Depth-depending YOUNG´s modulus of thin films for increased load carrying capacity

F. RICHTER, N. SCHWARZER, V. LINSS, I. HERMANN, T. CHUDOBA

Technical University Chemnitz,
D-09107 Chemnitz, Germany

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1. Introduction

- Protection of surfaces by hard coatings: how to find an appropriate thin film system for a given application?
- Today: mainly empirical approaches, based on hardness, scratch, wear test, etc..
- General aim of this work: To contribute to a higher degree of modelling for more straightforward design of thin film systems.
- Enormous complexity of the problem; advances will be possible only little by little.
- Here: Increase of the load carrying capacity due to a depth-depending YOUNG´s modulus for: spherical counterpart,

  normal load,

  plastic deformation

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2. Methodology

- Our approach: High-accuracy spherical indentation and theoretical modelling
- Can be utilised for:
  - determination of film parameters (E, s_Y, ..),
  - identification of failure mechanisms,
  - prediction of film/substrate performance,
  - design of film systems.
- **Modelling** based on modern potential theory,
- elastic stress and strain fields in substrate & ≤ 5 different layers,
- easy-to-use software ELASTICA™ available (≤ 3 layers),
- **experimental**: UMIS 2000 nanoindentation device (CSIRO, Australia)
- typical resolution: $\Delta P < 1\ \mu N$, $\Delta h < 0.1$ nm.
- compliance / T drift / zero point detection / indenter shape

• YOUNG´s modulus, E

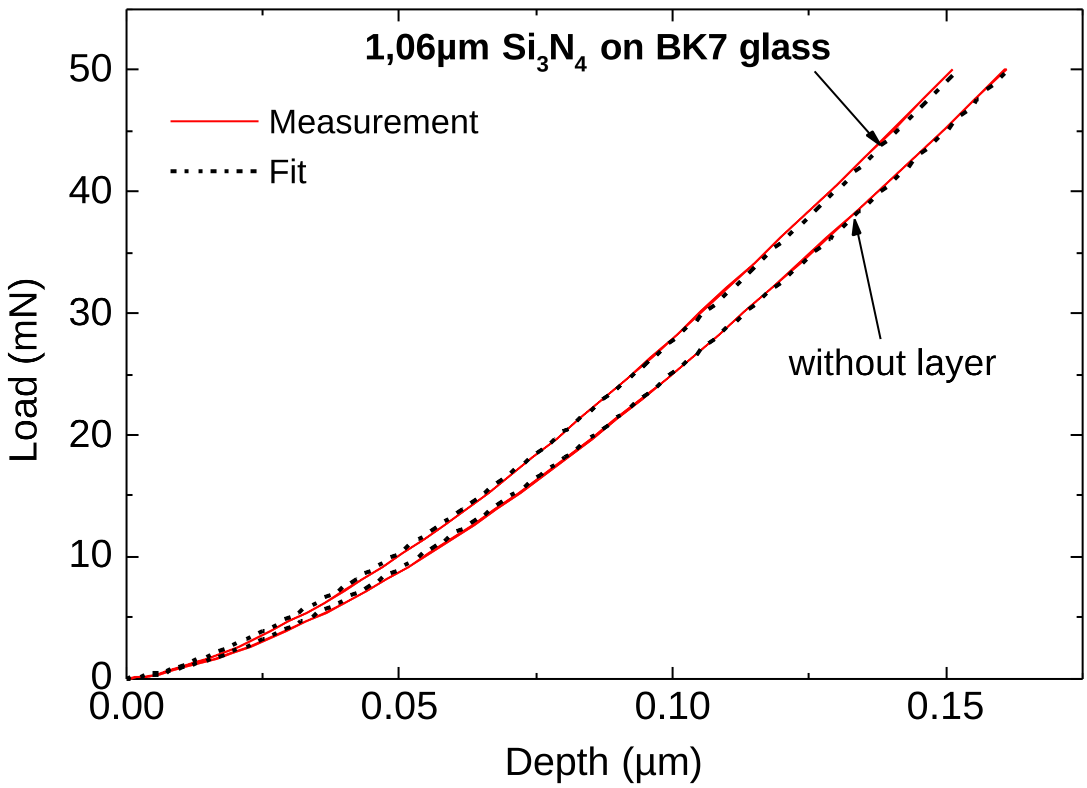
Conventionally, E is determined after OLIVER & PHARR → tolerable indentation depth:

H: $h_{max} / t_f \leq 0.1$ (BÜCKLE´s rule)

E: "h_{max} as small as possible"

Our method considers also the substrate
→ large h_{max} / t_f permitted!

Simulation of the load indentation curve:



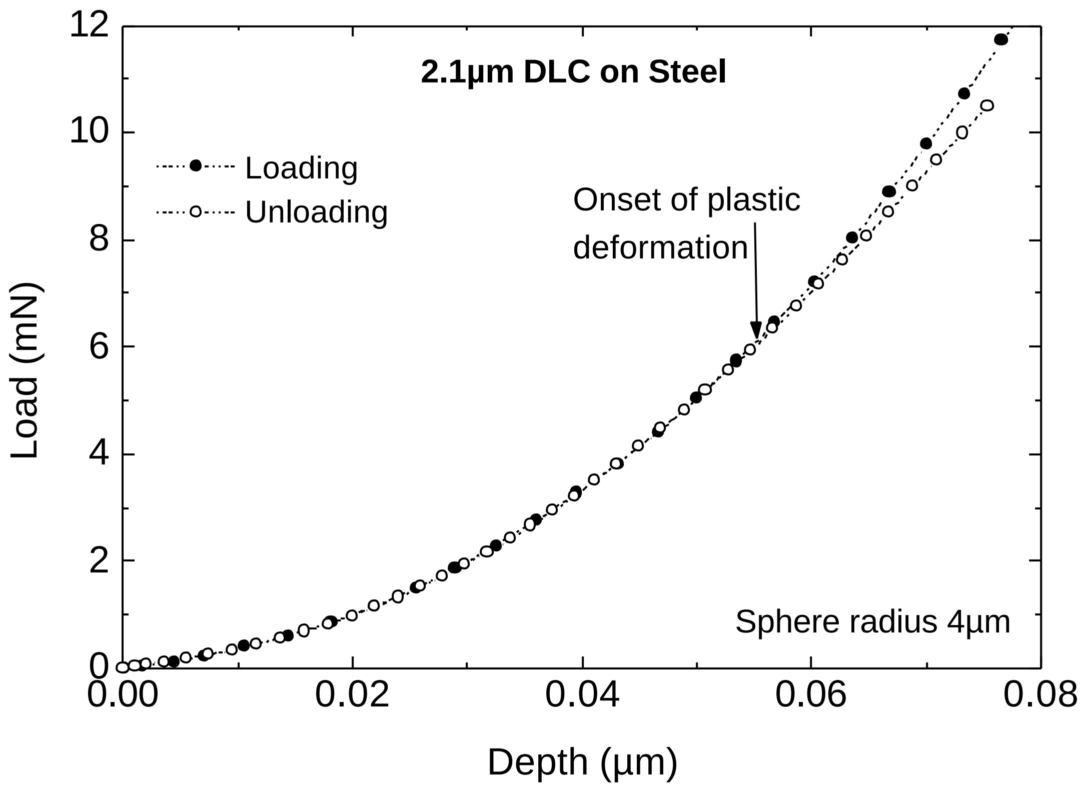
• yield strength, s_Y

The VON MISES yield criterion describes the onset of yield for a **general stress state,** defined by the components, s_{xx}, s_{yy}, s_{zz}, t_{xy}, t_{yz}, and t_{zx} :

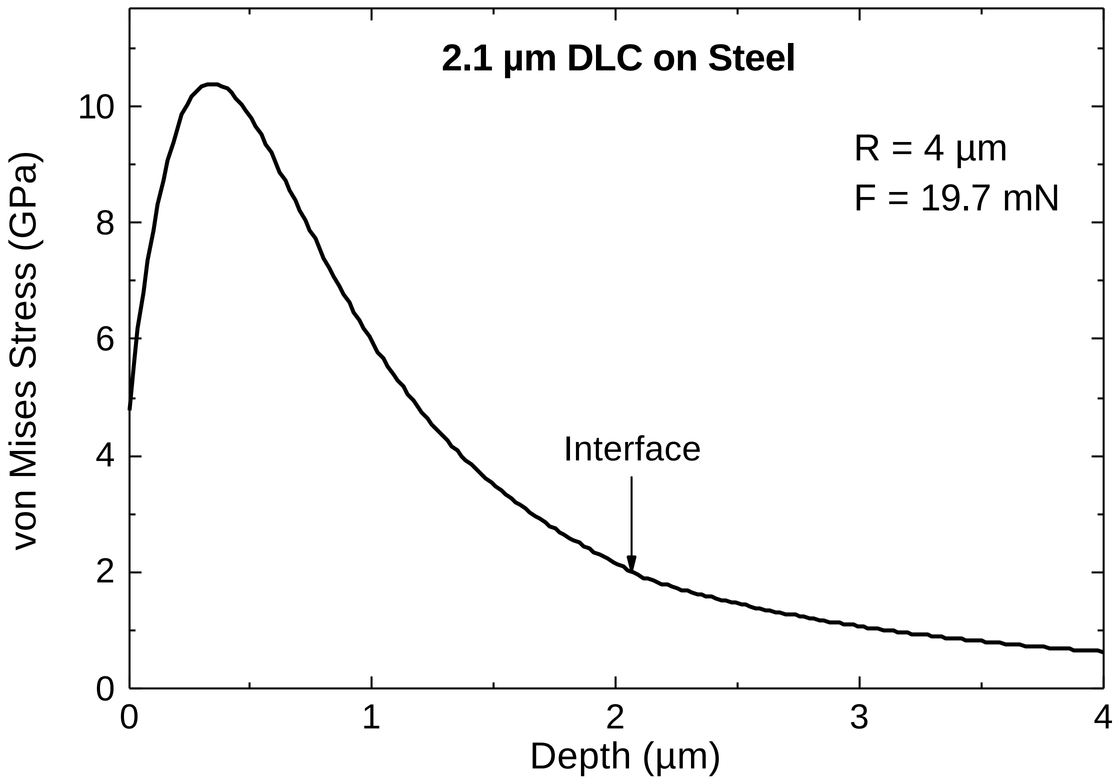
$$s_M = \sqrt{\frac{1}{2}\left(\left(s_{xx} - s_{yy}\right)^2 + \left(s_{yy} - s_{zz}\right)^2 + \left(s_{zz} - s_{xx}\right)^2 + 6 * \left(t_{xy}^2 + t_{yz}^2 + t_{zx}^2\right)\right)}$$

Plastic deformation for $s_M > s_{M,crit}$ = f(material)

Procedure: i) Detection of the onset of yield:



ii) Calculation of σ_M along the axis of symmetry:

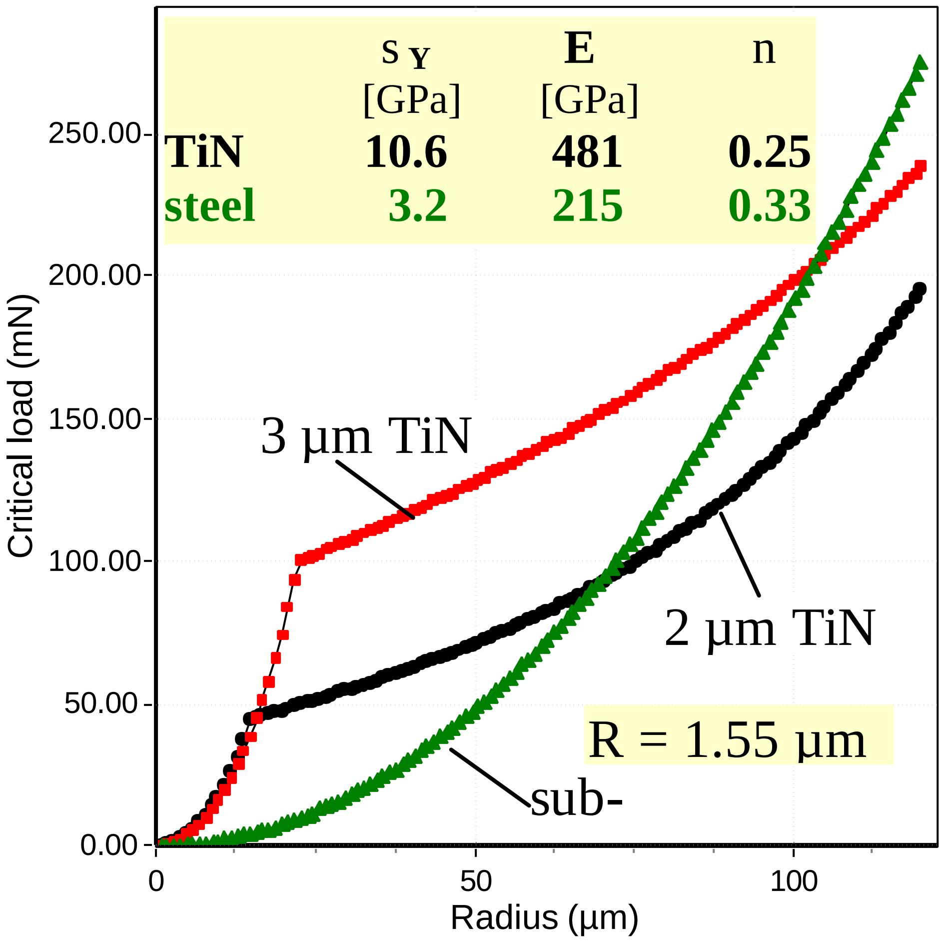


→ Critical load: 17.7 ± 1.1 mN

Critical yield stress: 10.4 ± 0.3 GPa

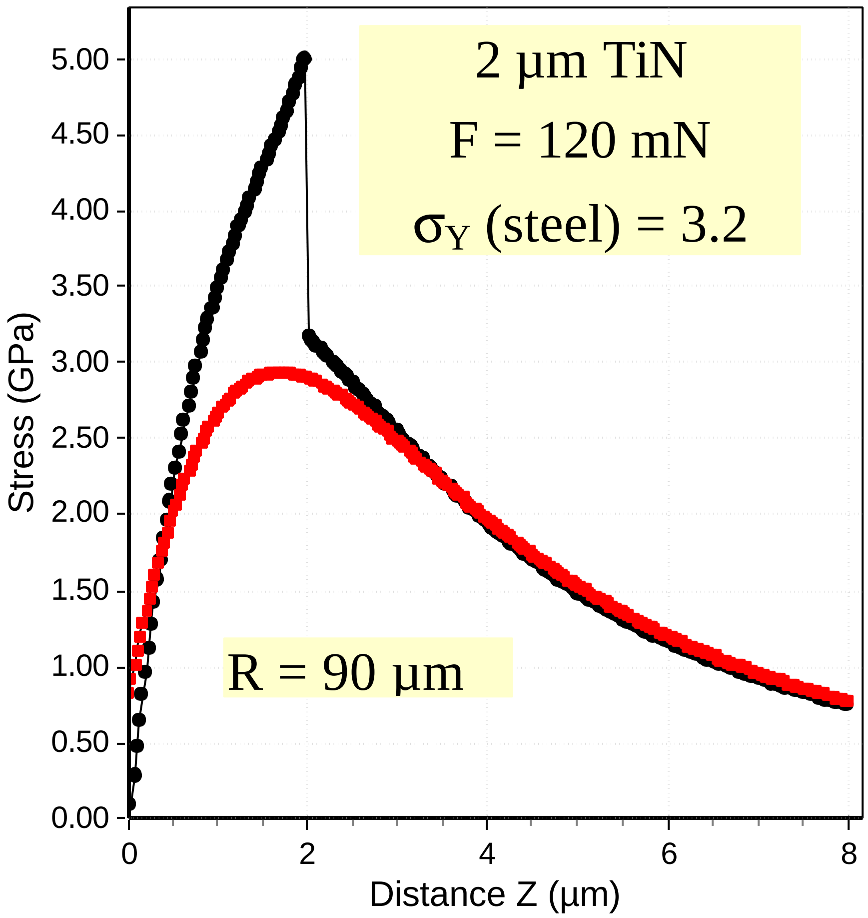
3. Load-carrying capacity of a film

- We assume plastic deformation as the relevant failure mechanism.
- Single layer (TiN on steel) as an example:



Above a certain radius of the counterpart, the critical load is higher <u>without</u> layer!

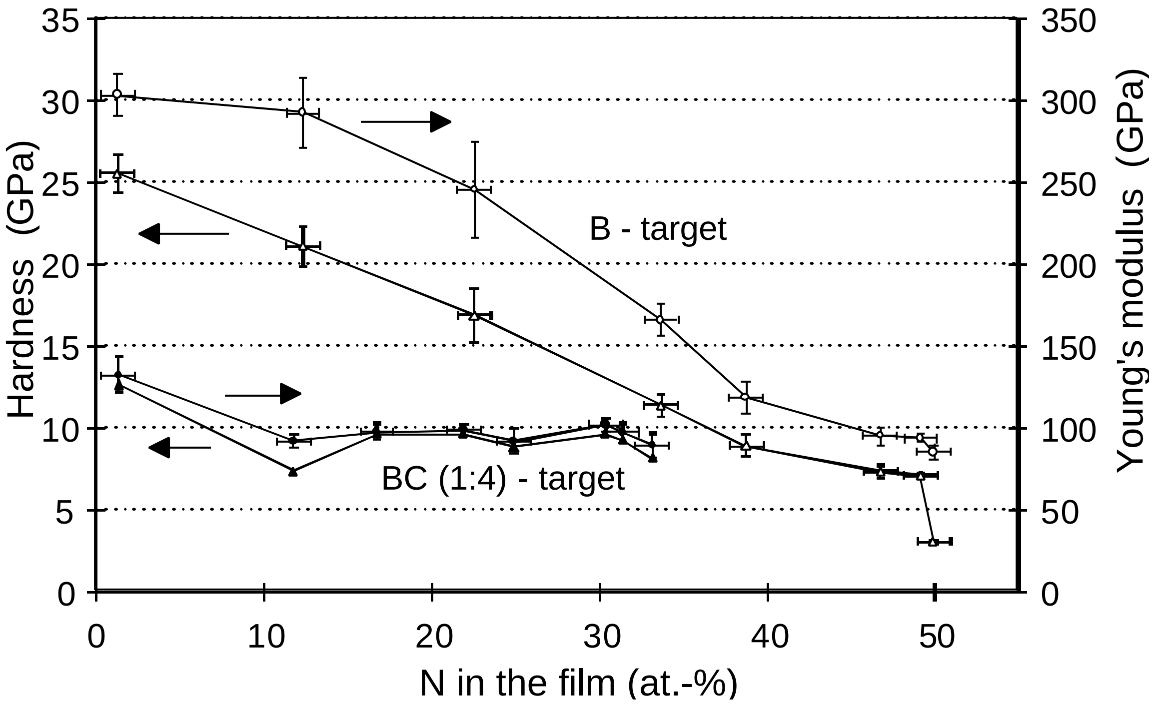
σ_M along the z-axis with and without TiN film :



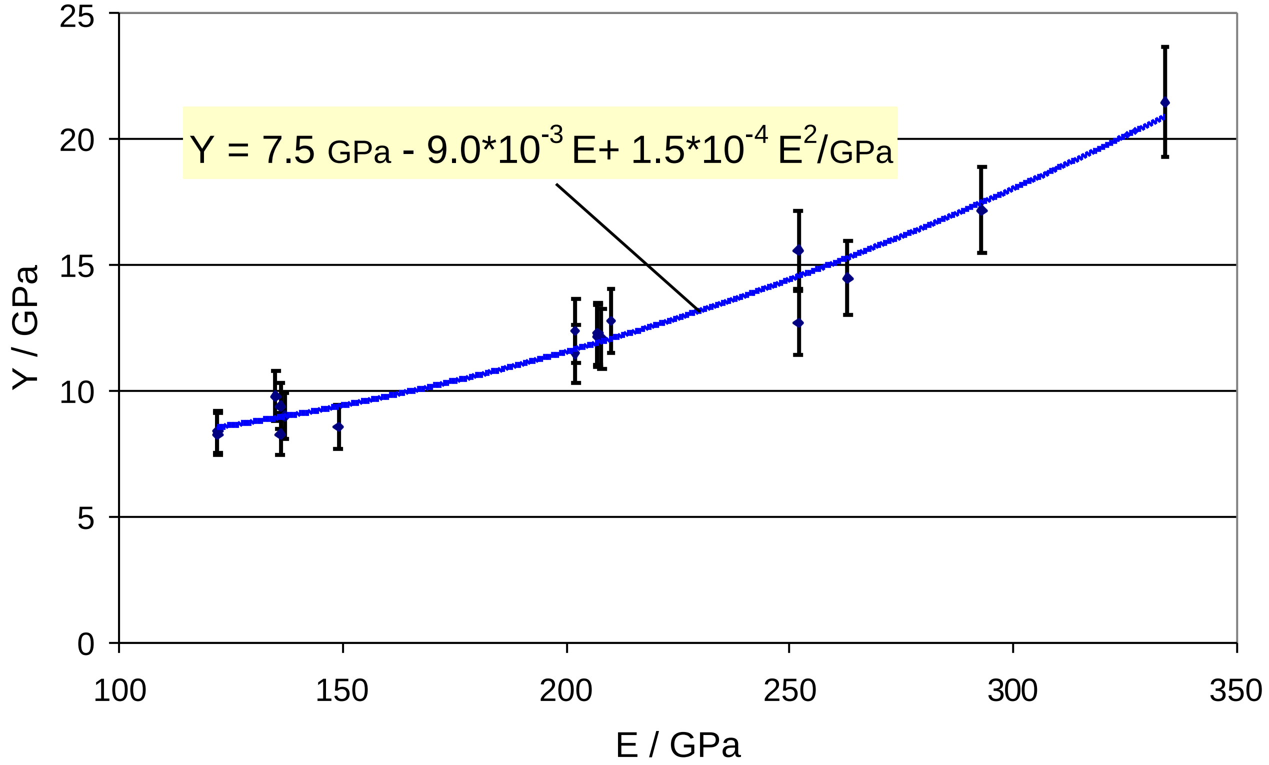
→ Stress concentration just below the interface due to TiN film; without film F_{crit} = 156 mN!

4. Film deposition and characterisation

- Ternary films (B,C,N) have been deposited using magnetron sputtering (cf. LINSS et al., B3-1-6)
- YOUNG´s modulus of these film can be varied by deposition parameters to a large extent:



Together with YOUNG´s modulus, the yield stress varies:

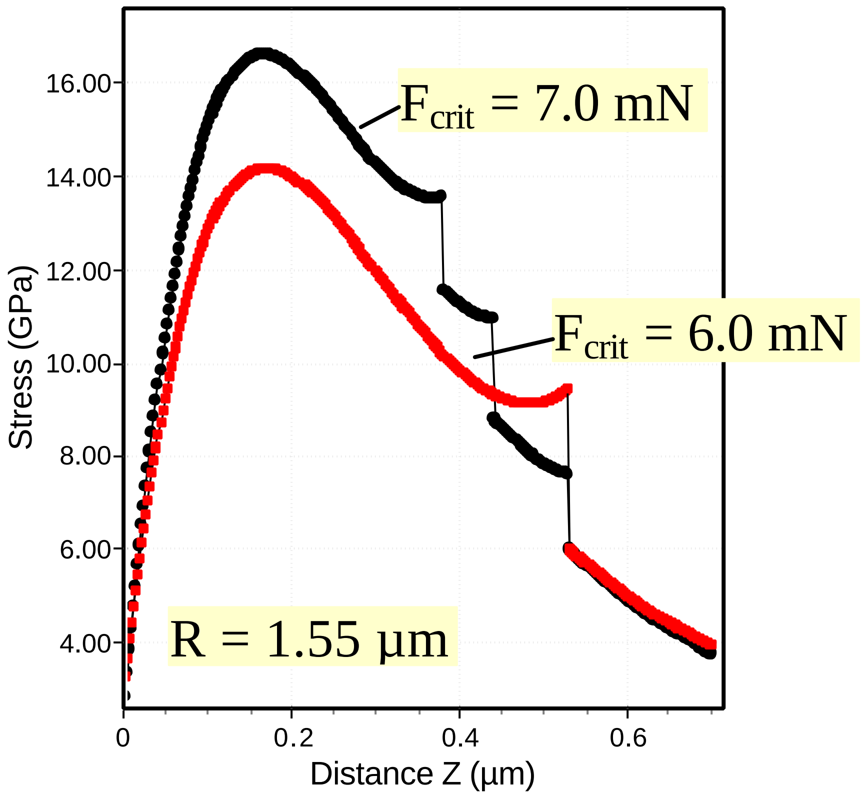


5. Design of film systems

Calculation based on three (B,C,N) materials i, ii, iii.
Optimum stack on fused silica for R = 1.55 µm:

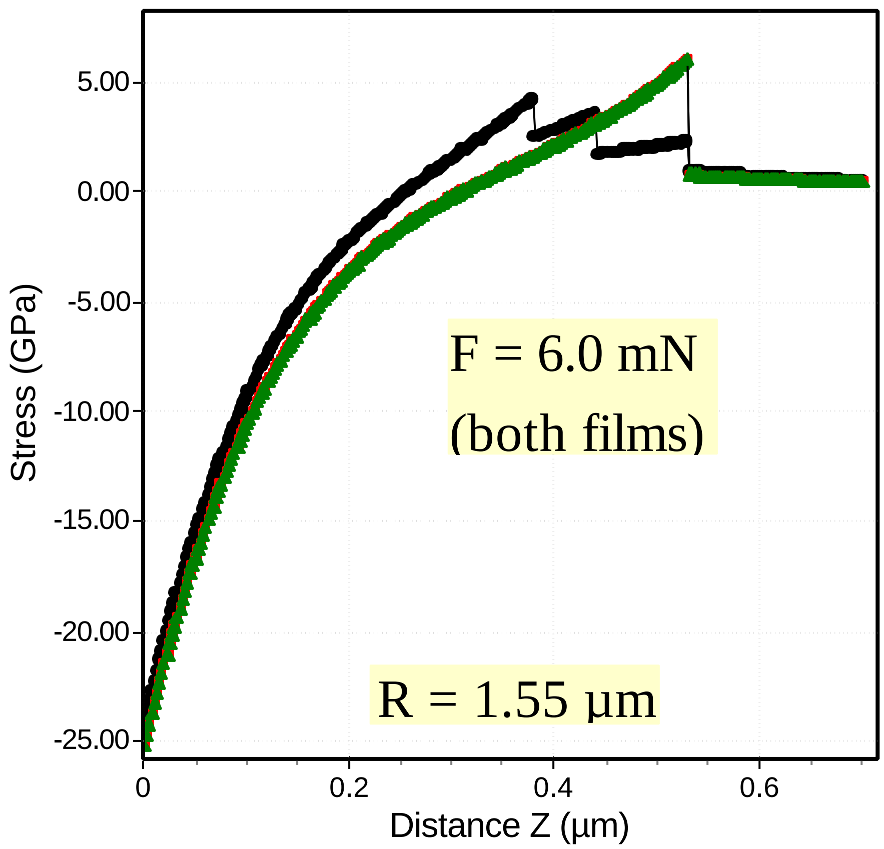
film	p_{N2}/p_{Ar}	E / GPa	σ_Y / GPa	t_f / nm
i	8 %	137	9.0	90
ii	4 %	207	11.9	60
iii	2 %	280	16.5	380

Optimum stack in comparison to a 530 nm single layer, σ_M along the z-axis:



→ maximum utilisation of the load carrying capacity of all single layers as well as the substrate

Tensile stress σ_{xx} along the axis of symmetry:

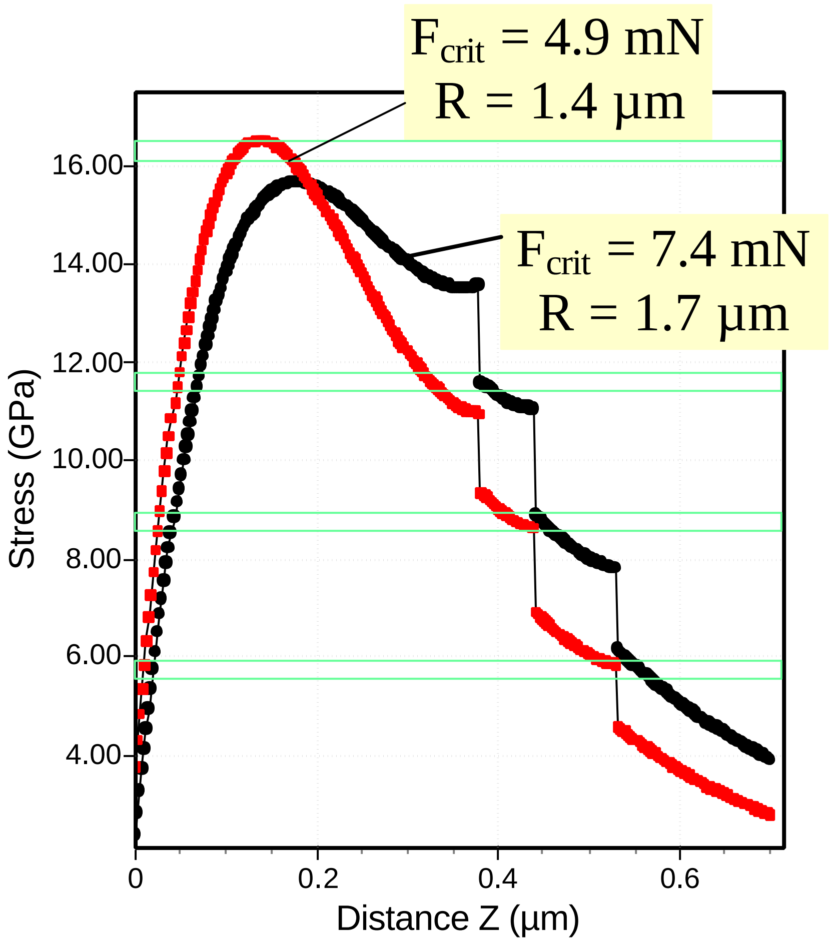


→ increase of critical load by 17 %

→ reduction of tensile stress near the interface (causing "star cracks")

→ very bad adhesion of the single layer; triple layer adhered well.

Variation of the radius of the counterpart, using radii of R = 1.4 µm and 1.7 µm as an example:



- bigger R → increased F_{crit}; stacks fails at the bottom
- smaller R → decreased F_{crit}; stacks fails in top layer
- In both cases, the bearable pressure is reduced.

6. Discussion and conclusions

- Finding optimum coating designs for mechanical contact is a very complex task where a lot of different parameters have to be taken into account.
- However, for exactly that reason it is unlikely that optimum results at low costs can be found by trail and error. Hence, a better understanding due to theoretical modelling is necessary.
- We have demonstrated a first step in this respect, restricting ourselves to a spherical counterpart under normal load.
- Ternary thin film materials from the (B,C,N) system, which offers a broad range of mechanical parameters, were chosen for experiments.
- Using our approach of theoretical modelling and spherical indentation, YOUNG´s modulus and yield strength of the films have been determined with high accuracy.

- Using these date, plastic deformation could be taken into account quantitatively when optimum layer stacks were designed. In contrast, "star crack" formation was included only qualitatively since critical tensile stress values of the films are still missing.

Future work shall include:

- the experimental determination of critical values for "star crack" formation and other inelastic effects as well as their inclusion in the modelling in a quantitative manner,
- roughness effects,
- more complex load conditions, indenter shapes and contact stress distributions,
- improvement of the computer model in order to perform the expensive calculations faster and with a higher degree of automation.