Functional nano-structured tungsten based coatings for systems for energy production.
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Outline
The stability of heterophase interfaces between metal systems, their kinetic, structural, and thermomechanical properties are a matter of concern for high demanding applications involved in the development of technological coatings for the first wall materials in fusion reactors and their prototypes (ITER). We would like to discuss preliminary results of X-ray experiments on model coatings made of tungsten, in particular the problems related to strain inhomogeneously in metal films on heterophase substrates. These analyses of nanostructured thin layers can be performed using laboratory grazing incidence diffraction, allows the accurate extraction of quantitative relevant information about the structure (strain and atomic positions) and the microstructure (crystallite size and microstrain), selectively probing the material on a depth of few nanometers.

Phase analysis
Residual stress analysis
Crystallite size and strain determination
Study of the anisotropy in the lattice deformation
Investigation of gradients of microstructure parameters vs depth

Snell, Fresnel & XRD
\[ n \cos \alpha' = \cos \alpha \]
\[ n = 1 + \delta i \beta = 1 - \alpha^2 + i\beta \cdot \alpha^2 = \frac{4\pi}{\lambda} \cdot \beta = \frac{\mu}{2k} \]

Inhomogeneous strain in films

Differences between the specular reflectivity (XRR) and diffraction signals (GID).

1 + R(\alpha) = T(\alpha) \rightarrow T(\alpha) = \frac{2\alpha}{\alpha + \alpha'}
T(\alpha) = \frac{2\alpha}{\alpha + \alpha'} \text{ for } \alpha < \alpha_1
T(\alpha) = \frac{2\alpha}{\alpha + \alpha'} + \sqrt{\alpha^2 - 1} \text{ for } \alpha > \alpha_1

The regular \( \psi \)-scan method unfortunately probes a volume that changes as a function of \( y \), averaging out the strain in the film, and preventing a mapping of the local strain

Snell’s law adapted to XRD: it provides the encoding of the probed depth information by the impinging beam angle

Depth profile of residual stresses in W films can be obtained using GID. A limitation of the method is that the material should be quasi-isotropic (untextured).
This requirement can be further relaxed if the anisotropy ratio of the material is small, that is the case of many metals like W and Mo. The result show that the strain is almost uniform in most of the film but it rapidly increases close to the surface. In a layer below the surface (< 100nm) the strain increases very fast. A small part of this effect seems related to the presence of a very thin oxide layer (thickness of about 1 nm).

References

Benefits
The analysis of the structures and microstructures of nanostructured thin layers can be performed using laboratory grazing incidence diffraction, provided accurate corrections are performed to handle the instrumental broadening effects related to the experiment geometry for an impinging beam close to the critical angle. These procedures allow the accurate extraction of quantitative relevant information about the structure and the microstructure, selectively probing the material on a depth of few nanometers.
Grazing incidence X-ray diffraction can be a workhorse technique for deriving crystallite size in nanoscale systems due to its non-destructive character, the fast data collection and the relative simplicity of the experimental setup. This information is relevant for an accurate description of nanocrystalline systems prepared as thin films and it can significantly improve the knowledge of their structure-properties relationships.
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