DYNAMIC SPALLATION OF FILM/SUBSTRATE INTERFACES TAILORED WITH SELF ASSEMBLED MONOLAYERS: A MULTISCALE MODEL OF INTERFACE ROUGHNESS EFFECT

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Abstract

Due to the flexibility that they offer in the selection of the end groups attached to the substrate and film materials, self-assembled monolayers (SAMs) composed of very short (nanometer-long) aligned polymer chains have been proposed as a unique way to tailor the electrical, thermal and mechanical properties of interfaces. In this combined experimental and computational study, we investigate the impact of the SAMs on the failure properties of a gold film/silicon substrate interface. In particular, we study SAMs with methyl (-CH3) and mercapto (-SH) terminated functional groups, introduced along the film/substrate interface through transfer printing.

In the experimental component of the project, we adopt a non-contact laser-based spallation technique to measure the failure strength of a silicon/SAM/gold system. Results show a strong dependence of the failure strength of the interface on the choice of SAM. Detailed AFM and XPS analyses performed on the post-spallation surfaces provide information on the roughness profile and chemical composition of the failure surface.

On the modeling side, we develop a multiscale model that combines a cohesive failure model derived from MD simulations of the spallation event with a continuum model of the bending response of a film printed on a rough interface of varying wavelength and amplitude.

References

[1] Awasthi, A. P., Grady, M. E., Kim, I. H., Sottos, N. R., and Geubelle, P. H. (2016) "Nanoscale mechanical tailoring of interfaces using self-assembled monolayers." To appear in *Mechanics of Materials*.

[2] Zhang, C., Awasthi, A. P., Geubelle, P. H., Grady, M. E., and Sottos, N. R. (2016) "Effects of interface roughness on the cohesive strength of self-assembled monolayers." Submitted.