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čtvrtek, 3. 4. 2025, 14.00,
posluchárna F2, MFF UK, Ke Karlovu 5

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Interplay between residual stress and microstructure features in thin Cr and Mo films deposited on various substrates

The presented study is a part of the project focused on the fundamental description of the laser ablation process. The laser ablation could introduce craters into a material which can play an important role in a modification of local material properties, especially microstructure. The microstructural properties inside the craters could then work as *post mortem* probes of condition (temperature, pressure) during ablation itself.

However, to describe these microstructural changes properly, well known original state of a material is the necessary prerequisite. For this purpose, the 100 nm thick epitaxial layers of Cr and Mo were deposited by magnetron physical vapour deposition (PVD) on various substrates: amorphous SiO_2 and single-crystalline MgO(100), MgO(110) and corundum Al_2O_3(0001). The microstructural properties such as residual stresses, grain sizes, layer morphology and crystallographic orientation have been studied in the mean of the X-ray diffraction and electron microscopy.

With the use of an amorphous substrate SiO_2, both Cr and Mo layer grow with the 110 fibre texture. Here, the surface energy plays the decisive role – the surface energy is the lowest at 110 crystallographic plane (Cr and Mo are both bcc metals).

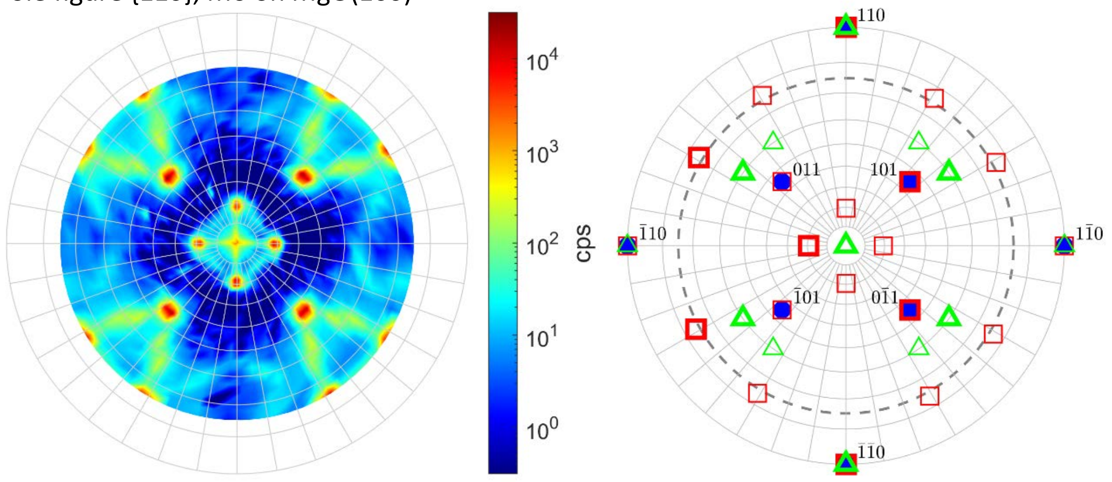
Using a single crystalline substrate, the minimalization of the deformation energy leading from the lattice misfit between the layer and substrate will play an important role. Therefore, deposited layers will grow in the specific orientation relation with the substrate. However, the presence of several variants or twins with different orientation was observed in some cases. Individual orientation relations can be deduced from the measured pole figures (example in **Figure 1a** and **1b**). The reason of forming such variants is to reduce overall deformation energy.

The residual stresses obtained by $\sin^2\psi$ method are shown in **Table 1**. The results show that the layers posses quite high residual stresses in the order of several GPa. In comparison to the yield strength (0.131 GPa for Cr and 0.324 GPa for Mo [1]), this points to a fact that there should be an inner mechanism leading to the material hardening. The analysis of the diffraction peaks broadening and also transmission electron microscopy show that the deposited layers consist of the small columnar crystallites with the size of d = 20-50 nm (see **Figure 1c**). The presence of such crystallites leads to an increase of the yield strength through the Hall-Petch relation $\sigma_{yield} \sim d^{-\frac{1}{2}}$ [2].

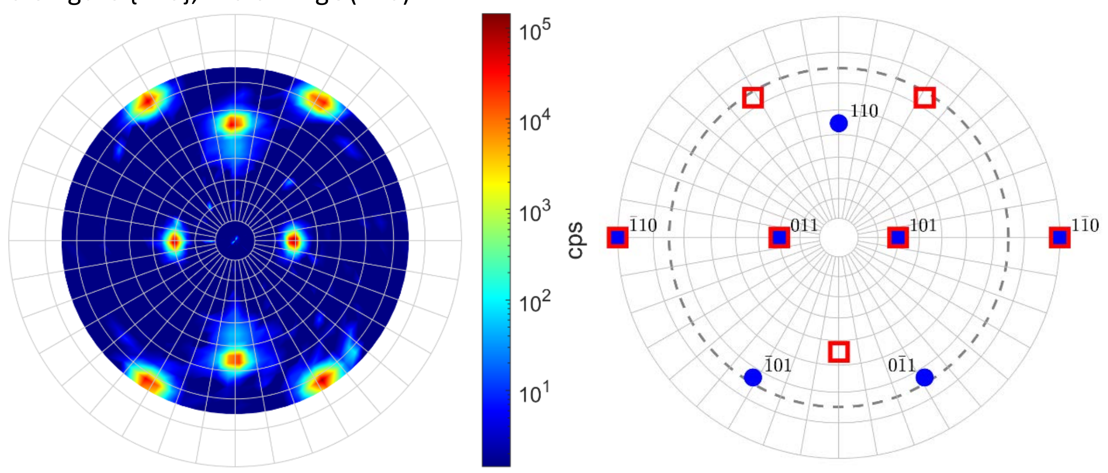
Table 1: Out-of-plane orientation of individual variants inside studied layers and their residual lateral stress σ_{lat}.

		MgO(100)		MgO(110)		Al_2O_3(0001)	
		out-of-plane orientation	σ_{lat} (GPa)	out-of-plane orientation	σ_{lat} (GPa)	out-of-plane orientation	σ_{lat} (GPa)
layer	Cr	100	1.4	2 variants with 211	4.1 3.9	unspecific fibre texture	-
	Mo	matrix: 100 twins: 212 minor v.: 101	-1.5 0 -0.8	2 variants with 211	2.3 2.1	3 variants with 110 (Δφ=60°)	1.5 1.6 1.3

a) Pole figure {110}, Mo on MgO(100)



b) Pole figure {110}, Mo on MgO(110)



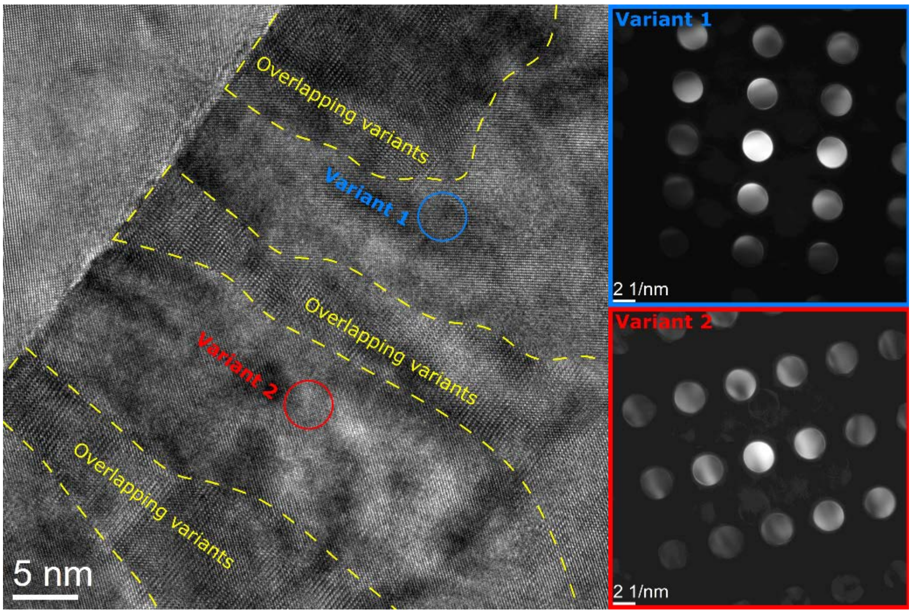


Figure 1: **a)** Pole figure 110 measured on Mo layer deposited on (100)-oriented MgO and the stereographic projection with theoretical positions of the peaks (blue circles – matrix, red squares – twins, green triangles – minor variants). **b)** Pole figure 110 measured on Mo layer deposited on (110)-oriented MgO and the stereographic projection with theoretical positions of the peaks (blue circles – variant 1, red squares – variant 2). **c)** High-resolution TEM image and convergent beam electron diffraction (CBED) patterns showing the variants in Mo layer deposited on (110)-oriented MgO substrate.

References:

[1] Theodore Gray, *Periodic Table (website)*, https://periodictable.com/, visited 8.8.2024

[2] Niels Hansen, *Hall–Petch relation and boundary strengthening*, Scripta Materialia 51 (2004) 801–806, doi: 10.1016/j.scriptamat.2004.06.002

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