Tribology and Mechanical Behavior of Coatings and Engineered Surfaces
Room Town & Country B - Session E2-1-ThM
Mechanical Properties and Adhesion I

Moderators: Carsten Gachot, Vienna University of Technology, Austria, **Bo-Shiuan Li**, Oxford University, UK

10:40am **E2-1-ThM-9 Effect of Thin Film Properties on Delamination Behavior and Interface Adhesion***, Alice Lassnig (alice.lassnig@oeaw.ac.at), S. Zak, R. Pippan,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria*; C. Mitterer,* Montanuniversität Leoben, Austria*; M. Cordill,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

Understanding the factors affecting thin film delamination and quantifying thin film adhesion to their substrates is important to ensure reliable multi-material components which are widely encountered in several technological applications.
Of special interest are brittle-ductile interfaces separating thin ductile films from rigid substrates since they are particularly weak. Standard routes to quantify such interfaces are 4 Point Bending tests or - if applicable- buckle-driven delamination by means of the stressed overlayer technique [1]. Improving the interface stability for nanosized thin films on brittle substrates is therefore crucial to ensure reliable bi- and multi-material devices.

In a recent study [2] we could demonstrate that intrinsic film properties such as grain size can significantly influence interface adhesion. Nanoindentation results allowed to estimate the film yield stress of the films when bonded to the substrate. The mixed-mode adhesion energy for each film ranged from 2.35 J/m^2 for the films with larger

grains to 4.90 J/m^2 for their small-grained counterparts while all the films showed similar residual stresses and same film thicknesses. A newly developed focused ion beam (FIB) cutting technique allowed to decouple and quantify the amount of elastic and plastic deformation stored in the buckled thin film. This surprising result could be understood by introducing a new finite element modelling technique to further help understand plasticity contribution as a toughening mechanism during thin film delamination [3] and to further adapt established models, which currently only account for purely elastic film delamination.

[1]A. Lassnig, B. Putz, S. Hirn, D.M. Többens, C. Mitterer, M.J. Cordill, Adhesion evaluation of thin films to dielectrics in multilayer stacks : A comparison of four-point bending and stressed overlayer technique . Mater. Des. 200 (2021) 109451. doi:10.1016/j.matdes.2021.109451.

[2]A. Lassnig, V.L. Terziyska, J. Zálešák, T. Jörg, D.M. Többens, T. Griesser, C. Mitterer, R. Pippan, M.J. Cordill, Microstructural Effects on the Interfacial Adhesion of Nanometer-Thick Cu Films on Glass Substrates: Implications for Microelectronic Devices. ACS Appl. Nano Mater. 4 (1) (2021) 61–70. doi:10.1021/acsanm.0c02182.

[3]S. Zak, A. Lassnig, M. J. Cordill, R. Pippan, Finite element-based analysis of buckling-induced plastic deformation. Journal of the Mechanics and Physics of Solids 157 (2021) 104631. doi: 10.1016/j.jmps.2021.104631.

11:00am **E2-1-ThM-10 Buckling-Induced Delamination: Connection between Mode–Mixity and Dundurs´ Parameters***, Stanislav Zak (stanislav.zak@oeaw.ac.at), M. Cordill,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

Modern electronics and micromechanical devices consist of various combinations of layered materials and/or coatings with different material properties. In recent years, differences in the elastic moduli and Poisson's ratios are becoming more pronounced (e.g. when bendable electronic components are designed). Therefore, a strong push to investigate interface stability with a more in–depth view on the elastic material properties mismatch influence is needed. Measurements of the adhesion energy of the thin film on the different substrate materials can be made using the spontaneous (compressive stress induced) buckling method described by Hutchinson and Suo. This method induces lateral deformation of the thin film with respect to the substrate (to form delaminated buckles), which causes a significant shear loading contribution to the delamination crack front and therefore, the inevitable mode II appearance. Additionally, the shear loading can be highly influenced by the differences in deformations of the film and substrate due to their elastic mismatch which can be high for modern material combinations, such as those found in flexible devices. Therefore, the original approach to elastic mismatch by Hutchinson and Suo is revised and extended in this work. Since the elastic mismatch on the interface between two different materials can be described by the Dundurs' parameters, a wide range of parameters are used to evaluate the mode-mixity at the delamination crack front. Finite element (FE) modelling is combined with analytical solutions to evaluate parameters describing the mode–mixity of the delaminated buckles as a function of elastic mismatch (both according to Hutchinson and Suo and also with the use of more real-like models). The FE approach enables relatively simple and quick evaluation of stress intensity factors for arbitrary models via domain integration method. Therefore, several FE model configurations can be analysed together with numerically obtained stress/strain fields in the buckled samples. The resulting map of the mode-mixity as a function of Dundurs' parameters will lead to more precise experimental measurements of the mode I and mode II adhesion energy components for modern material combinations.

11:20am **E2-1-ThM-11 Colored Picosecond Acoustics Versus Scotch Tape Adhesion Test: Confrontation on a Series of Similar Samples With a Variable Adhesion***, A. Vital-Juarez,* IEMN UMR CNRS 8520, France*; J. Desmarres,* CNES, France*; **Arnaud DEVOS (arnaud.devos@iemn.fr)**,* IEMN UMR CNRS 8520, France

The study of the bonding at interfaces between thin layers is of great importance in optical and electronic applications as well as in the field of space exploration. A large number of methods have been developed to characterize the adhesion of a thin film to a substrate. Among them, Scotch Tape test is still one of the most popular methods.

Acoustic waves and especially ultra-high frequency acoustic waves are also sensitive to adhesion defects as they affect the way acoustic waves are reflected at the concerned interface.

In this paper, we prepare a dedicated series of identical thin-film samples with a variable adhesion at the interface between the film and its substrate. For that several avenues have been explored: introduction of a weak layer between the film and the substrate; reinforcement of the weak layer adhesion using ion beam implantation. The samples are then characterized using two much different techniques: colored picosecond acoustics for measuring thickness and acoustic reflection coefficient at the interface and scotch tape test to have an independent evaluation of the adhesion. An excellent correlation is found between techniques regarding adhesion that confirms the capability of APiC to perform adhesion test in a totally non destuctive manner and furthermore locally.

11:40am **E2-1-ThM-12 High-Throughput Screening of Adhesion and Friction of Solid Interfaces***, **Maria Clelia Righi (clelia.righi@unibo.it)**,* University of Bologna, Italy **INVITED**
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High-throughput studies have become a valuable tool for material advancement, which is of tremendous importance for industry and closely tied to various societal challenges like clean energy production. We designed and implemented an advanced workflow, based on the FireWorks platform, to perform first principles calculations using the VASP package. Starting from two elemental solids, the workflow can generate the surfaces of interest and match them to form an interface. The interfacial adhesion, load-displacement curves, shear strength and charge displacements are automatically calculated and the results are stored in a public database [1].

In a first application of the high-throughput approach tohomogeneous interfaces we generated a database of the shear and cleavage strengths for over hundred interfaces formed by matching two equivalent surfaces of different elemental crystals [2]. We discovered the existence of a power-law between the adhesion and the shear strength for these interfaces. Moreover, the ratio of the strengths can provide an estimate of the material failure mode[3]. The analysis also showed that the mechanical properties of elemental crystals are closely related to their electronic structure [4].

In a more recent advancement, we created a database for heterogeneous interfaces focusing in particular to metal-on-metal surfaces relevant for technological applications and 2D layers adsorbed on solid substrates. The analysis of the overall trends and the comparisonof the data obtained for heterogeneous interfaces with the homogeneous counterparts improved the scientific and mechanistic understanding of interface mechanics and tribology [5].

[1] G. Losi, O. Chehaimi and M. C. Righi, ”A workflow for high throughput screening of the tribological properties of heterogeneous interfaces”, in preparation.

[2] Restuccia, P. et al., “Ideal adhesive and shear strengths of solid interfaces: A high throughput ab initio approach” Comp. Mat. Sci. 154, 517 (2018).

[3] Wolloch, M. et al., “High-throughput screening of the static friction and ideal cleavage strength of solid interfaces” Scientific reports, 9, 1 (2019).

[4] M. Wolloch, G. Levita, P. Restuccia, M. C. Righi, “Interfacial Charge Density and Its Connection to Adhesion and Frictional Forces,” Phys. Rev. Lett., 121, 2 (2018).

[5] G. Losi, O. Chehaimi and M. C. Righi, ”High throughput screening ofsolid interfaces for tribological applications”, in preparation.

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