

Motivation:

Modern electronics and micromechanical devices consist of various combinations of layered materials and/or coatings with different material properties. In such applications, differences in the elastic moduli and Poisson's ratios are becoming more pronounced. Therefore, a strong push to investigate interface stability with a more in-depth view on the elastic material properties mismatch influence is needed. One way to investigate thin film adhesion using spontaneous buckling was described by Hutchinson and Suo. With this method, a significant shear loading occurs at the delamination crack front and, consequently, there will always be the I+II mixed mode conditions. Therefore, a numerical study of the mode-mixity dependence on the material properties mismatch is being performed to extend the original approach for more precise use in modern applications.

Dundurs parameters are ideal to describe the elastic mismatch of the interface between two different materials. Hence a wide range of Dundurs parameters is used to evaluate the mode-mixity during the buckling delamination with use of the finite element (FE) modelling and analytical solutions. The FE approach enables relatively simple and quick evaluation of stress intensity factors for arbitrary models via domain integration method, thus, several FE model configurations can be analysed together with numerically obtained stress/strain fields in the buckled samples. The resulting dependence of the mode-mixity on the Dundurs parameters will lead to more precise experimental measurements of the mode I and mode II adhesion energy components for modern material combinations.

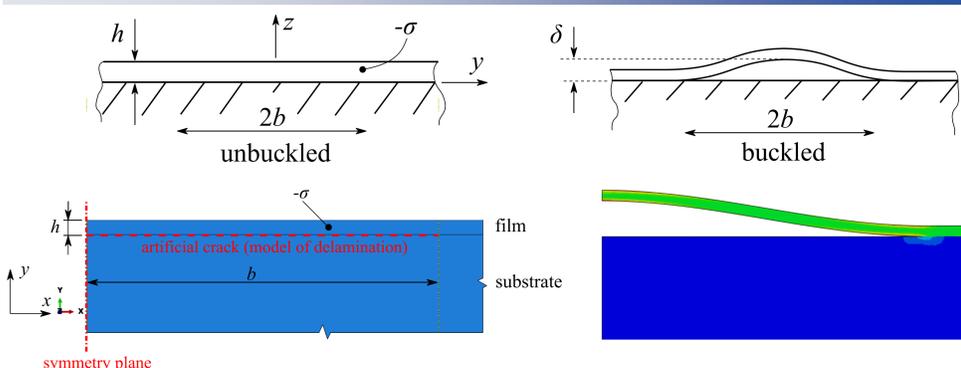
Problem description

The compressive stress induced buckling delamination method by Hutchinson and Suo [1] is complex but easy to use method to assess the adhesion energy of the thin film on substrate as a function of the mode mixity-angle Ψ :

$$\tan(\Psi) = \frac{K_{II}}{K_I} = \frac{4 \cos(\omega) + \sqrt{3}\xi \sin(\omega)}{-4 \sin(\omega) + \sqrt{3}\xi \cos(\omega)} \quad \text{with} \quad \xi = \frac{\delta}{h}$$

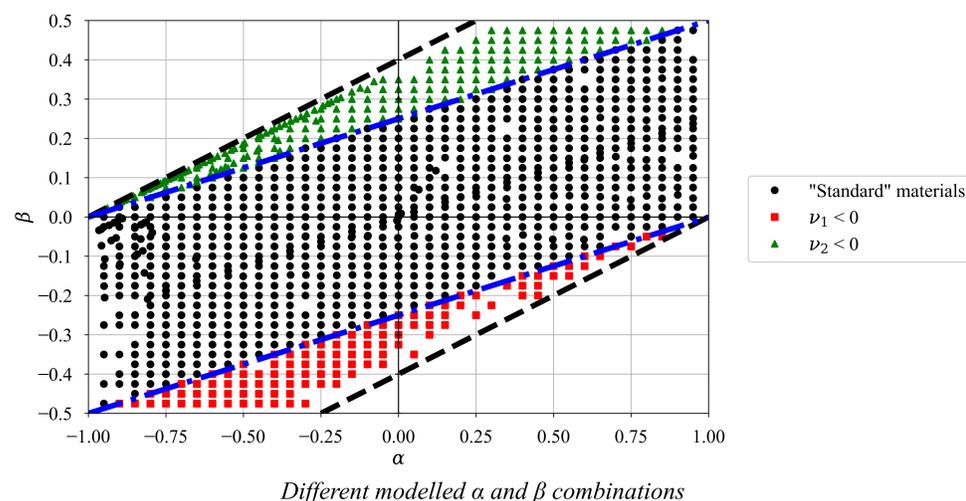
The Ψ defines the ratio between normal and shear loading at the delamination crack front from measured buckle height δ , film thickness h and phase factor ω . In the case of the buckling delamination, the phase factor ω purely comes from the Dundurs parameters α and β . Despite the clear influence, the original work tackles only ω for cases $\beta = 0$ and $\beta = \alpha/4$ and the subsequent research assumes strong simplification $\alpha = \beta = 0$, therefore, $\omega = 52.1^\circ$. Such simplification is rather inadequate and the real elastic mismatch with correct phase factor ω should be used.

Model



Original (top row) and numerical (FE, bottom row) models

The Hutchinson and Suo model relies on the 2D approximation of the buckled thin film cross-section, whereas the analytical methods are based on the simple Euler's beam theory and calculations by Suo and Hutchinson of different types of delamination cracks [2]. They present method to evaluate the adhesion energy $\Gamma(\Psi)$ from known buckle dimensions, residual stress in the film, film material properties and assumption of $\omega = 52.1^\circ$. To expand the knowledge on the influence of the elastic mismatch on the mode-mixity, a numerical, FE model was created using Abaqus code. This FE model uses the same 2D simplification and a symmetry plane. In addition, the numerical procedures allows for the use of large deformations theory, instead of the simplified Euler's beam theory, furthermore improving the accuracy of results. The model was evaluated for different combination of input parameters, such as film and substrate material properties, film thickness, buckle width and compressive stress.

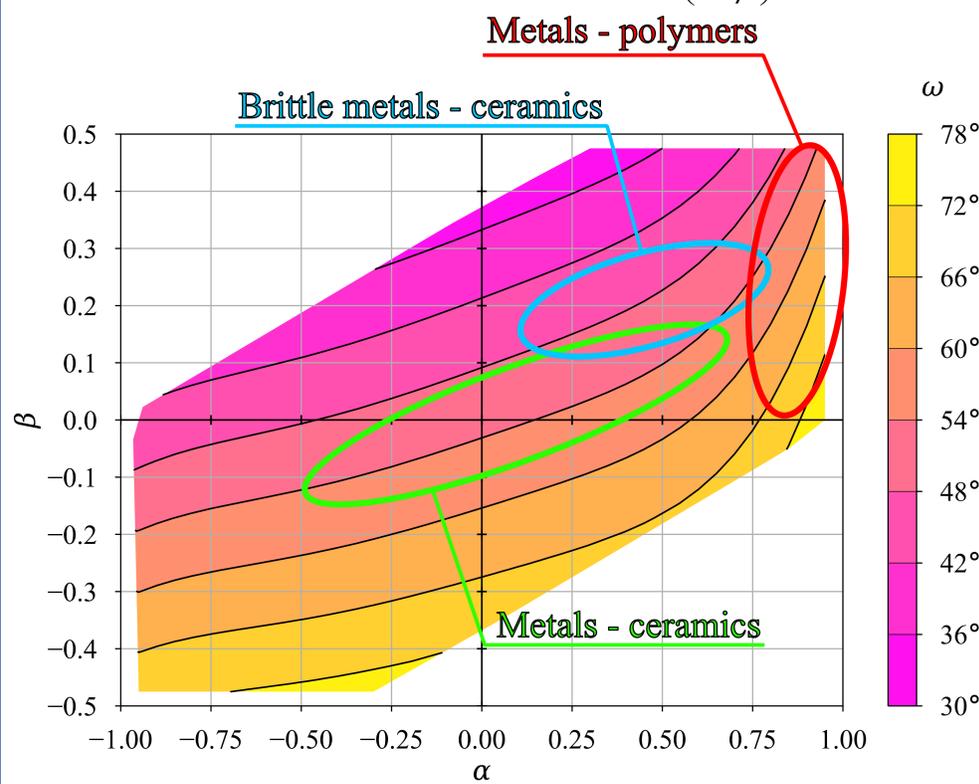


Results

Properly calibrated and validated model was used for evaluation of the K_I and K_{II} stress intensity factors at the delamination crack tip. Their values were subsequently used for reverse calculation of the phase factor ω for possible α and β combinations. However, with assumption of $\beta \neq 0$, a complex value of mode-mixity had to be used [1]:

$$\frac{\text{Im}(Kh^{i\varepsilon})}{\text{Re}(Kh^{i\varepsilon})} = \frac{4 \cos(\omega) + \sqrt{3}\xi \sin(\omega)}{-4 \sin(\omega) + \sqrt{3}\xi \cos(\omega)} \Rightarrow \omega(\alpha, \beta)$$

$$\text{where } K = K_I + iK_{II} \quad \text{and} \quad \varepsilon = \frac{1}{2\pi} \ln\left(\frac{1-\beta}{1+\beta}\right)$$



While standard metallic thin films on ceramic or glass/Si substrates are in the region of $\beta = \alpha/4$ and the evaluated ω is in range between 50° and 60° , more progressive material combinations leads to vastly different ω -values. Hard and brittle metals (such as HEAs or metallic glasses) on ceramic substrates above the $\beta = \alpha/4$ lead to ω in range between 40° and 50° while metallic films on polymer (compliant) substrates with α around 0.9 can vary the ω from 55° to 80° . Some concrete values for real material combinations are as follows:

Thin film material	Substrate material	α	β	$\omega / ^\circ$
W	SiO ₂	0.73	0.30	50.90
Cu	Al ₂ O ₃	-0.50	-0.09	52.50
WTi	glass	0.46	0.17	49.97
Au	polyimide	0.81	0.14	61.63
Mo	polyimide	0.94	0.15	69.77

Summary

The difference in elastic material properties of thin film and substrate proves to be more important than it was assumed for many years. Current model shows need for better use of ω in further studies, because modern materials combinations lead to elastic mismatch which highly influences the mode-mixity at the delamination crack front through the ω ranging between 30° and 80° . This completely invalidates old $\omega = 52.1^\circ$ assumption for some materials.

[1] John W. Hutchinson, Zhigang Suo, Mixed Mode Cracking in Layered Materials, Advances in Applied Mechanics 29 (1992) 63–191. [https://doi.org/10.1016/S0065-2156\(08\)70164-9](https://doi.org/10.1016/S0065-2156(08)70164-9).
[2] Zhigang Suo, John W. Hutchinson, Interface crack between two elastic layers, International Journal of Fracture 43 (1990) 1–18. <https://doi.org/10.1007/BF00018123>.