

March 2004 MIT NANOAM Meeting
Thursday 18th March, 2004-MARRIOTT

Longfellow Room, Third Floor

8:30	-	9:00	Breakfast
9:00	-	9:30	Opening Remarks (<i>W. C. Carter & D. J. H. Cockayne</i>)
9:30	-	10:20	Influence of the IGF Chemistry on Grain Growth Mechanism and Room Temperature Mechanical Properties of Si_3N_4 (<i>R. Satet</i>)
10:20	-	10:50	Coffee
10:50	-	11:40	Structural Characterisation of Interfaces in Si_3N_4 Ceramics by Electron Microscopy (<i>M. Doeblinger</i>)
11:40	-	12:30	Continuum Thermodynamic Approaches to IGFs (<i>M. Tang & C. M. Bishop</i>)
12:30	-	12:50	Short Poster Advertisements
12:50	-	14:20	Lunch EC e-TIP Program (<i>J. Wiggins, OU</i>) Creep of RE-doped Si_3N_4 (<i>S. Wiederhorn, NIST</i>) SiC as parallel to Si_3N_4 (<i>J. Kruzic, LBL</i>) Equilibrium Oxide Surface Layers (<i>J. Luo, Clemson</i>) POSTERS
14:20	-	15:10	Investigating Thermodynamic Properties of Amorphous IGFs in Si_3N_4 and SiC by Electron Diffraction, HR-ELSP, and HRTEM (<i>C. Koch</i>)
15:10	-	16:00	Atomistic Simulations of IGFs in Si_3N_4 (<i>S. H. Garofalini</i>)
16:00	-	16:30	Coffee
16:30	-	17:00	Liquid Density Functional Theory (<i>A. P. Sutton</i>)
17:00	-	17:50	Nanoscale Dispersion Forces and Graded Interface Models: Application To Atomically Structured Grain Boundaries in SrTiO_3 (<i>R. H. French</i>)
17:50	-	18:40	Ab-initio Calculations of the Electronic Structure and Optical Properties of Binary, Ternary and Quaternary Y-Si-O-N crystals Ab-initio Calculations of all Polymorphs of SiC Theoretical Investigations on the $(\text{ZrO}_2)_x(\text{SiO}_2)_{1-x}$ Gate Dielectric Materials (<i>W.Y. Ching</i>)
18:40	-	19:00	Recap of Tuesday/Wednesday Sessions (<i>One from each session</i>)
19:30	-		Dinner-Polcari's

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MODIFIED Friday 19th March, 2004-MARRIOTT

Salon 5 and 6, Second Floor

8:30	-	9:00	Breakfast
9:00	-	9:50	Do Stable SiO _x Films Form on Si Surfaces Below the Wetting Limit? (<i>Y.-M. Chiang, A. Ramos, & M. Tang</i>)
9:50	-	10:40	REELS Studies of Nanometric SiO ₂ Films on Si (<i>F. Paumier</i>) XPS and REELS Studies of Si-Mg-Re-O-N Glasses (Re=La, Lu, Y) (<i>M. Gautier-Soyer</i>)
10:40	-	11:10	Coffee
11:10	-	11:25	Additional Items from WP2 (<i>W. Y. Ching</i>)
11:25	-	11:50	Additional Items from WP4 (<i>M. Rühle</i>)
11:50	-	12:05	Overview of Wednesday Sessions (<i>M. J. Hoffmann, C. M. Bishop, & Y.-M. Chiang</i>)
12:05	-	12:50	Status Overview (<i>R. M. Cannon</i>)
12:50	-	14:20	Lunch Differential Binding Energy for RE Elements in Si ₃ N ₄ (<i>G. Painter, ORNL</i>) Observations on Interfacial Segregation in Si ₃ N ₄ Materials (<i>N. Shibata, ORNL</i>) Grain Boundary Structure and Chemistry in Y-doped and Annealed Si ₃ N ₄ and the Effect on Fracture (<i>A. Ziegler, LLNL</i>) POSTERS
14:20	-	15:00	Comparison of Computational Techniques and Models (<i>Led by A. P. Sutton</i>)
15:00	-	15:30	Overview of Physical Samples (<i>Led by Y.-M. Chiang and M. J. Hoffmann</i>)
15:30	-	16:00	Coffee
16:00	-	17:00	Status of Achievements and Collaborations (<i>Led by R. H. French</i>)
17:00	-	17:30	Changing Work Plans for the Rest of the Current Program (<i>Led by D. J. H. Cockayne</i>)
17:30	-	19:00	New Directions (<i>Led by W. C. Carter</i>) EU Opportunities (<i>J. Nucci, MPI</i>) Opportunities to Relate to the IT Industry (<i>R. H. French</i>) Non-equilibrium Properties (<i>A. P. Sutton</i>)
19:30	-		Dinner-Sydney's Grill

March 2004 MIT NANOAM Meeting Supplemental Informal Discussions

Tuesday 16 March, 2004-MIT

pm	MIT 13-5002	Coarse-graining (Led by C. Koch)	MIT, MPI
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Wednesday 17 March, 2004-MIT

am	MIT 13-5002	Experiments in Si ₃ N ₄ (Led by M. Hoffmann)	Karlsruhe, MPI, MIT, LBL
pm	MIT 13-5002	Relations to Phase-field Models (Led by C. M. Bishop)	MIT, LBL, MPI, Rutgers, UM-KC
pm	MIT 13-3038	Surface Films (Led by Y.-M. Chiang)	UPenn, MIT, CEA, UM-KC
19:00	Dinner	Legal Seafood	

Saturday 20th March, 2004-MIT

am	MIT 13-5101	TEM Interpretation & Collaboration (Led by M. Rühle)	Oxford, MPI, ORNL, Karlsruhe, CEA, Dupont, LBL, MIT
am	MIT 13-5002	Glasses-Atomic Structure and Properties (Led by R. Satet)	ORNL, Karlsruhe, CEA, Dupont, LBL, MIT
am	MIT 13-4106	Experiments and Microstructural Models in Si ₃ N ₄ (Led by R. M. Cannon)	Karlsruhe, MPI, MIT, LBL
12:00	MIT 13-5101	Final Words (R. M. Cannon)	
12:30	Lunch	Bertucci's	

Meeting Participants

Paul Becher (ORNL)
Catherine Bishop (MIT-OU)
Rowland Cannon (LBL)
Craig Carter (MIT)
Yet-Ming Chiang (MIT)
Wai-Yim Ching (UM-KC)
David Cockayne (OU)
Markus Doeblinger (OU)
Paulo Ferreira (MIT)
Roger French (UPenn-Du Pont)
Stephen Garofalini (Rutgers)
Martine Gautier-Soyer (CEA-Saclay)
Michael Hoffmann (Karlsruhe)
Toby Hudson (OU)
Christoph Koch (MPI)
Jamie Kruzic (LBL)
Jian Luo (Clemson)
Chris Marsh (OU)
Julie Nucci (MPI)
Lizhi Ouyang (UM-KC)
Gayle Painter (ORNL)
Fabien Paumier (CEA-Saclay)
Ana Ramos (MIT)
Manfred Ruehle (MPI)
Raphaelle Satet (Karlsruhe)
Bill Shelton (ORNL)
Naoya Shibata (ORNL)
Adrian Sutton(OU)
Ming Tang (MIT)
Shelley Wiederhorn (NIST)
Jason Wiggins (OU)
Graham Winkelman (OU)
Zaoli Zhang (MPI)
Alexander Ziegler (LLNL)