated dislocations, and thus must be at the atomic scale. Three main features are relevant here: mobility, recombination via dislocation mechanisms and intensive pipe/core diffusion. A Kinetic Monte Carlo (KMC)-based approach describing microstructure evolution under displacement cascade damage and incorporating the elastic interaction between defects is used to investigate the spatial and size distribution of defect clusters produced in displacement cascades [5]. The method of Parametric Dislocation Dynamics (PDD) is being extended to determine dislocation interaction with nano-voids, precipitates and Self Interstitial Clusters (SIA's), accounting for the first time for the flow of vacancies to dislocation cores during irradiation (i.e. dislocation climb) [9]. The microstructure predicted by KMC simulation is then be used to serve as input to DD simulation to investigate radiation effects on plastic deformation in a realistic way. The effective properties of dislocations in radiation-damaged steels (e.g. stress-velocity relationship and back stress) are then passed on to 3-D PDD simulations of dislocation microstructure evolution under neutron irradiation. From these simulations, the rates of dislocation reactions (i.e. generation, recovery, hardening, and interactions with dislocation cells and sub-boundaries) are determined. These parameters are used in a comprehensive rate theory model of radiation damage and in-reactor deformation. This model focuses on rate-independent (in-reactor) plasticity, high-temperature creep and creep-fatigue. The developed materials models are integrated within the Finite Element framework through the commercial Finite Element Codes.

4. Conclusions

Because the operational environment of structural materials in fission or fusion energy systems is very severe, experiments can be costly. Without guidance from theory and modeling, development efforts on the basis of an experimental program alone are decidedly non-optimal. Predictions of the emerging multi-scale hierarchy outlined here are expected to be essential in future developments of radiation-resistant structural materials in nuclear energy applications.

Acknowledgements

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Linking multiscale materials modeling with experiment at the mesoscale using 3D X-ray microscopy

Dr. Ben C. Larson

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ABSTRACT

Recently developed 3D X-ray microscopy techniques using high-brilliance synchrotron X ray microbeams at the Advanced Photon Source (APS) now provide non-destructive, submicron-resolution 3D measurements of local crystal structure, lattice orientation, and strain tensors in single crystal and polycrystalline materials. This capability provides an unprecedented opportunity to directly link experiment with multi-scale modeling of the microstructure and evolution of materials, a critical step for detailed testing the predictions of models at mesoscopic length scales (~ tenths of microns to hundreds of microns). In this presentation, the 3D x-ray microscopy technique will be illustrated using thermal grain growth in polycrystalline Al and dislocation density tensor measurements in thin, plastically deformed single crystal Si plates, and the direct link between 3D x-ray microscopy and computer modeling on mesoscopic length scales will be discussed in connection with deformation in metals. The ability to make detailed, quantitative comparisons between non-destructive, micron-resolution 3D x-ray microscopy measurements and finite element modeling will be demonstrated using 3D maps of local lattice rotations and local dislocation density tensors associated with nano/micro indentation induced deformation in Cu. Direct statistical based comparisons between 3D x-ray microscopy measurements and discrete dislocation calculations of deformation in homogeneously strained metals will be demonstrated as well, and discussed in connection with dislocation patterning on mesoscopic length scales. The ability of 3D x-ray microscopy to characterize strong dislocation patterning will be illustrated through direct, spatially resolved measurements of elastic strain in dislocation-rich cell walls and dislocation-poor cell interiors in deformed Cu.

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Some mathematical and numerical issues in multiscale modeling

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ABSTRACT

To put multiscale modeling on a solid foundation, we need to study the following problems:

1. The connection between different physical models, e.g., how continuum elasticity models can be derived from quantum mechanics models
2. How to impose general, non-periodic boundary conditions for different physical models?
3. How to interface the different models so that the coupled model is uniformly accurate?
4. In general, how to develop sub-linear scaling algorithms that use higher levels of adaptivity?

I will discuss some recent progress that has been made on these issues, using both classical atomistic models and electronic structure models as examples.

(Joint work with Carlos Garcia-Cevera, Xiantao Li, Jianfeng Lu and Pingbing Ming)

Making and breaking of chemical bonds under mechanical load

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ABSTRACT

Brittle fracture as well as adhesion, or friction and wear are prominent examples for mechanical problems with clearly observable macroscopic consequences that are directly related to the processes of the formation and destruction of chemical bonds. Modelling such processes requires us to propagate the atomistic information through the scales to obtain macroscopic information. If chemical specificity and chemical accuracy are required, only few approaches are available.

I will quickly review latest achievements in concurrent coupling techniques, in particular the "earn on the fly" (LOTF) technique with applications to brittle fracture of diamond and silicon. The main focus of this talk will be the simulation of friction and wear processes between amorphous diamond-like carbon (DLC) films. Sequential techniques must be applied there to first obtain reasonable starting configurations for the atomic structure and topology of the films. Then different levels of approximations are required to assess the evolution of the friction contacts. Considerable attention must be paid there to extracting relevant information from large scale atomistic simulations, which in turn first requires an atomistic model for the hydrocarbons that can describe well the making and breaking of the atomic bonds. I will introduce such a new potential, report about comparison to large-scale tight binding simulations and present results for the evolution of an atomistically determined friction coefficient during running-in of such a contact.

Depinning Transition in Solid Mechanics

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ABSTRACT

The depinning transition describes the onset of steady flow of a driven elastic system interacting with a random potential. Many examples of such a transition can be encountered in solid mechanics: friction, crack propagation, dislocation trapping, or plasticity of amorphous solids. It is argued that the onset of low is generically a second order phase transition which can be characterized by a few critical exponents. This observation leads to specific predictions concerning size effects of the fluctuations of the driving force, and even the probability distribution function of instantaneous critical depinning forces. The examples of crack propagation in a brittle solid, and glass plasticity are discussed more extensively.

1. Introduction

In statistical physics, the depinning transition describes the onset of motion of an elastic manifold interacting with a random potential. At the critical forcing that separates a pinned regime where the manifold reaches a static equilibrium configuration and a propagating regime where the manifold acquires a finite velocity, a genuine second order phase transition occurs. Flow above and at threshold consists in a series of micro-instabilities. Such a transition is encountered in a variety of different contexts,[1] and controls critical currents in superconductors, magnetic walls, wetting contact lines, etc.

In Solid Mechanics also this general phenomenology is at play for different phenomena such as solid friction,[2] individual dislocation in crystals,[3] crack propagation in brittle heterogeneous materials,[4] or plasticity of amorphous media[5]. However, depending on the dimensionalities of the problem (elastic manifold and embedding space) and the type of elastic interactions, different universality classes are encountered. The consequences of such depinning transitions will be discussed, focusing mainly on crack arrest and amorphous media plasticity.

Not only does this framework accounts for a threshold forcing, but it also provides a natural explanation for rate independent laws. A determining property of depinning problems is the elastic coupling between the different parts of the system which interact with the random potential. This makes the flow intrinsically collective, and hence the individual nature of potential wells is not probed. On the contrary, general (or universal) laws emerge irrespective of the detailed nature of the potential. One of the most remarkable features is that the random pinning potential does not need to be characterized in full details, but may be reduced to a few

characteristic features. Only the mean value and standard deviation of the macroscopic critical forcing at a given reference scale is enough to predict its effective distribution at a different scale. Up to rescaling factors involving the above two moments, the shape of the distribution of the critical forcing (energy release rate for cracks, yield stress for amorphous media plasticity) is universal. Moreover, the scaling of the standard deviation with the system size is shown to display a non-trivial but universal power-law behavior.

2. Crack propagation

Let us consider a semi-infinite mode I crack limited by a straight crack front in an infinite domain. Along the crack surface, the microscopic toughness $K_c(x)$ is assumed to vary randomly. A uniform loading is applied at infinity such that the stress intensity factor would be equal to K_0 for a perfectly straight crack front. Only a weak disorder is considered so that the statistical distribution of K_c is narrow. A so-called "extremal dynamics" is considered so that at each time step, the remote loading is adjusted so that at only one point along the front the stress intensity factor reaches its threshold value. At this point, the front is advanced by a constant or random quantity, and a new local toughness is encountered. The same rule is repeated over and over again. The front thus becomes rough, and meanders around an overall straight line. Its geometry is described by a function $h(x)$. The very concept of the stress intensity factor, even if computed all along the crack front, is a non-local quantity. For a small perturbation expansion to first order in h, it can be computed [6] as

$$K(x) = K_0\left(1+\frac{1}{\pi}\int\frac{(h(y)-h(x))}{(y-x)^2}dy\right) \qquad (1)$$

This equation describes the "elastic coupling" along the crack front.

If the loading is weak, the front may advance for a transient period and reach a static configuration where $K(x)<K_c(x)$ for all x. In contrast, a larger loading will lead to an unlimited propagation. The critical loading which separates these two regimes would correspond for a straight crack to a uniform stress intensity factor K^* which defines the macroscopic toughness of the material. This can be seen as a homogenization procedure relating the random local toughness field to the macroscopic toughness. Only for the special case of an extremely anisotropic toughness field, (called "weak pinning") does this procedure reduces to the arithmetic average of the local toughness (see Ref. [7] for a discussion). The generic case is rather the "strong pinning" regime, where the macroscopic toughness is larger than the average.

The extremal dynamics is an easy way to access the critical stress intensity factor, as $K_0(t)$ is adjusted at each time step. K^* is the maximum value of $K_0(t)$, provided finite size effects are taken care of to avoid rare (insignificant) events.

The morphology of the crack front in the steady state displays an interesting self-affine property. Namely, the front remains (statistically) invariant under an affinity of arbitrary scale ratio λ along the x axis and λ^ζ along the h direction

$$h(\lambda x) = \lambda^{\zeta} h(x) \qquad (2)$$

where the "roughness" exponent ζ is a universal critical exponent whose value is numerically estimated to be 0.38. Universal means that this value is independent on the statistical distribution of the local toughness, $K_c(x)$.

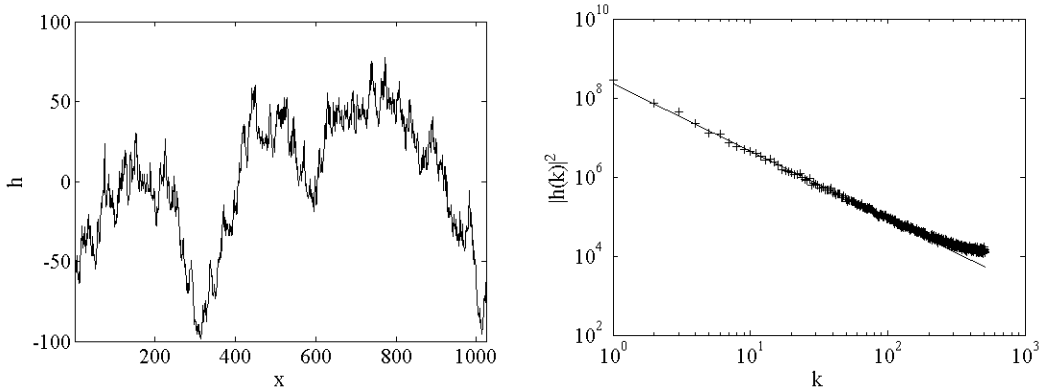

Figure 1: (left) An example of the crack front shape and (right) its averaged power spectrum (symbol +) together with a power-law fit (straight line).

However, the crack front morphology is seldomly accessible experimentally, and hence this property may appear as rather useless. However, the same exponent appears in more significant observables.

Let us consider the instantaneous macroscopic critical stress intensity factor $K(t)$. It was mentioned that its maximum value gives the macroscopic equivalent toughness. However its entire statistical distribution is not of much interest as it reflects the local toughness distribution, and hence is dependent on the details of the system under study. The immediate vicinity of K^* is more interesting as it reflects globally pinned configurations. Indeed, let us imagine that the loading is kept constant at a value $K^*(1-\varepsilon)$ slightly below the macroscopic toughness. We can reconstruct the propagation scenario from $K(t)$. It consists in "bursts" of propagation (or avalanches) separated by arrest events where $K(t)$ exceeds $K^*(1-\varepsilon)$. The duration of the "bursts" diverge as ε goes to zero. The bursts are spatially localized and have an extension along the front axis which scales with a correlation length, ξ. The corresponding growth along the front direction results from the self-affinity property, and scales as ξ^{ζ}. From Eq. (1), dimensional analysis provides the relation between ε and ξ, $\varepsilon \propto \xi^{\zeta-1}$, which can be rephrased as classically encountered in critical phenomena as:

$$\xi \propto (K^* - K)^{-\nu} \qquad (3)$$

where $\nu = 1/(1-\zeta) \approx 1.61$. From this observation, one can study the critical depinning force at those instants where the position of the active site exceeds a given distance d. Those instants correspond to a pinned configuration over a scale d, and hence for large distances, they will reflect properties of the critical point. Indeed, it is observed that the probability distribution

function (pdf) of the macroscopic toughness conditioned by the distance acquires a universal shape. The width of the distribution of (K^*-K) indeed decreases as a power-law of d with an exponent $-1/\nu$. If we consider the statistical distribution of $u = (K^*-K)d^{1/\nu}$, one obtains a d-independent function, $\Psi(u)$, as shown in Figure 2. The latter distribution is to be interpreted as the effective distribution of macroscopic toughness for a finite size system, i.e., a crack front length of order d.

This property is quite remarkable. Indeed for all distributions of the local toughness, the macroscopic toughness assumes the same statistical distribution. It only depends on two parameters, namely the asymptotic macroscopic toughness (the limit value obtained for a crack front of infinite size), and a standard deviation of the distribution, σ_0, observed at an arbitrary reference length scale, L_0. This property was used in order to analyze the statistics of arrest cracks for indentation of a variety of different ceramic materials [9].

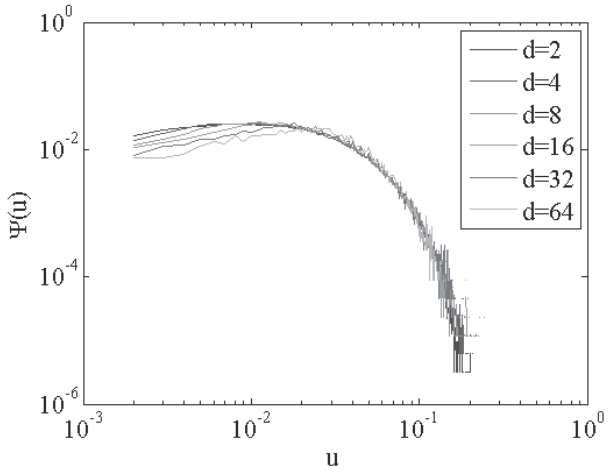

Figure 2: Scaled distribution of the critical depinning toughness showing its independence from the distance d between consecutive active sites.

3. Plasticity of amorphous media

Amorphous media (such as amorphous silica or soda lime glass) can undergo irreversible strains under load and thus appear to behave plastically at a macroscopic level. However, in contrast with crystalline media where dislocation motion and generation is known to be at the origin of plasticity, no extended defects such as dislocations can be defined for such amorphous systems. The present understanding of the mechanism of this plasticity is the occurrence of conformational changes in confined regions of space under the action of an external stress [10]. This view is supported by Molecular Dynamics simulations [11,12]. However, the size of the considered domains and the time duration of a simulation make it difficult to consider large strains in a quasi-static limit. A complementary view is proposed here so as to offer a coarse-grained picture of this phenomenon, which may allow for bridging the scale from atomic scale simulations to a continuum deterministic description. Modeling in this spirit has been proposed in Refs. [5,13].

A two dimensional medium is considered discretized at a scale ℓ. Each element contains one potential "shear transformation zone" which requires a random shear stress threshold in order to change conformation. The latter induces locally a local restructuring which gives rise to a plastic strain, and redistributes the shear stress over the entire medium based on the elastic Green function for an elementary local slip. Here again we choose an extremal dynamics which consists in selecting the site for which the difference between the local stress and the yield threshold is minimum. Figure 3 shows an example of a cumulative plastic shear strain map (where the average has been subtracted off), and an incremental map (for a total of 10 slip events per site).

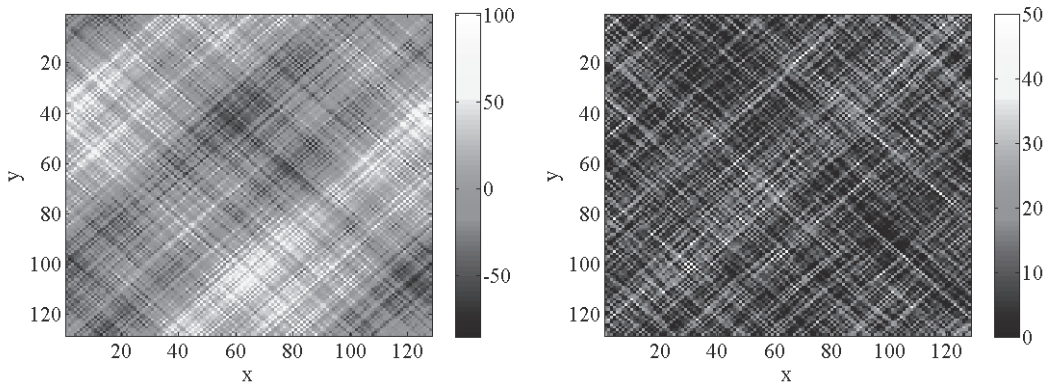

Figure 3: Cumulative (mean subtracted) and incremental shear strain over a square domain with periodic boundary conditions. The self-organization of the shear bands is clearly visible.

We do observe in the steady state a similar self-organization of the yielding as shown in Figure 3. In this example, the elastic coupling is provided by the stress redistribution after each elementary slip. It provides the natural orientation at $\pm\pi/4$ of the plastic strain field. It is interesting to note that at steady state, the yield stress is constant, and hence we are exactly at the borderline of localization. Indeed, the plastic strain pattern is not concentrated over a single slip system (localized), nor uniformly spread over the entire domain. These two cases can however be enforced by adjusting the stress redistribution kernel in order to reproduce either a strain weakening or a strain hardening character at the macroscopic level.

Here again the instantaneous yield stress is not universal as it depends on the local threshold stress distribution. However, if we condition this probability by the distance between consecutive active sites, we have access to globally pinned configurations which reveal a universal distribution of yield stress which can again be characterized only by two of its moments, (mean and standard deviation).

6. Conclusions

The above two examples illustrate the occurrence of *universal* pdf forms for yield stress or toughness, with non trivial power-law scaling with system size. The origin of this behavior is to be found in the criticality of the onset of depinning, and the long range elastic couplings which make the phenomenon intrinsically collective. We insisted on the statistical distribution of the

macroscopic driving force, however a number of other features characterizing the morphology of the crack front or the distribution of cumulative plastic strain can be analyzed within the same framework and can be characterized by related critical exponents. Unfortunately, these critical exponents cannot be obtained today through an analytic derivation, and hence they require the use of numerical simulations.

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Multiscale computations of fracture: quantum to continuum

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ABSTRACT

The prediction of the strength of materials from fundamental principles poses a formidable challenge. Since bond breaking is involved, a first principles attack on the problem requires quantum mechanical modeling at the bond breaking level. However, it has become apparent that even at the nanoscale, strength seems to be dominated by defects in the specimen. To study such defects in terms of basic physics, quantum mechanics is usually necessary to model bond breaking. However, to account for defects, the models must be substantially larger than can be treated by quantum mechanics with modest computational power. Here a coupled method for quantum/molecular/continuum mechanics is described. A method for coupling quantum mechanics with molecular mechanics is summarized, as well as methods for coupling molecular mechanics with continuum mechanics [1].

The coupled method is then applied to the analysis of the strength of crystalline carbon nanotubes and nanoscale graphene sheets with defects. Both holes and slitlike defects that are similar to cracks are considered. The results show that the strength in crystalline carbon diminishes rapidly with flaw size and in fact agrees quite closely with the Griffith formula when the surface energy is obtained by a quantum calculation. Computations of the strength of amorphous carbon nanostructures have also been made [2]. The environment-independent interatomic potential of Marks, which is well suited to amorphous carbon, is used. These manifest much less decrease in strength with increasing flaw size, indicative of a flaw tolerance.

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In pursuit of imperfection: can modelling help?

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ABSTRACT

The beauty of the perfection of crystals grabs attention, but materials scientists know that it is the imperfection in crystalline materials that can hold the interest. Whilst most of the basic properties of crystal defects were established long ago, important details have lain undiscovered. Not all are amenable to experimental investigation, but, with the aid of modern computing power, modelling by simulation can be a powerful aid to the researcher. This paper will review a few topics in an attempt to justify this claim. It will focus on radiation damage, dislocation-obstacle interactions and interfaces in metals.

Displacement cascades are the primary source of radiation damage in fast neutron- and ion-irradiated metals. Atomic-scale computer simulation has revealed details of the population and clustering of defects in cascades and their dependence on parameters such as the energy and mass of the primary knock-on atom. Simulation is also being used to investigate the interaction of dislocations with defects in irradiated metals under external stress. Processes such as defect absorption and transformation have been identified, and parameters associated with the obstacle strength of defects have been determined. This information is required for reliable modelling at the continuum level in the multi-scale framework. Finally, simulation can provide information of defect processes in boundaries to supplement conventional models based on crystallography. Examples include absorption of a crystal dislocation by a moving twin boundary and its transformation into a defect source of twinning dislocations, and the interaction between a moving boundary and point defect clusters that leads to either defect absorption by the boundary or boundary pinning.

Coupling of Atomistic and Continuum Scales

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ABSTRACT

The paper describes various multiscale approaches aimed at bridging between atomistic and continuum scales developed by the author. The multiscale approaches are grouped into two main categories: information-passing and concurrent. In the concurrent multiscale methods both, the discrete and continuum scales are simultaneously resolved, whereas in the information-passing schemes, the discrete scale is modelled and its gross response is infused into the continuum scale. Most of the information-passing approaches provide sublinear computational complexity, (i.e., scales sublinearly with the cost of solving a fine scale problem), but the quantities of interest are limited to or defined only on the coarse scale.

1. Introduction

A modelling and simulation approach is termed multiscale if it is capable of resolving certain quantities of interest with a significantly lower cost than solving the corresponding fine-scale system. Schematically, a multiscale method has to satisfy the so-called Accuracy and Cost Requirements (ACR) test:

$$\boxed{\begin{array}{l} \textit{Error in quantities of interest} < \textit{tol} \\ \dfrac{\textit{Cost of multiscale solver}}{\textit{Cost of fine scale solver}} \ll 1 \end{array}}$$

This paper focuses on two categories of multiscale approaches: information-passing and concurrent. In the information-passing multiscale approach (see Section 2), the discrete scale is modelled and its gross response is infused into continuum (or discrete coarse-grained) scale, whereas in the concurrent approach (see Section 3), both, the discrete and continuum scales (or coarse-grained) are simultaneously resolved.

Loosely speaking, the information-passing multiscale approach is likely to pass the so-called ACR (Accuracy and Cost Requirements) test provided that:
(i) the quantities of interest are limited to or defined only on the coarse scale (provided that this quantities are computable from the fine scale), and
(ii) special features of the fine scale problem, such as scale separation and self-similarity, are taken advantage of.

On the other hand, for the concurrent multiscale approach to pass the ACR test, the following conditions must be satisfied:
(i) the interface (or interphase) between the fine and coarse scales should be properly engineered (see Section 3), and
(iia) the information-passing multiscale approach of choice should serve as an adequate mechanism for capturing the lower frequency response of the fine-scale system, or alternatively,
(iib) the fine scale model should be limited to a small part of the computational domain.

The ACR condition (iia) represents a stronger requirement typically satisfied by multigrid-based concurrent methods (see Section 3.2), but not by domain decomposition based (Section 3.1) concurrent methods. It is important to note that even though concurrent approaches

may pass the ACR test, their computational cost will typically exceed that of the information-passing methods. Nevertheless, they offer a distinct advantage over the information-passing methods by virtue of being able to resolve fine scale details in critical regions. Therefore, concurrent multiscale approaches are typically pursued when the fine scale information is either necessary, or if not resolved, may pollute significant errors on the coarse scale information of interest.

2. Information-passing multiscale methods

In the information-passing multiscale methods, calculations at finer scale, and of high-computational complexity, are used to evaluate certain quantities for use in a more approximate or phenomenological computational methodology at a longer length/time scale. This type of scale bridging is also known as sequential, serial or parameter-passing. For nonlinear problems, fine and coarse scale models are two-way coupled, i.e., the information continuously flows between the scales.

In this section we review several information-passing bridging technique including: the Generalized Mathematical Homogenization (GMH) theory [1-4], which constructs an equivalent continuum description directly from molecular dynamics (MD) equations; and the Multiscale Enrichment based on the Partition of Unity (MEPU) method [5], which gives rise to the enriched coarse grained formulation

2.1 Generalized Mathematical Homogenization (GMH) theory

In the GMH approach a multiple scale space-time asymptotic expansion is employed to approximate the displacement field

$$\boldsymbol{u}(\boldsymbol{x},\boldsymbol{y},\tau,t,s_i)=\boldsymbol{u}^0+\varepsilon\boldsymbol{u}^1\ldots$$

where $\boldsymbol{x}$ is a differentiable continuum coordinate; $\boldsymbol{y}=\boldsymbol{x}/\varepsilon$ the discrete coordinate denoting position of atoms in a unit cell and $0<\varepsilon\ll 1$; τ the fast time coordinate, which tracks vibration of atoms for finite temperature applications; t the usual time coordinate; s_i the slow time coordinates, which from the physics point of view capture dispersion effects, whereas from the mathematics point of view eliminate secularity of asymptotic expansions. We first outline the $O(1)$ GMH theory without consideration of slow time scales.

The primary objective of GMH is to construct continuum equations directly from Molecular Dynamics (MD) equations

$$m_i(\mathbf{Y}_i)\ddot{\mathbf{u}}_i(\mathbf{X}_i,\mathbf{Y}_i,t,\tau)=\frac{1}{\varepsilon}\sum_{j\neq i}\mathbf{f}_{ij}(\mathbf{x}_{ij})$$

where $\boldsymbol{f}_{ij}$, $\mathbf{x}_{ij}$ are the interatomic force and the radius vector between atoms i and j, respectively; and m_i is the mass of atom i. Capital and lower case letters denote initial and current positions of atoms, respectively. For simplicity pairwise interatomic potential is considered, which may be inadequate for solids. Expanding $\mathbf{x}_{ij}=\varepsilon\mathbf{x}_{ij}^0+\varepsilon^2\mathbf{x}_{ij}^1+\ldots$ in asymptotic sequence and the force field $\boldsymbol{f}_{ij}$ in Taylor's series expansion around the leading order term $\varepsilon\mathbf{x}_{ij}^0$ yields a set of coupled continuum-atomistic governing equations:

(i) Fine scale equation:

$$\frac{m_i}{\varepsilon}\frac{\partial^2\mathbf{u}^1}{\partial\tau^2}=\sum_{j(\neq i)}\mathbf{f}_{ij}\left\{(\mathbf{F}(\mathbf{u}^0)\cdot\left[\mathbf{X}_{ij}+\varepsilon\left(\mathbf{u}^1(\mathbf{x}_j)-\mathbf{u}^1(\mathbf{x}_i)\right)\right]\right\}$$

subjected to the deformation gradient $\mathbf{F}(\mathbf{u}^0)$ and temperature T obtained from the continuum equations.

(ii) Coarse scale mechanical equation

$$\rho_0\frac{\partial^2\mathbf{u}^0(\mathbf{X},t)}{\partial t^2}-\nabla_{\mathbf{X}}\cdot\langle\mathbf{P}\rangle=0\qquad\mathbf{P}(\mathbf{X},t,\tau)=\frac{1}{2\Theta}\sum_{i=1}^{n}\sum_{j\neq i}[\mathbf{f}_{ij}\otimes\mathbf{X}_{ij}]$$

(ii) Heat flow (coarse scale) equation

$$C\frac{\partial\langle T\rangle}{\partial t}-\nabla_{\mathbf{X}}\cdot\langle\mathbf{q}(\mathbf{X},t,\tau)\rangle=-2\langle\mathbf{P}\rangle:\nabla_{\mathbf{X}}\frac{\partial\mathbf{u}^0(\mathbf{X},t)}{\partial t}$$

$$\mathbf{q}(\mathbf{X},t,\tau)=\frac{1}{2\Theta}\sum_{i=1}^{n}\sum_{j\neq i}[(2\frac{\partial\mathbf{u}^0}{\partial t}+\frac{\partial\mathbf{u}_i^1}{\partial\tau})\cdot(\mathbf{f}_{ij}\otimes\mathbf{X}_{ij})]$$

where $\mathbf{P}$ and $\mathbf{q}$ are the First Piola-Kirchhoff stress tensor and thermal flux vector, respectively; T the temperature; ρ the density; Θ the volume of the atomistic unit cell; $\boldsymbol{\nabla}_X\cdot(\,)$ the divergence operator with respect to the initial coordinates; $\mathbf{X}_{ij}$ the initial separation between atoms i and j.

The temporal averaging operator is defined as

$$\langle\chi(\tau)\rangle=\frac{1}{\tau_0}\int_0^{\tau_0}\chi(\tau)d\tau$$

where τ_0 is a characteristic time period of the function $\chi(\tau)$.

It can be seen that the First Piola-Kirchoff stress derived from the $O(1)$ GMH theory coincides with the mechanical term in the virial stress formula.

The motivation for introduction of slow time scales was given in [6], where it has been shown that in absence of slow time scales the scaling parameter $\varepsilon=O\left(\sqrt{\bar{t}}\right)$ becomes time dependent, where $\bar{t}$ is the normalized time coordinate. Consequently, as $\bar{t}\to\infty$ the asymptotic expansion becomes no longer uniformly valid.

Higher order GMH theory incorporating slow time scales leads to the nonlocal continuum description. Alternatively, a close form solution for slow time scales can be obtained leading to an algebraic system of equations with a single time scale [2].

2.2 Multiscale Enrichment based on the Partition of Unity

Multiscale Enrichment based on Partition of Unity (MEPU) [5] is a synthesis of the generalized mathematical homogenization and Partition of Unity methods and is closely related to XFEM [7]. MEPU can be used to enrich the coarse scale continuum description or the coarse-grained discrete formulations. It is primarily intended to extend the range of applicability of the mathematical homogenization theory to problems where scale separation may not be valid, such as in the case of nonperiodic solutions or problems where the coarse solution may rapidly vary over the domain of a unit cell.

MEPU belongs to the category of methods employing hierarchical decomposition of the approximation space in the form of

$$\boldsymbol{u}=\boldsymbol{u}^c+\boldsymbol{u}^f$$

where $\boldsymbol{u}^c$ and $\boldsymbol{u}^f$ are the coarse and fine scale solutions, respectively. Note that in GMH $\boldsymbol{u}^c=\boldsymbol{u}^0(\boldsymbol{x})$ and $\boldsymbol{u}^f\approx\varepsilon\boldsymbol{u}^1(\boldsymbol{x},\boldsymbol{y})$. In MEPU, on the other hand,

$$\mathbf{u}=\sum\mathbf{N}(\boldsymbol{x})\mathbf{d}+\sum\mathbf{H}(\boldsymbol{x})\mathbf{N}(\boldsymbol{x})\mathbf{a}$$

where $\mathbf{N}$ are the coarse scale element shape functions; $\mathbf{H}(\boldsymbol{x})$ the influence function obtained from the unit cell solution; $\mathbf{d},\mathbf{a}$ the nodal and enrichment degrees-of-freedom, respectively. The influence functions can be either discrete (obtained from the atomistic unit cell) or continuous. MEPU allows consideration of nonperiodic fields by associating different unit cells with different Gauss points in the coarse scale elements.

3. Concurrent multiscale methods

In this section we present a class of multiscale approaches for systems, whose behaviour depends on physics at multiple scales. For problem such as fracture, multiple scales have to be simultaneously resolved in different portions of the problem domain. Multiscale methods based on the concurrent resolution of multiple scales are often coined as embedded, concur-

rent, integrated or hand-shaking multiscale methods. Various domain decomposition based methods and multigrid based methods are used to communicate the information between the subdomains represented by different mathematical models.

In the remainder of this section we outline the basic ideas of the domain decomposition [8, 9] and multigrid [10, 11] based concurrent multiscale methods common to several aforementioned approaches. We emphasize that the above multiscale methods are concerned with a concurrent bridging of dissimilar mathematical models representing different scales, as opposed to the classical domain decomposition, multigrid and enrichment methods, which are primarily concerned with efficient solution of a single scale mathematically similar models.

3.1 Domain Decomposition based Concurrent Multiscale Method

The strong form of equilibrium equation in the interface Ω^I is given by blending

$$\left\{\Theta^c(x)\sigma_{ij}\right\}_{,j} + \Theta^c(x)b_i + \sum_{\alpha}^{n^I}\left[\left\{\sum_{\beta}^{n\alpha\beta}\left(\Theta^A_{\alpha\beta}f_{i\alpha\beta}\right) + \Theta^A_{\alpha}b_{i\alpha}\right\}\delta(x-x_\alpha)\right] = 0$$

$$\Theta^A_{\alpha} = 1-\Theta^c(x_\alpha) \qquad \Theta^A_{\alpha\beta} = 1-0.5\left\{\Theta^c(x_\alpha)+\Theta^c(x_\beta)\right\}$$

subjected to weak compatibility condition in the overlap region [10]. In the above, n^I is the number of atoms in the interphase, δ is the Dirac delta, $f_{i\alpha\beta}$ *is i*-th component of interatomic force between atoms α and β; $\Theta^c(x)$ is continuum blend function evaluated based on the proximity of the point x in the interphase to the continuum region. The above equation can be extended on the whole problem domain by defining $\Theta^c(x) = 0$ in the atomistic region and $\Theta^c(x) = 1$ in the continuum domain. For derivation of the weak form and implementation details see [10, 11].

3.2 Multigrid based Concurrent Multiscale Method

The motivation for use of multigrid ideas for multiscale problems was given in [12, 13]. To convey the basic ideas, consider a one-dimensional two-scale elliptic problem

$$\frac{d}{dx}\left(K(x)\frac{du}{dx}\right) + b(x) = 0 \quad x \in (0,L) \quad u(0) = u(L) = 0$$

with oscillatory periodic piecewise constant coefficients K_1, K_2 and *0.5* volume fraction.

The above equation is discretized with *2 (m-1)* elements - each element possessing constant coefficients. The eigenvalues can be computed in a closed form:

$$\lambda^i = \frac{\frac{4\tilde{K}}{h}\sin^2\left(k\frac{\pi}{2m}\right)}{1+\sqrt{1-q\sin^2\left(k\frac{\pi}{2m}\right)}}, \quad \lambda^{2m-k} = \frac{\frac{4\tilde{K}}{h}\sin^2\left(k\frac{\pi}{2m}\right)}{1-\sqrt{1-q\sin^2\left(k\frac{\pi}{2m}\right)}}$$

where $1 \le k < m$; *2h* the unit cell size; $\tilde{K}$ the overall coefficients and q the ratio between geometric and arithmetic averages of the coefficients given as:

$$\tilde{K} = \frac{2K_1K_2}{K_1+K_2}, \quad \sqrt{q} = \frac{\sqrt{K_1K_2}}{(K_1+K_2)/2}$$

Note that in many applications of interest and in particular those described at the atomistic scale $K_1 \gg K_2$ or $K_2 \gg K_1$ or $0 < q \ll 1$. Consequently, the eigenvalues are clustered at the two ends of the spectrum, with one half being $O(1)$ and the other half being $O(1/q)$. More importantly, the $O(1)$ eigenvalues are identical to those obtained by the problem with homogenized coefficients. This character of the spectrum suggests a computational strategy based on the philosophy of multilevel methods. In such a multilevel strategy smoother is designated to capture the higher frequency response of the fine scale model represented by a linear combination of the $O(1/q)$ eigenmodes. The auxiliary coarse model is then engineered to effectively capture the remaining lower frequency response of the fine scale problem. For a periodic heterogeneous medium, such an auxiliary coarse model coincides with the boundary

value problem with homogenized coefficients as evidenced by the identical eigenvalues. The resulting multiscale prolongation Q operator is given by

$$Q = Q^c + Q^f$$

where Q^c, Q^f are the classical (smooth) prolongation and the fine scale correction obtained from the discretization of the influence functions, respectively. The rate of convergence of the multigrid process for the two-scale problem is governed by [12, 13]:

$$\|e_{i+1}\| = q\|e_i\|/(4+q)$$

where $\|e_{i+1}\|$ is the norm of error in iteration *i+1*. For example, if either K_1/K_2 or K_2/K_1, is 100, then the two-scale process converges in three iterations up to the tolerance of 10^{-5}.

In principle, any information-passing approach described in Section 2 can be used as an auxiliary coarse model to capture the lower frequency response of the fine scale problem. The multiscale prolongation depends on the choice of the information-passing approach.

To this end we describe the application of multigrid ideas to bridging diverse time scales. The space-time variational multigrid method developed in [14] is aimed at bridging between atomistic scale and either coarse grained discrete or continuum scales. The method consists of the wave-form relaxation scheme aimed at capturing the high frequency response of the atomistic vibrations and the coarse scale solution in space and time intended to resolve smooth features of the discrete medium. The waveform relaxation decomposes the system into very small subsystem (for instance, atom-by-atom decomposition) which can be integrated in parallel and take advantage of unstructured time integrators. The waveform relaxation can be also interpreted as atom-by-atom minimization of MD Hamiltonian.

The a coarse model correction at a certain time step $u^f + Qe^c$ can be calculated from the Hamilton principle on the subspace of coarse scale functions

$$H(\boldsymbol{e}^c) = \sum w^f \left(\boldsymbol{u}^f + Q\boldsymbol{e}^c\right) + \sum \frac{1}{2} m\left(\dot{\boldsymbol{u}}^f + Q\boldsymbol{e}^c\right)^T \left(\dot{\boldsymbol{u}}^f + Q\boldsymbol{e}^c\right) \to \min_{e^c}$$

The method has been used to simulate a polymer structure and compared to the classical explicit integration. Significant speed-ups have been observed in particular on parallel machines.

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