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Size Effects on Deformation and Fracture of Scandium Deuteride Films

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Motivation

Neutron targets are typically a metal-hydride film.

Scandium deuteride (ScD_2) films are of interest since they:

- reach steady-state neutron yield quickly
- have relatively good thermal stability
- do not exhibit crater formation during use

However, these films have been observed to crack and delaminate. This has prompted a series of studies on the fracture properties of these films that utilized both channel cracking within films and pillars.

This work seeks to explore if there is a significant size effect.

Materials and Methods

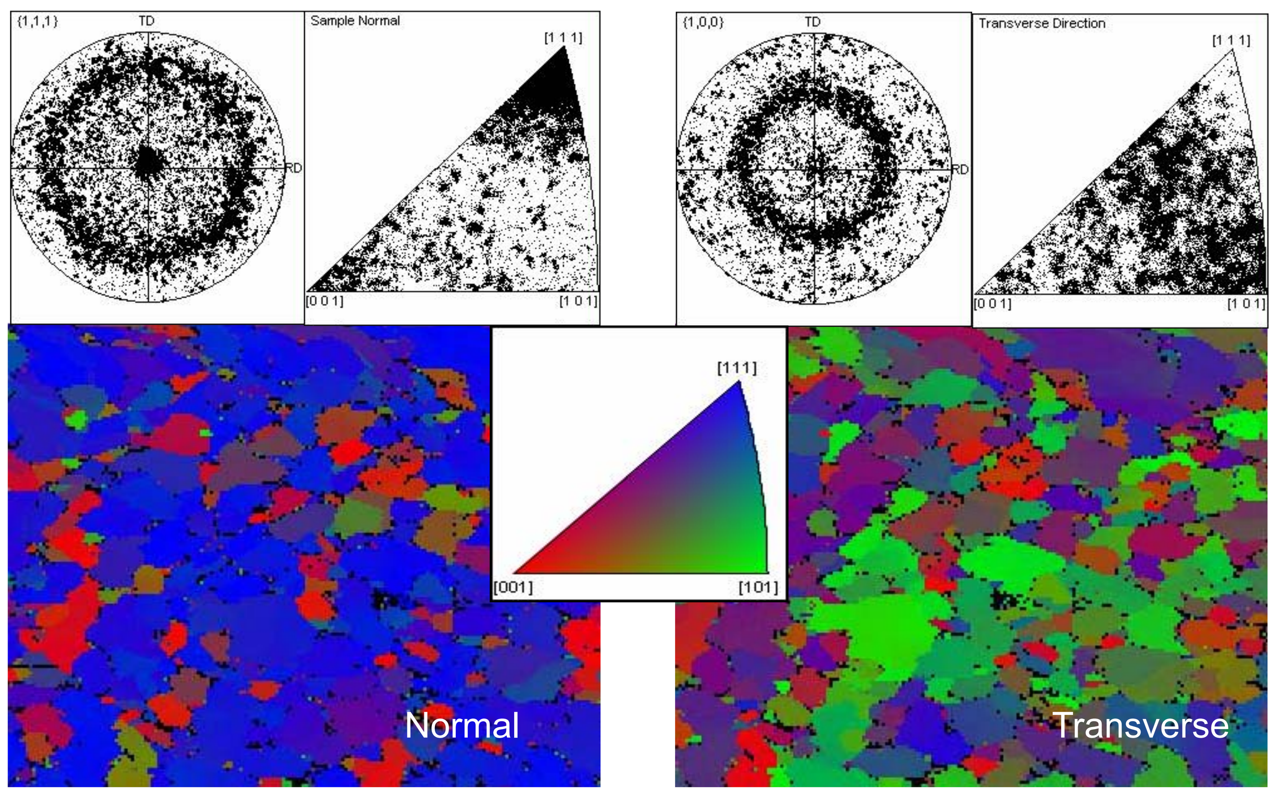
Sc films were sputter deposited onto molybdenum and fused silica substrates.

Films underwent thermal deuterium charging and film stresses all transitioned to tensile.

Thermal misfit strains during cool down lead to cracking and network of islands.

Micropillars were milled from islands using a FIB (300, 800, 1600 nm diameter).

Structure of ScD_2

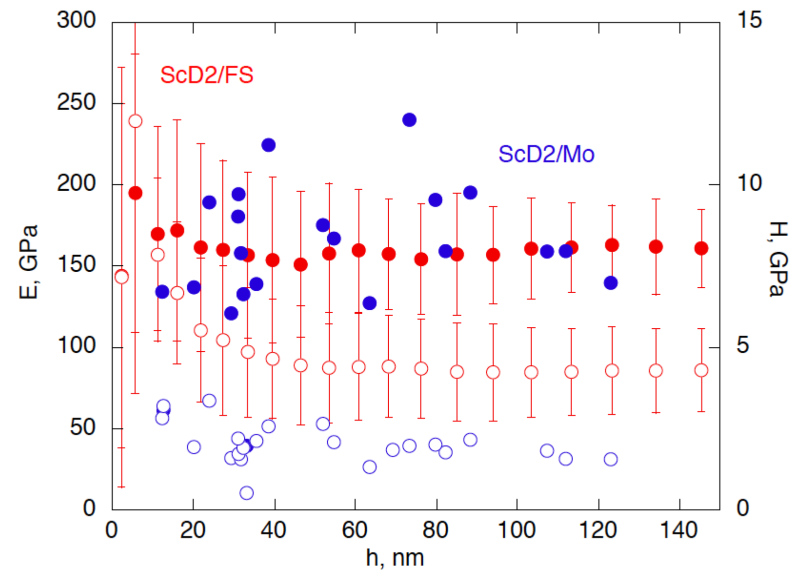


X-ray diffraction scans, pole figures and electron backscatter diffraction maps showed that the film surface had a face centered cubic structure with a (111) normal orientation typical of deuterides. Cross section EBSD showed a mix of (110), (100), and to a lesser degree (111) oriented grains in the transverse orientations.

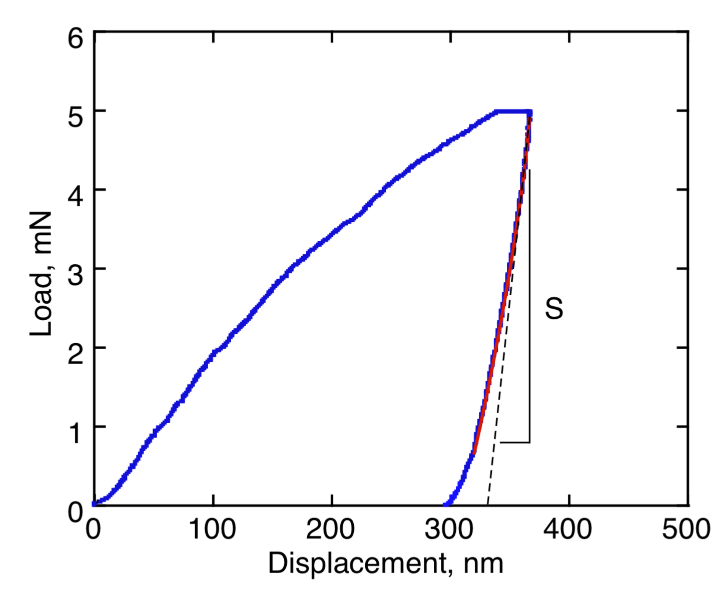
Mechanical Properties from Nanoindentation

Scandium deuteride films have a higher modulus and hardness than the scandium films.

Scandium deuteride films on fused quartz had a modulus near 150 GPa and hardness of 4 GPa. Films on Mo substrates had lower hardness values.



Calculating modulus from the elastic unloading of micropillars.

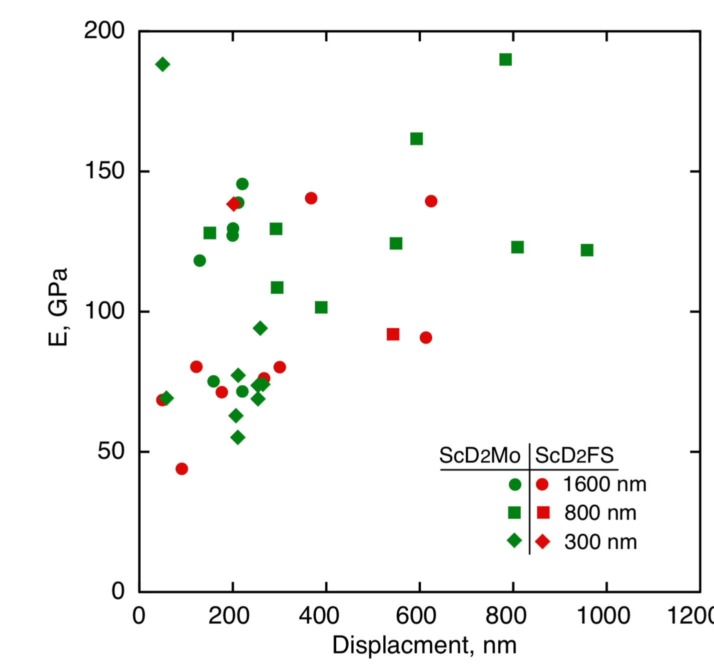


pillar as a tapered cylinder
(Singh et al. 2011; Lee et al. 2007)

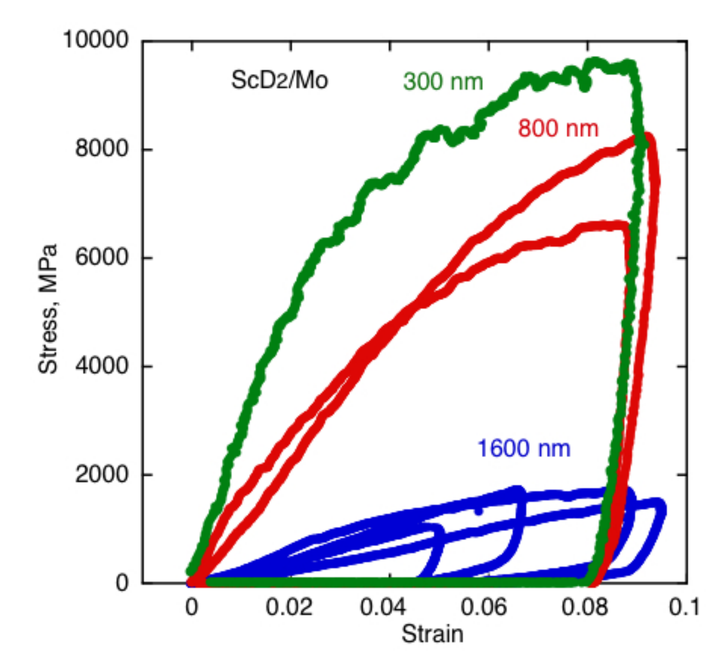
$$E = \frac{\pi d_o^2 L_o S_{pillar}}{4 L_p^2}$$

pillar as a right circular cylinder
(Greer et al. 2007; Uchic et al. 2004)

$$E = \frac{P L_o S_{pillar}}{\pi d_o \left(d_o + L_o \sin\theta\right)}$$

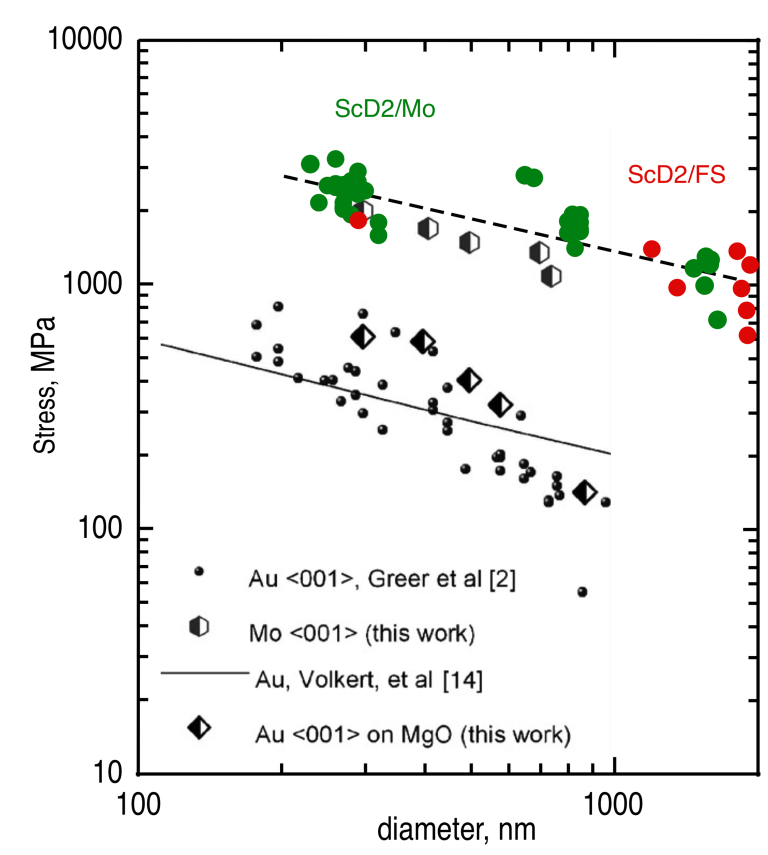


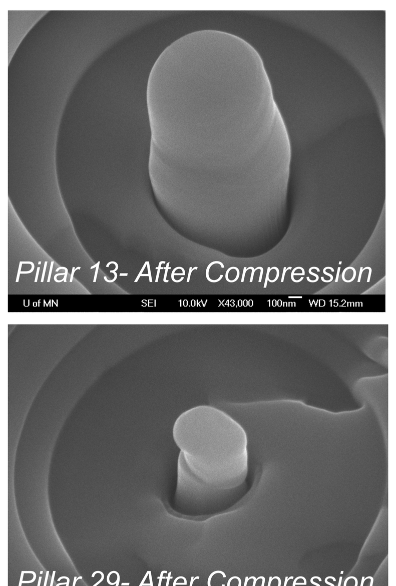
Stress- strain response of pillars with 300 nm- 1600 nm diameters.



Stress from top diameter

Smaller pillars exhibited higher stress.



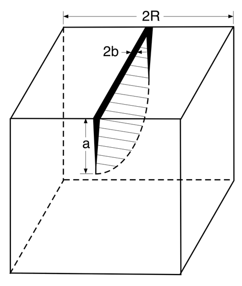


Scatter at small pillar diameters is probably due to grain size being equal to or on the order of the pillar diameter.

Cracking during compression testing of micropillars also provided a measure for fracture toughness.

Through thickness cracking:
(Broek, 1991; Ostlund et al. 2009)

$$K_{Ic} = \frac{\sqrt{3EbR^{3/2}}}{4a^2(1-\nu^2)}$$



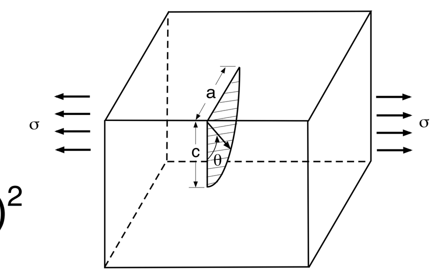
Treating the crack as corner crack under an applied tensile stress gradient: **(Tada et al. 2000)**

$$K_{Ia} = \frac{2}{\pi}\sigma\sqrt{\pi a}\,F(\theta)$$

where

$$F(\theta) = 1.0 - 0.72\sqrt{\sin\theta} + 0.11\,(\sin\theta)^2$$

$$(10^\circ < \theta < 80^\circ)$$



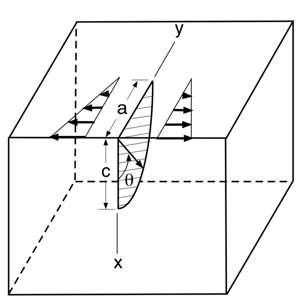
Treating the crack as corner crack under a uniform applied tensile stress: **(Tada et al. 2000)**

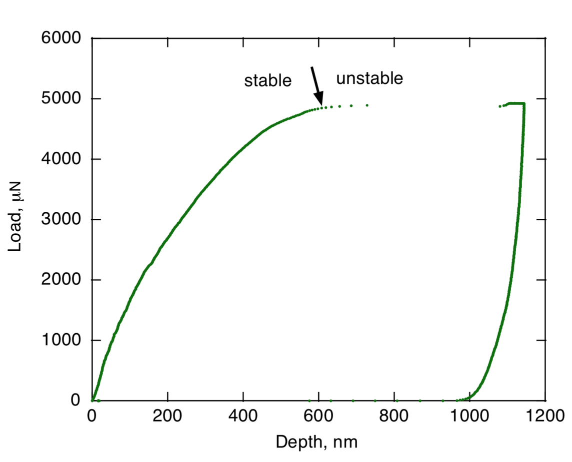
$$K_{Ia} = \frac{2}{\pi}\sigma\sqrt{\pi a}\,F_Q(\theta)$$

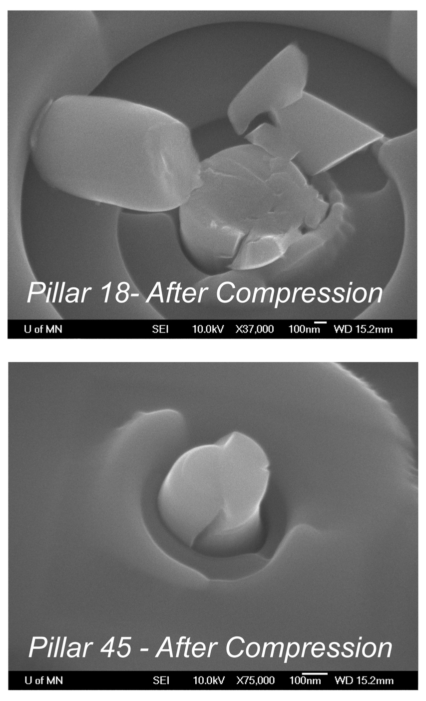
where

$$F_Q(\theta) = F(\theta)\cdot F\left(\frac{\pi}{2} - \theta\right)$$

$$F(\theta) = 1.211 - 0.186\sqrt{\sin\theta}$$







Cracking occurred in the 300 and 1600 nm pillars for the ScD_2/Mo pillars, while the ScD_2/FS system has cracking in the 1600 nm pillars only.

Method for calculating Fracture Toughness		ScD_2/FS	ScD_2/Mo	
		1600 nm	1600 nm	300 nm
		MPa-m$^{1/2}$	MPa-m$^{1/2}$	MPa-m$^{1/2}$
Corner Crack	Uniform stress field	2	1	
Corner Crack	Stress gradient	0.4	0.5	
Through Thickness Crack	Treating as a beam	1.4		0.4-0.7
Channel Cracking		1.0-1.9		

Conclusions

- Compression testing did not show a clear size effect on mechanical properties
- Residual stress induced channel cracking suggests that the fracture toughness of this film system is near 1.4 MPa-m$^{1/2}$
- Fracture during micropillar tests give fracture toughness values from 0.4 to 2.0 MPa-m$^{1/2}$ with full beam fracture giving a value of 1.4 MPa-m$^{1/2}$

Acknowledgements

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