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# DEPENDENCE OF INTERFACIAL TOUGHNESS ON INTERFACIAL TOPOGRAPHY

*E. D. Reedy, Jr.*
*Sandia National Laboratories, Albuquerque, NM, 87111*
*edreedy@sandia.gov*

*N. R. Moody, J. A. Zimmerman, and T. D. Nguyen*
*Sandia National Laboratories, Livermore, CA, 94551*

*H. S. Park,*
*Vanderbilt University, TN, 37235*

## Introduction

Material interfaces play a critical role in determining a layered structure's performance and reliability. Our goal is to develop an understanding of how patterns of small-scale interfacial heterogeneities affect interfacial crack propagation. We are concentrating our efforts on a tungsten/silicon interface because there are many techniques for patterning silicon and furthermore the use of brittle materials avoids the complication of having to account for the contribution of bulk dissipation on interfacial toughness. Presented here are some initial results of our ongoing study. We are performing detailed finite element analyses to develop a fundamental understanding of the effect of interfacial topography on crack growth at the nano/micro-scale. The finite element modeling effort is currently focused on a rippled interface. This geometry allows us to investigate the effect of ripple wavelength and magnitude on interfacial crack propagation. Preliminary finite element results predict a significant increase in the apparent toughness of patterned tungsten/silicon interfaces relative to that of a planar interface. We are also performing atomistic simulations to guide the development of physics-based, cohesive zone models that more accurately represent the nano-scale separations that are modeled in the finite element analysis. Our experimental work is focused on developing techniques to measure the effect of interfacial topography on interfacial toughness and also creating interfaces with well-defined surface patterns of controlled shape and dimension. We are depositing submicron-thick tungsten coatings on patterned silicon substrates to create well-defined interfacial geometries. The interfacial toughness of these bimaterials is being measured using four-point bend techniques as well as with stressed-metal overlayers.

## Finite Element Simulations

The finite element modeling effort is currently focused on simulating crack growth along a rippled interface between a 0.25 micron-thick tungsten layer and a silicon substrate. This relatively simple geometry allows us to investigate the effect of ripple wavelength and magnitude on interfacial crack propagation using a 2-D, plane strain idealization (Fig. 1). Two types of loadings are being studied---one simulates a buckle-driven delamination like that which we expect to generate in our stressed-metal overlayer experiments (Fig. 1) while the other applies various ratios of normal and tangential edge displacements in a fixed grip configuration to generate any desired mixed-mode loading (mode mixity is a measure of the crack-tip interfacial tangential-to-normal stress at a characteristic length-scale). These particular geometries were chosen because the solution for a flat interface is known and consequently provides a baseline to compare against. Crack growth was modeled using cohesive zone elements that define interfacial separation in terms of an effective interfacial traction vs. separation relationship. The particular cohesive zone formulation used in this study is similar to that used by Tvergaard and Hutchinson [1]. Simulating interfacial crack propagation using cohesive zone elements is computationally attractive since crack growth is a natural outcome of the solution and moreover this approach leads to mesh-independent results since a length scale is embedded within the traction-separation relationship (with the proviso that the mesh is sufficiently refined to resolve the cohesive zone behind the crack-tip). Note that the characteristic length of the finite element model is ~10 microns while the critical separation distance in the trac-

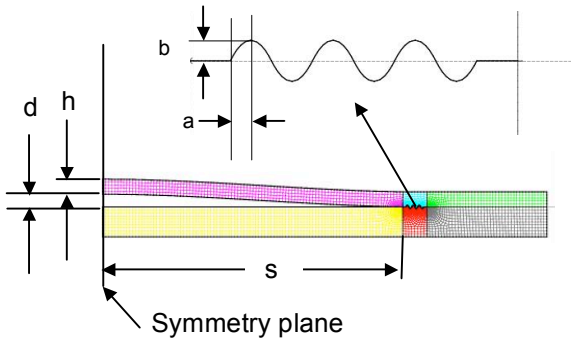


Figure 1. Pull left-hand side of the layer's edge up to model a growing buckle.

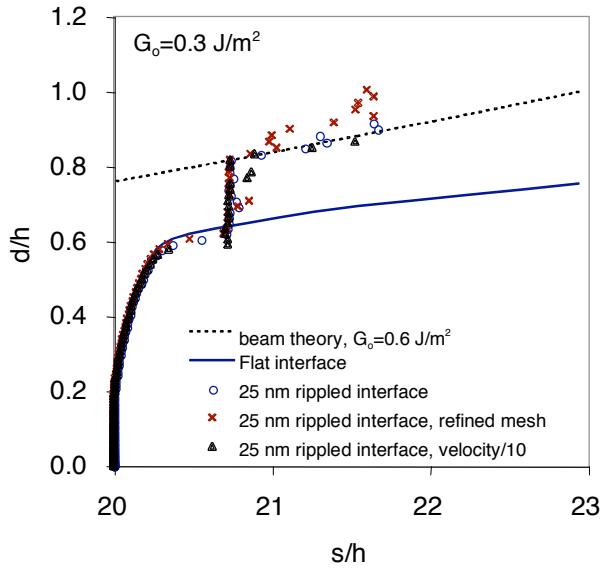


Figure 2. Predicted normalized edge displacement d vs. delamination length s.

tion-separation relationship is one nanometer.

Initial work verified the finite element simulations by examining convergence with mesh size and applied boundary velocity. This was especially important in these explicit dynamics simulation since the calculations show "stick-slip" behavior as the crack runs along a rippled interface. The sensitivity of calculated results to cohesive zone model parameters was also studied. Our most important finding is that the finite element simulations do predict a significant increase in the apparent interfacial toughness when the interface is non-planar. These results are for material, interface, and geometric properties representative of the tungsten/silicon system we plan to test. Figure 2 plots the normalized buckle height (d/h) versus the length of the delamination (s/h). The calculations indicate that the apparent fracture toughness is twice that of the intrinsic interfacial toughness when there is a 25-nm ripple (a=b=25 nm in Fig. 1). Other calculations suggest that the apparent

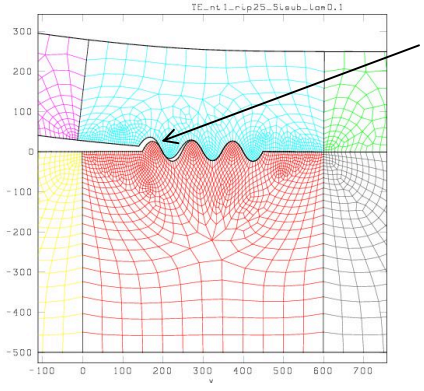


Figure 3. Example of deformed geometry (displacement magnified by a factor of 5).

toughness increases with ripple height. The finite element results indicate that the interface does not simply unzip in a continuous manner, but rather the crack is pinned in back of the ripple with crack growth occurring in front of the pinned region (Fig. 3).

## Molecular Dynamics Simulations

Our initial work has concentrated on developing atomistic models to analyze incoherent interfaces of regular geometry. A model representative of realistic incoherent bi-material interfaces was created by equilibrating a <100> oriented block of gold on top of a <110> oriented block of gold using the modified embedded atom method. Figure 4 shows the type of failure predicted under a tensile loading. We also perform shear simulations by translating one edge relative to the other. Much of our work has focused on determining the effect of atomistic system size on calculated results. To accomplish this we performed a comprehensive suite of simulations that varied the system's height, width and depth. These results were then used to determine how the energetic characteristics varied with system size for both tensile and shear loadings. This was quantified by defining the work needed to fail an incoherent interface as the energy to failure (area under the calculated stress-strain curve) normalized by the interfacial area. Using this measure, we have determined that relatively small atomistic systems are sufficient to determine the work needed to create interfacial failure.

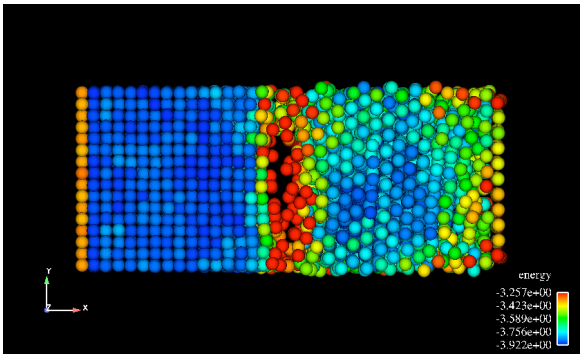


Figure 4. Incoherent interface subjected to a tensile loading (atoms colored by potential energy).

## Experiments

The experimental effort is currently focused on both developing techniques to measure the effect of interfacial topography on interfacial toughness as well as creating interfaces with well-defined surface topographies of controlled shape and dimension to test.

We have adapted a four-point bend, interfacial fracture test to nanoscale film fracture (in collaboration with the W. W. Gerberich's group at the University of Minnesota). This testing method imposes a nominally balanced

crack-tip mode mixity [2] (i.e., the magnitude of the crack-tip interfacial shear stress is similar to that of the interfacial normal stress at the length scale of interest). A loading technique that uses cyclic compression has been developed to nucleate a starter crack with a uniform front along the interface of interest. This, along with the reduction in friction at the loading supports, is critical for accurate interfacial toughness measurements. We are also using compressively stressed, thin film tungsten overlayers to measure interfacial toughness. These submicron-thick, tungsten overlayers are sputter deposited in such a way as to generate an intrinsic residual stress that can exceed two GPa. Such highly compressed films can generate delamination buckles that impose a nominally mode II–like crack-tip loading. The magnitude of the interfacial toughness can be inferred by analyzing the size and type of buckle pattern. By using both four-point bend and stressed overlayer tests, with their significantly different mode mixity, allows us to explore the effect of mode mixity on crack propagation along patterned interfaces.

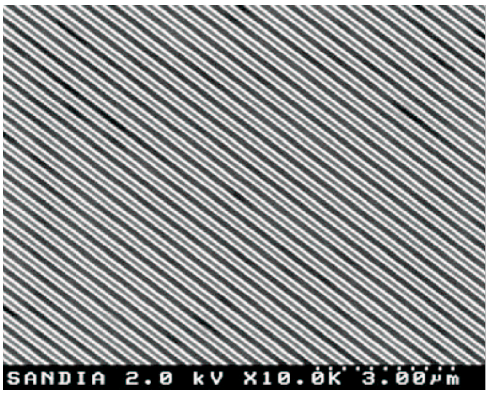


Figure 5. Nanoimprint lithography creates 200-nm sinusoidal patterns over large sample surfaces

We have also been working to create interfaces with well-defined surface topographies. For example, nanoimprint lithography has been used to create well-formed 200-nm wavelength sinusoidal patterns on a test wafer (Fig. 5). This pattern is well suited for experiments aimed at gaining a fundamental understanding of how patterned surfaces affect interfacial crack propagation. We will be able to study crack growth both along and also across the rippled interface.

## Conclusions

Our most important finding to date is that finite element simulations do predict a significant increase in the apparent toughness of patterned tungsten/silicon interfaces like those we plan to test. The calculations indicate that the apparent fracture toughness is twice that of the intrinsic interfacial toughness when there is a 25-nm ripple. Experiments with a rippled tungsten/silicon interface are now underway.

## Acknowledgements

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## References

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2. P.G. Charalambides, J. Lund, A. G. Evans, and R. M. McMeeking, *Journal of Applied Mechanics*, 1989, 56 pp 77-82.