Molecular Modeling in Industry for Electronic Materials: Nanoscale Perspectives

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Honeywell Performance Materials and Technologies

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Understanding Modeling Scales Needed

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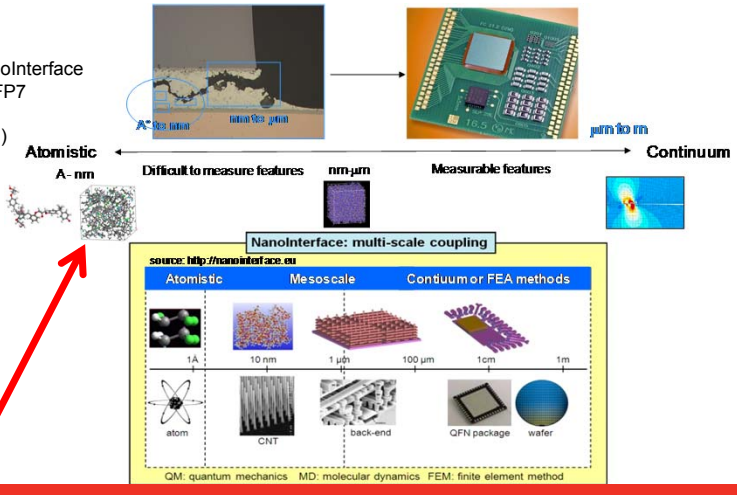
From the NanoInterface Consortium; FP7 (NMP3-SL-20080214371)



The impact of the atomistic/molecular interface is usually ignored by using bulk properties….This can be addressed by use of molecular modeling

The expanse of scales is huge when all of the materials are considered that must work together

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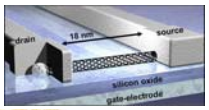
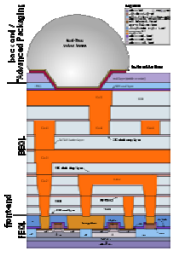
http://newsroom.intel.com/community/intel_newsroom/blog/2014/08/11/intel-discloses-newest-microarchitecture-and-14-nanometer-manufacturing-process-technical-details



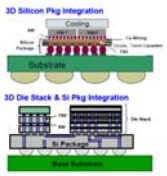
http://www.infineon.com/cms/en/about-infineon/press/press-releases/2004/132191.html

Feb 3, 2015; Scientific Computing

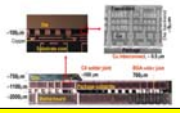
http://www.levitech.nl/technology/integrated-circuit/



(Knickerbocker 2012 NSF workshop)



K.N. Tu Microelectronics Reliability Volume 51, Issue 3, March 2011, Pages 517–523



From the NanoInterface Consortium; FP7 (NMP3-SL-20080214371)

Integration

As feature sizes shrink and densities increase, the critical molecular (or nano) interfaces that initiate and propagate failure become more and more important

With a molecular model, all interfaces reduce to nanoscale issues.

Different Molecular Modeling Scales: Different Information

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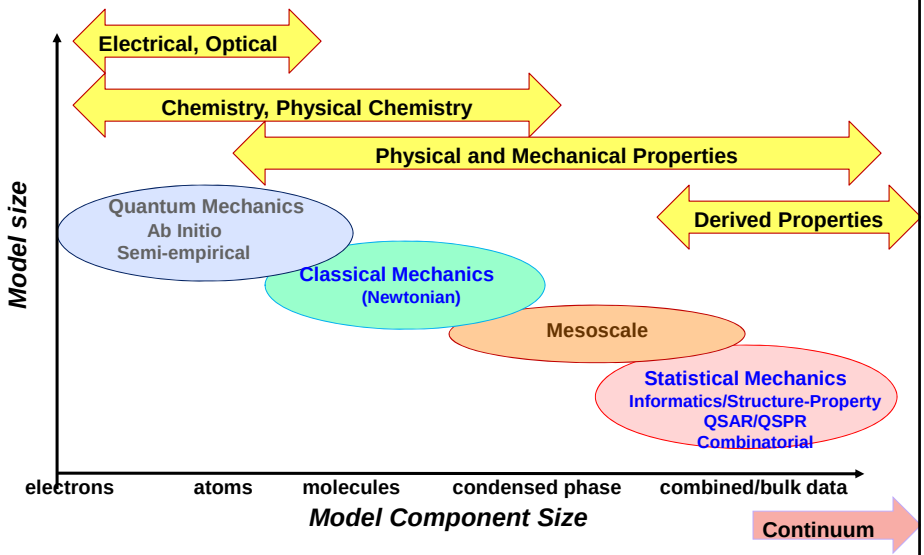

Causes of hi k gate dielectric electrical leakage

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Grain boundary effects on the electronic structure of Hafnium Oxide for hi k dielectrics

G. Bersuker et al. / Solid-State Electronics 65–66 (2011) 146–150

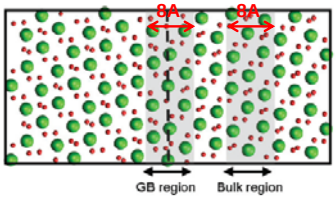

Fig. 3. *Ab initio* model of the (1 0 1) grain boundary in monoclinic HfO_2. Large green and small red balls represent Hf ions and O ions, respectively. The dashed line shows the position of the grain boundary plane. The shaded regions indicate ~8 Å wide regions at the grain boundary and in the bulk. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

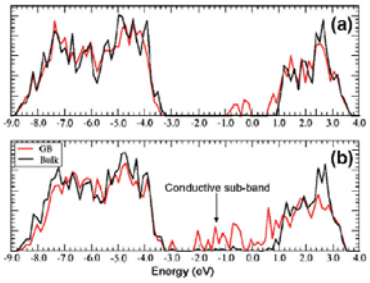

Fig. 5. Density of states associated with the bulk of the monoclinic HfO_2 grain (black line) and the grain boundary (red line). (a) and (b) correspond to low and high concentrations of V_O^0 at the grain boundary, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Molecular models can help in understanding the crystal structure effects on the electronic properties such as electrical leakage

Leakage in a dielectric for flat panel displays

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(From Molecular Modeling and Multiscaling Issues for Electronic Materials v1 Chapter 2)

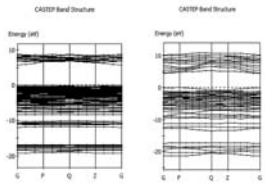
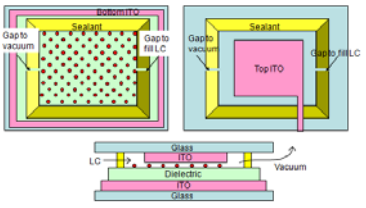


Figure 4. Band structure of a silicate before (left) and after (right) bond cleavage to form SiOH groups.



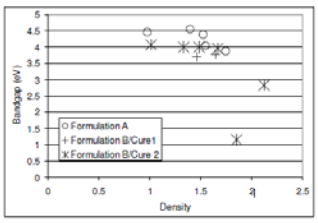


Figure 6. Bandgap (Fermi to Conduction Band gap in eV) comparisons of formulations A and B.

Other molecular models in this materials study included:

- Cure thermodynamics
- Cure volume shrinkage
- Film Mechanical stability

•Iwamoto; Microelectronics Reliability 2009

Understanding the molecular effects can impact understanding at higher scale levels

Enhancing Formulation work

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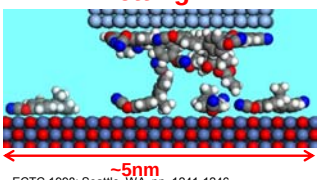
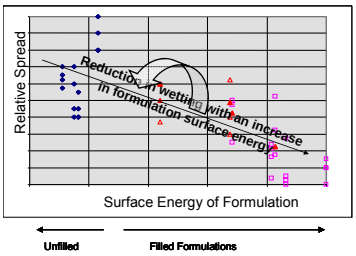
Wetting

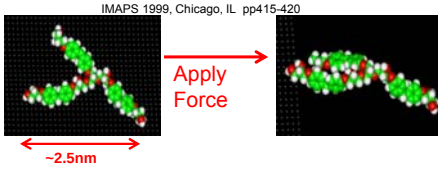


ECTC 1998; Seattle, WA, pp. 1241-1246



Adhesion

IMAPS 1999, Chicago, IL pp415-420



Eurosime 2010 April 26-28, Bordeaux, France

Used to understand wetting and adhesion in:

- **Die attach**
- **Molding compound**
- **Underfill**
- **Dielectrics**
- **Etchants/cleaners**

Understanding the surface/interface effects has aided formulation development

Molecular Coffin-Manson and stress cycling trends

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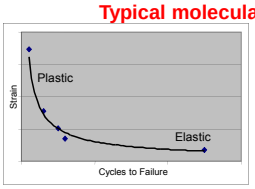
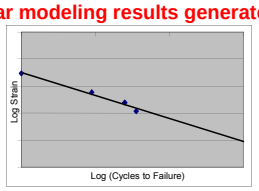
$\varepsilon = M N^z$
(ε = strain, N = #cycles)

A log-log plot gives a linear relationship between strain and cycles

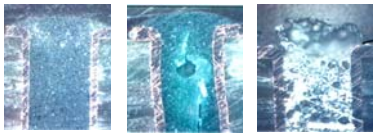
Typical molecular modeling results generated from small oligomer models





- **Both Coffin-Manson and Weibull relationships can be found in relative molecular models**

Package and Board Viafills



JME-AS 500cycles | Competitor A 200cycles | Competitor B 200 cycles

(Condition B: -55 to 125C; liq/liq; 10 min. cycle)

N. Iwamoto, "Simulating Stress Reliability Using Molecular Modeling Methodologies" 32nd International Symposium on Microelectronics; Chicago, Ill, Oct. 26-28, 1999; 1999 Proceedings pp. 415-420

Engineering reliability issues are mirrored on the molecular interface level

Grain Boundary Studies and Mechanical Failure Using Large MD Models

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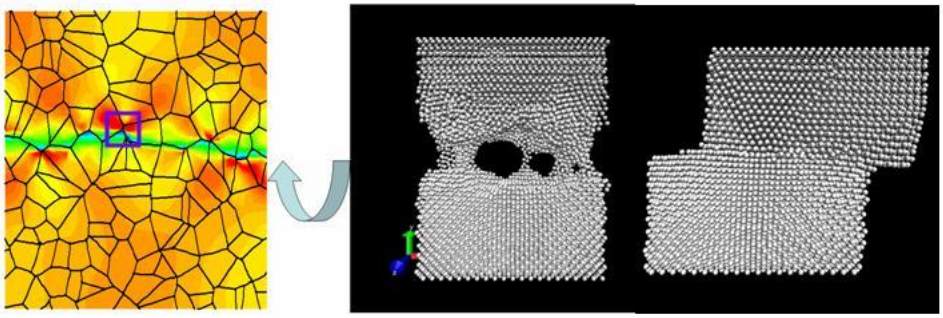

Polycrystal failure simulation using cohesive elements

Molecular dynamics simulation of bicrystal interface

V. Sundararaghavan and N. Zabaras, "Combined MD and continuum approaches towards modeling inter-granular failure using cohesive zone models", 2006 TMS Annual Meeting & Exhibition (D. F. Bahr, J. Lucas and N. R. Moody, organizers), San Antonio, TX, March 12-16, 2006

Atomistic crystal structure studies have been pursued by academia and National Labs for mechanical failure especially for metals.

Mesoscale Models Derived from Molecular Scales

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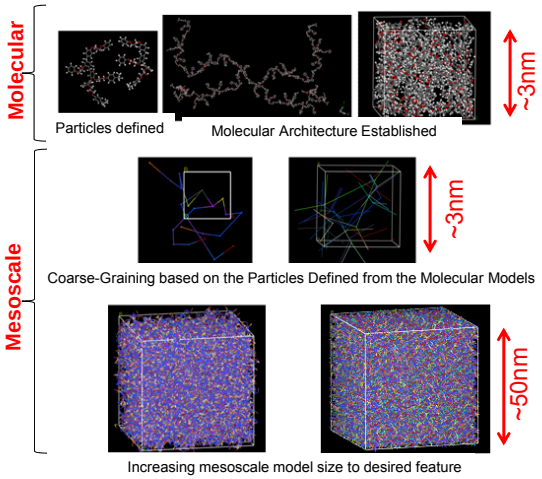

Developed within the EU consortim: NanoInterface Consortium; FP7 (NMP3-SL-20080214371

•Direct parameterization from molecular models can be used in order to scale from molecular to mesoscale

Molecular Modeling and Multiscaling Issues for Electronic Material Applications Ch 14 in vol 1, and Ch 6 in vol 2.

Properties extracted include: modulus, void formation, yield, energy gain/losses, relative strain to break, moisture effects on strength.

Mesoscale Cu Oxide to Epoxy Adhesion: Impact of Moisture On A Molding Compound

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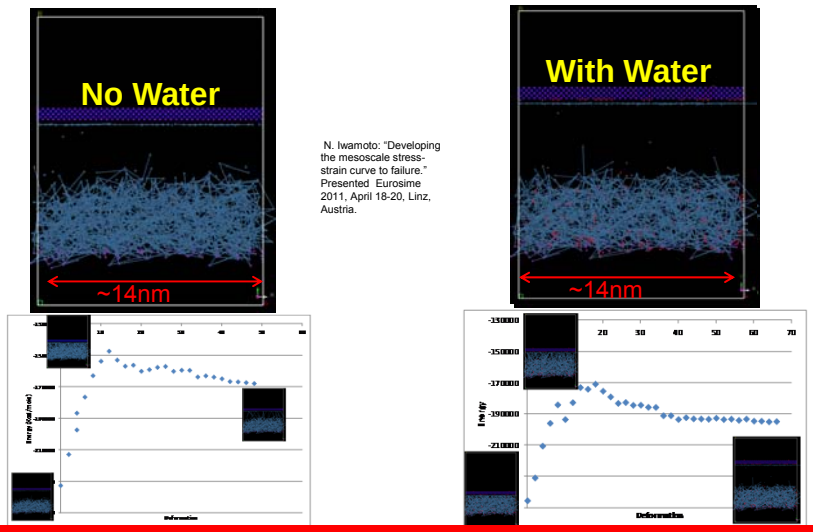

N. Iwamoto: "Developing the mesoscale stress-strain curve to failure." Presented Eurosime 2011, April 18-20, Linz, Austria.

Water tends to lower the energies, and plasticize the response (higher deformation)

Molecular modeling: bridging the link between chemical composition and performance

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- **Molecular modeling should be integrated with other models to improve predictions**
  - Fills-in the atomistic understanding and how chemistry (and chemical structures) contributes to performance (i.e. identify what can initiate and propagate failure?)
    - Immediate Needs:
      - Meshing the results of molecular models into larger scales and into life equations
    - Future Needs:
      - Dynamically change chemical and physical properties in engineering models based on molecular models
      - Develop life-equations that take into account chemical and property changes.
- **Materials Genome Initiative (DOE/DOD/NFS/NIST)…2X Faster, 2X Cheaper**
  - What's the best way to get the right materials chemistry into engineering models and products faster?
    - Software? Data bases? Informatics? Standards etc??….. All also identified issues in the ITRS roadmap

Is Nanoscale Hype?....Not to molecular modeling, where the perspective has always been nanoscale.