
OVERVIEW ON MATERIALS RESEARCH ACTIVITIES AT UCLA

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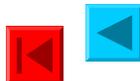
August 27-28, 2001



OBJECTIVES - 1

➤ Technology:

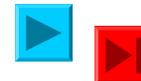
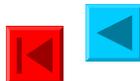
- 1. To develop new-engineered materials by computational design for future energy sources in magnetic- and laser- based systems;*
- 2. To design materials at the nano- and micro-scale for applications in the Nuclear, Aerospace and Microelectronics Industries;*
- 3. To utilize plasma as the fourth state of matter for experimental development of novel materials processing techniques.*



OBJECTIVES - 2

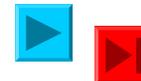
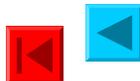
➤ **Fundamental:**

- 1. To provide predictive relations between the microstructure of the material at the microscopic scale with its mechanical properties at the macroscopic scale by computational modeling;*
- 2. To study the collective behavior of defects in materials by large-scale computer simulations;*
- 3. To investigate the fundamental aspects of pattern formation, non-equilibrium phase transitions and instability phenomena.*

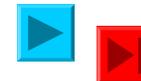
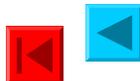


UCLA GROUP AT A GLANCE!

- *Joined UCLA in 1977. Participated in most fusion system and material studies for ~ 25 years.*
- *Over 200 Publications (more than 150 refereed journal articles).*
- *Research covers the physics and mechanics of materials, radiation interaction with solids, energetic (plasma, ions & laser) material processing, and thermo-mechanical design.*
- *33 graduates with M.S. degree, 16 with the Ph.D. degree and 28 post-doctoral or research staff. 5 graduates hold professorships.*



CURRENT RESEARCH TEAM - 1



Current Research Team - 2

➤ Research Staff:

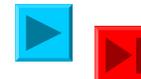
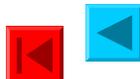
1. *Shahram Sharafat -- Senior Research Engr. (Part time till 12/01).*
2. *Shih-his Tong – Post Doc. -- Computational Geometry*
3. *Xueli Han - Associate Research Engr. -- Micromechanics*

➤ Ph.D. Students:

1. *Gregory Johnson -- Nucleation of Nano-clusters.*
2. *Jianming Huang -- DBTT Dislocation Modeling.*
3. *Ming Wen -- Atomistic-Continuum Models of Defects.*
4. *Zhiqiang Wang – Interface Effects on Surface Deformation.*
5. *Qiyang Hu – Material System Design of Laser Optics.*

➤ M.S. Students:

1. *Gigio Sakota -- Rate Theory of Irradiated Materials.*



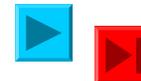
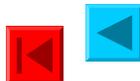
RESEARCH PROJECTS - 1

- **Laser Effects on Surface Deformation and Roughening of Optics.**

- **Funding Agency:**
Department of Energy / Office of Fusion Energy Sciences/ Laser IFE

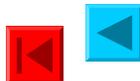
- **Duration & Funding:**
Three Years:(August 2000-July 2003) ~ 130K/ yr

- **Objectives:**
 1. Determine the physical mechanisms responsible for damage and degradation of the optical qualities of IFE final optics.
 2. Design material systems for IFE final optics that are resistant to damage of a single laser pulse, and to the progressive damage of multiple pulses.



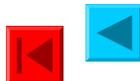
RESEARCH PROJECTS - 2

- **Large-scale Dislocation Dynamics Simulations for Computational Design Of Semiconductor Thin Film Systems .**
- **Funding Agency:**
National Science Foundation/ DMR & IT.
- **Duration & Funding:**
Three Years:(September 2001- August 2004) ~ 100K/ yr
- **Objectives:**
 1. Investigate single and collective dislocation interaction phenomena in anisotropic materials, which determine plasticity and failure of semiconductor devices .
 2. Large-scale simulations and optimization of semiconductor systems to provide guidelines for engineering design of new generations of microelectronics .



RESEARCH PROJECTS - 3

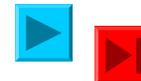
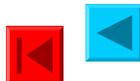
- **Computational Design of Fusion Materials (with UCSB).**
- **Funding Agency:**
Department of Energy / Office of Fusion Energy Sciences/ Fusion Materials Science
- **Duration & Funding:**
Three Years:(April 2001-April 2004) ~ 80 K/ yr
- **Objectives:**
 1. Develop predictive Monte Carlo and Rate Theory Computer Models for Microstructure and non-equilibrium phase evolution;
 2. Suggest Fe and V alloy designs for optimum mitigation of the effects of helium and non-equilibrium phases on mechanical properties.



RESEARCH PROJECTS - 4

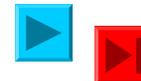
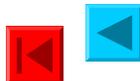
- **Plasticity and Fracture Mechanisms of Fusion Materials.**
- **Funding Agency:**
Department of Energy / Office of Fusion Energy Sciences/ Fusion Materials Science
- **Duration & Funding:**
Five Years:(July 1998-July 2003) ~ 185K/ yr + ~ 50K/ yr (JUPITER-II).
- **Main Objective:**
Computer Modeling of the main phenomena involved in plastic flow localization and associated fracture instabilities under irradiation.

Modeling is strongly tied to national and international research programs to assist in optimized alloy designs and material selection.



Specific Objectives of Research on Plasticity and Fracture

- **Radiation hardening,**
- **Helium effects on grain boundary fracture,**
- **Stress-induced impurity segregation and cracking,**
- **Ductile-to-brittle-transition behavior,**
- **Mechanisms of Flow Localization and Failure,**
- **Applications to FCC (e.g Cu) and BCC (e.g. Fe and V) for optimum alloy designs.**



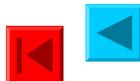
Recent Publications Funded by OFES (5 yr period)

1. N.M. Ghoniem and A. Elazab, "Thermo-mechanical Design of the Grazing Incidence Metal Mirror of the Prometheus-IFE Reactor", *Fusion Engineering and Design*, 29: 89-97, 1995.
2. A. Elazab and N.M. Ghoniem, "Mechanical Response and Fatigue Analysis of the First Wall structure of the Prometheus IFE Reactor", *Fusion Engineering and Design*, 27: 536-543, 1995.
3. A. Elazab and N.M. Ghoniem, "Visco-elastic Analysis of Mismatch Stresses in Ceramic Matrix Composites under High-Temperature Neutron Irradiation", *Mechanics of Materials*, 20: 291-303, 1995.
4. H. Huang, N.M. Ghoniem, J. Wong, and M. Baskes, "Molecular Dynamics Determination of Defect Energetics in Beta-SiC Using Three Representative Empirical Potentials", *Mod & Sim in Mat Sci & Eng*, 3: 615-627, 1995.
5. H. Huang and N.M. Ghoniem, "Formulation of a Moment Method for n-dimensional Fokker-Planck Equations", *Phys. Rev. E*, 51, 6: 5251-5260, 1995.
6. D. Walgraef and N.M. Ghoniem, "Non-linear Dynamics of Self-organized Microstructures Under Irradiation", *Phys. Rev. B*, 52,6: 3951-3962, 1995.
7. A. Elazab and N.M. Ghoniem, "Investigation of Time for sub-critical Crack Propagation in SiC-SiC Composites", *J. Nucl. Mater.*, 219: 101-109, 1995.



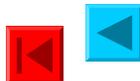
Recent Publications Funded by OFES (5 yr period)

8. A. Elazab and N.M. Ghoniem, "Stability and Evolution of Crack Systems in Dissipative Materials", ASME, *Applied Mechanics Division (AMD-Vol. 200)/ Materials Division (MD-Vol. 57)*, 57: 55-73, 1995.
9. A. Elazab and N.M. Ghoniem, "Time-Dependent Micro-mechanics in Damaged High-Temperature Ceramic Composites, ASME, *Applied Mechanics Division (AMD-Vol. 99)/ Materials Division (MD-Vol. 55)*, 55:235-38,1995.
10. D. Walgraef, J. Lauzeral, and N.M. Ghoniem, "Theory and Simulations of Defect Ordering in Irradiated Materials", *Phys. Rev. B*, 53,22: 14782-14794, 1996.
11. H. Huang and Nasr Ghoniem, "A Swelling Model For Stoichiometric SiC At Temperatures Below 1000 °c Under Neutron Irradiation", *Jour. Nucl. Mater.*, 250: 192-199 (1997).
12. D. Walgraef, N.M. Ghoniem, and J. Lauzeral, "Deformation Patterns in Thin Films Under Uniform Laser Irradiation", *Phys. Rev. B*, 56, No. 23: 15361-15377 (1997).
13. J. Lauzeral, D. Walgraef, and N.M. Ghoniem, "Rose Deformation Patterns in Thin films Irradiated By Focused Laser Beams", *Phys. Rev. Lett.* 79, No. 14: 2706-2709 (1997).
14. N.M. Ghoniem, "Clustering Theory of Atomic Defects", *Radiation Effects and Defects in Solids*, 148: 269-318 (1999).



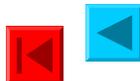
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15. N.M. Ghoniem, "Atomic Processes During Damage Production and Defect Retention", *J. Nucl. Mater.*, 258-263: 113-123 (1997).
16. H. Huang, N.M. Ghoniem, T. Diaz de la Rubia, M. Rhee, H. Zbib and J. Hirth, "Stability Of Dislocation Short-Range Reactions In Bcc Crystals", *J. Eng. Mat. & Tech.*, 121(2): 143 (1999).
17. N.M. Ghoniem, "Curved Parametric Segments For The Stress Field Of 3-D Dislocation Loops", *J. Eng. Mat. & Tech.*, 121(2): 136 (1999).
18. L. J. Perkins, B. G. Logan, M.D. Rosen, M.D. Perry, T. Diaz de la Rubia, N.M. Ghoniem, T. Ditmire, S. Wilkes and P.T. Springer, "The Investigation of High-Intensity-Laser Driven Micro Neutron Sources for Fusion Materials Applications at High Fluence", *Nuclear Fusion*, 40(1): 1-19 (2000).
19. N. M. Ghoniem, L. Sun, "Fast Sum Method for the Elastic Field of 3-D Dislocation Ensembles", *Phys. Rev. B*, 60(1): 128-140 (1999).
20. D. Walgraef and N.M. Ghoniem, "Modeling laser-Induced Deformation patterns: Nonlinear Effects and Numerical Analysis ", *J. Comp.-Aided Mat. Design*, 6(2&3): 323-335 (1999).
21. G. A. Johnson and N.M. Ghoniem, " Hierarchical Modeling of C and Si Nano-cluster Nucleation Utilizing Quantum and Statistical Mechanics ", *J. Comp. - Aided Mat. Design.*, 6(2&3): 337-347 (1999).



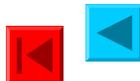
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22. N.M. Ghoniem, S.H. Tong, and L.Z. Sun, "Parametric Dislocation Dynamics: A Thermodynamcis-based Approach to Investigations of Mesoscopic Plastic Deformation", *Phys. Rev. B*, B1(1):913-927(2000).
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24. Nasr M. Ghoniem, "Computational Methods For Mesoscopic, Inhomogeneous Plastic Deformation", *Proceddings of First Latin American Symposium on Materials Instabilities*, Valpareso, Chile, Kluwer Publication, 2000.
25. L.Z. Sun, N. M. Ghoniem, S. Tong and B.N. Singh, "3-D Dislocation Dynamics Study of Plastic Instability in Irradiated Copper", *J. Nucl. Mater.*, 283:741(2000)
26. S.J. Zinkle and N.M. Ghoniem, "Operating Temperature Windows for Fusion Reactor Structural Materials", *Fusion Engineering and Design*, 51-52(2000), pp55
27. N.M. Ghoniem, B. N. Singh, L. Z. Sun, and T. Diaz de la Rubia, "Interaction and Accumulation of Glissile defect Clusters Near Dislocations", *J. Nucl. Mater*, 276: 166-177 (2000).
28. S. Sharafat, A. Kobayashi, S. Chen, and N. Ghoniem, "Production Of High-Density Ni-Bonded Tungsten Carbide Coatings Using An Axially Fed DC-Plasmatron", *J. Surface and Coatings Technology*, 130: 164-172 (2000).



Recent Publications Funded by OFES (5 yr period)

29. S. Sharafat, A. Kobayashi, V. Ogden, and N. Ghoniem, "Development of composite thermal barrier coatings with anisotropic microstructure", *Vacuum*, 59: 185-193 (2000).
30. L.Z. Sun, N.M. Ghoniem, and Z.Q. Wang, "Analytical and Numerical Determination of the Elastic Interaction Energy between Glissile Dislocations and Stacking Fault Tetrahedra in FCC Metals", *J. Mat. Sci. & Engr.*, A309–310: (2001) 178–183.
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32. Jianming Huang and Nasr M. Ghoniem, "The Dynamics of Dislocation Interaction with Sessile Self-Interstitial Atom(SIA) Defect Cluster Atmospheres", In the Press, *J. Comp. Mat. Science*, 2001.
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Recent Publications Funded by OFES (5 yr period)

35. N.M. Ghoniem, J.M. Huang, and Z.Q. Wang, "Affine Covariant-contravariant Vector Forms for the Elastic Field of Parametric Dislocations in Isotropic Crystals", submitted to *Phil. Mag. Lett.*, 2001.
36. N.M. Ghoniem and J.M. Huang, "Computer Simulations of Mesoscopic Plastic Deformation with Differential Geometric Forms for the Elastic Field of Parametric Dislocations : Review of Recent Progress," Invited Paper at the 5th Euro-Conference on Mechanics of Materials, Delft, Netherlands, March 6-9, 2001, Also in press *J. de Physique*, 2001.
37. D. Walgraef and N.M. Ghoniem, "The Effects of Crystal Anisotropy and Adherence Forces on Laser Induced Deformation Patterns in Thin Films," submitted to *Phys. Rev.*
38. N.M. Ghoniem, D. Walgraef and S. J. Zinkle "Theory and Experiment of Nanostructure Self-organization in Irradiated Materials," Invited Perspective Article, in press *J. Comp. Aided Mat. Design*.

