Nano/Micro–Engineered Interfaces for Improved Performance and Reliability

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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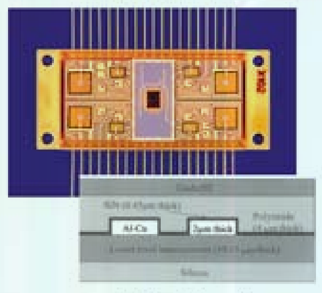
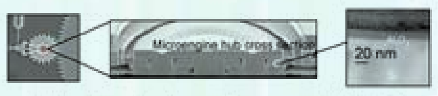
Problem

- The performance and the reliability of many devices are controlled by interfaces between thin films.
- The intrinsic toughness of such interfaces is often quite low because there is little energy dissipation in the surrounding bulk materials.
- A method to engineer thin film interfaces with improved toughness is needed to enhance thin film performance and reliability.

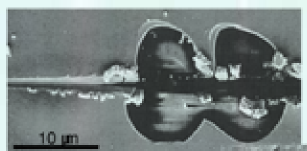


Thin films in microelectronics

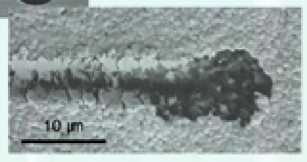


Tribological coatings on MEMS

Approach



Nanoscratch tests on a smooth (single-crystal sapphire) Al_2O_3 substrate coated with Ta_2N



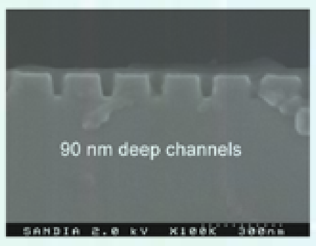
Nanoscratch tests on a rough (1 μm rms polycrystalline alumina) Al_2O_3 substrate coated with Ta_2N

- Our goal is to determine how patterned nano-scale interfacial roughness can be used to increase the apparent interfacial toughness of brittle, thin-film material systems.

- Well defined experiments using nano/micro patterned interfaces.
- Detailed finite element crack growth simulations to understand how patterned nano-scale roughness can increase apparent interfacial toughness.
- Atomistic simulations to guide the development of more realistic interfacial separation models for use in finite element modeling of nano-scale fracture.

Experimental

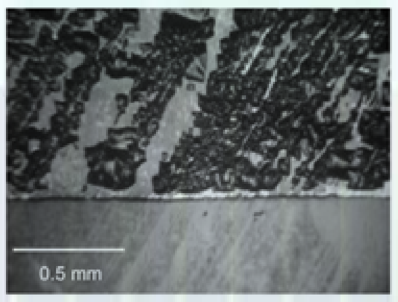
- Generated interfaces with patterned roughness using a commercially available, thermal nanoimprint lithography (T-NIL) tool.
- T-NIL can nano-pattern large areas by stamping a high precision master pattern into a polymer resist coating that is than etched to transfer the pattern to the underlying silicon wafer.
- A highly compressed tungsten film is sputter deposited on top of the patterned silicon interface to create the samples tested.



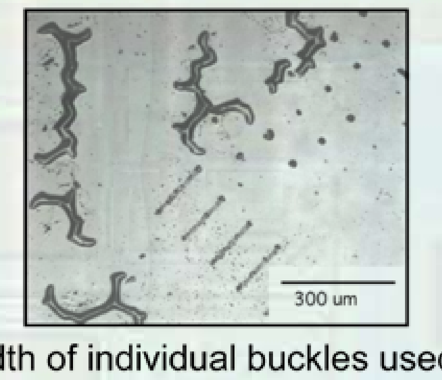
Square-toothed pattern of 60-nm wide by 90-nm deep channels on a silicon surface.

Performed experiments that demonstrated the effect of a nano-scale interfacial roughness pattern on interfacial toughness.

Key Results: Experimental



Buckles align with pattern.



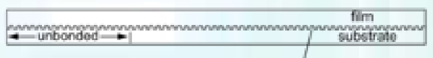
Width of individual buckles used to infer interfacial toughness.

- Tested an interface with a square-toothed pattern of 60-nm wide by 90-nm deep channels on a silicon surface.
- The highly compressed tungsten film (~ 3 GPa) triggered spontaneous buckle formation.
- Buckles aligned with the pattern.
- One can infer apparent interfacial toughness from buckle width.
- The apparent interfacial toughness increased from 0.6 J/m^2 for a similarly prepared atomistically smooth surface to 0.9 J/m^2 for the patterned interface.

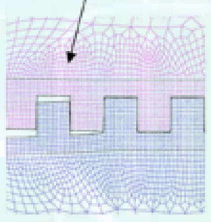
Fracture Analysis

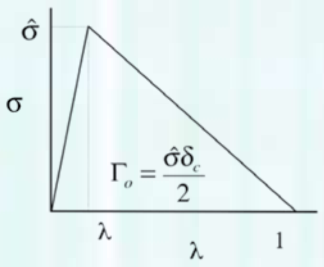
Determined how geometric and material parameter choices affect the apparent toughness of interfaces with patterned nano-scale roughness.

- Used an explicit, transient dynamics finite element code that is well-suited for analyzing discontinuous crack growth.
- The code models material separation using a specified traction-separation relationship.



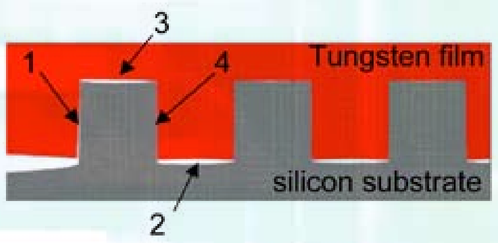
Analyzed idealized problem of a thin, bimaterial strip loaded by displacing the top edge relative to the bottom edge.





- Key parameters are the interfacial strength $\hat{\sigma}$ and the work of separation/unit area Γ_o.

Key Results: Fracture Analysis



- The apparent interfacial toughness scales directly with real interfacial area.
- Also depends on the ratio of interfacial strength $\hat{\sigma}$ to the stress characterizing the tendency for an interfacial segment to crack

Crack growth is discontinuous

1. Crack stalled by high energy needed to kink 90°.
2. Crack initiation at end of W tooth.
3. Crack initiation at end of Si tooth.
4. Side wall fails in shear.

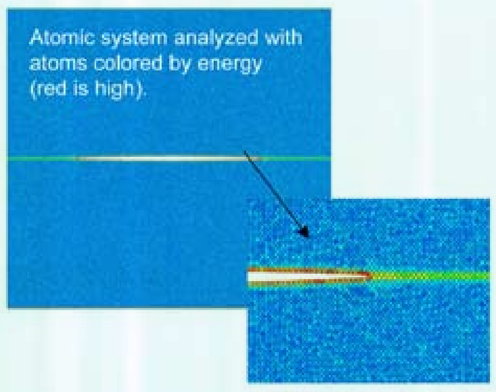
$$\sigma_c = \sqrt{\frac{E^*\Gamma_o}{\pi a}}$$

where
E^* is a bimaterial modulus
Γ_o = intrinsic interfacial toughness
a = the characteristic length scale of the pattern

Key Results: Atomistic Simulations

- Atomistic simulations used generic interatomic potentials and incorporated a brittle interface.
- Determined local tractions across the fracture plane as a function of local separation distance.
- Found that the work of separation is a factor of two higher in shear than in normal separation.
- In contrast, finite element interfacial separation models typically assume there is no intrinsic variation in separation energy with the mode of loading.

Performed atomistic simulations that suggest modifications to the interfacial separation models currently used in nano-scale, finite element fracture analyses.



Significance

- Thin films and coatings are used widely in many challenging applications.
  - Microelectronics
  - Protective coatings
  - Nuclear weapon components
- Interfacial failure is often the controlling failure mode determining performance and reliability.
- Have shown that nano-scale patterned interfacial roughness could be used to improve the performance of brittle, thin-film material systems.

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