IOP PUBLISHING JOURNAL OF PHYSICS D: APPLIED PHYSICS

J. Phys. D: Appl. Phys. **42** (2009) 185406 (6pp) doi:10.1088/0022-3727/42/18/185406

A proposal for an unusually stiff and moderately ductile hard coating material: Mo_2BC

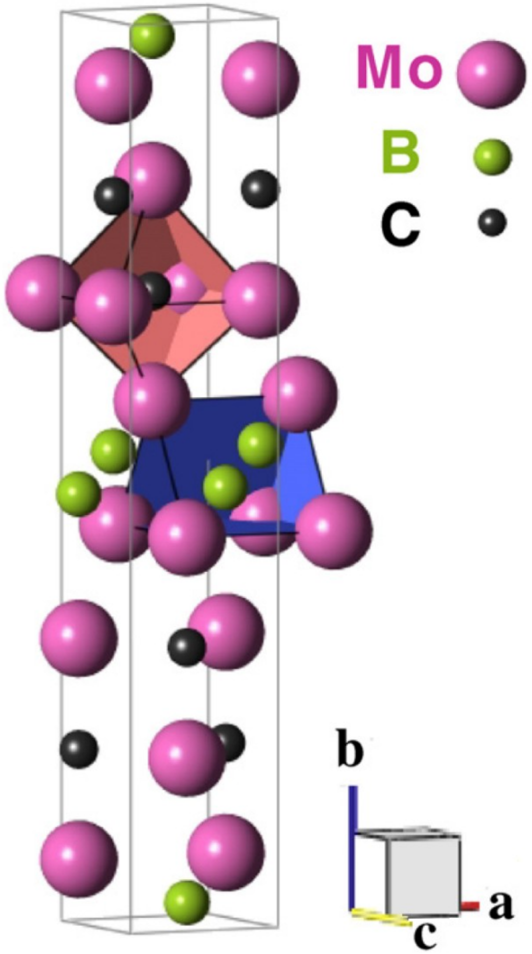
J Emmerlich[1,3], D Music[1], M Braun[1], P Fayek[1], F Munnik[2] and J M Schneider[1]

[1] Materials Chemistry, RWTH Aachen University, Kopernikusstr. 16, D-52074 Aachen, Germany
[2] Forschungszentrum Dresden Rossendorf, Bautzner Landstrasse 400, D-01328 Dresden, Germany

Introduction

- Protection of tools – thin films
- Most thin films – hard but brittle
- Combination of hardness and moderate ductility to prevent formation and spreading of cracks
- Nanolaminate Mo_2BC
- Prepared by magnetron sputtering

Mo_2BC coatings



Material	B (GPa)	B/G
TiN	295	1,39
$Ti_{0,25}Al_{0,75}N$	178	1,44
c-BN	376	0,98
Mo_2BC	324	1,72

- Combination of great hardness and moderate ductility
- Stiff Mo-B and Mo-C layers with metallic interlayer bonding
- B – bulk modulus
- G – shear modulus
- B/G > 1,75 ductile materials
- Mo_2BC thin films were synthesized using DC magnetron sputtering on Al_2O_3 at a substrate temperature of ~900 °C

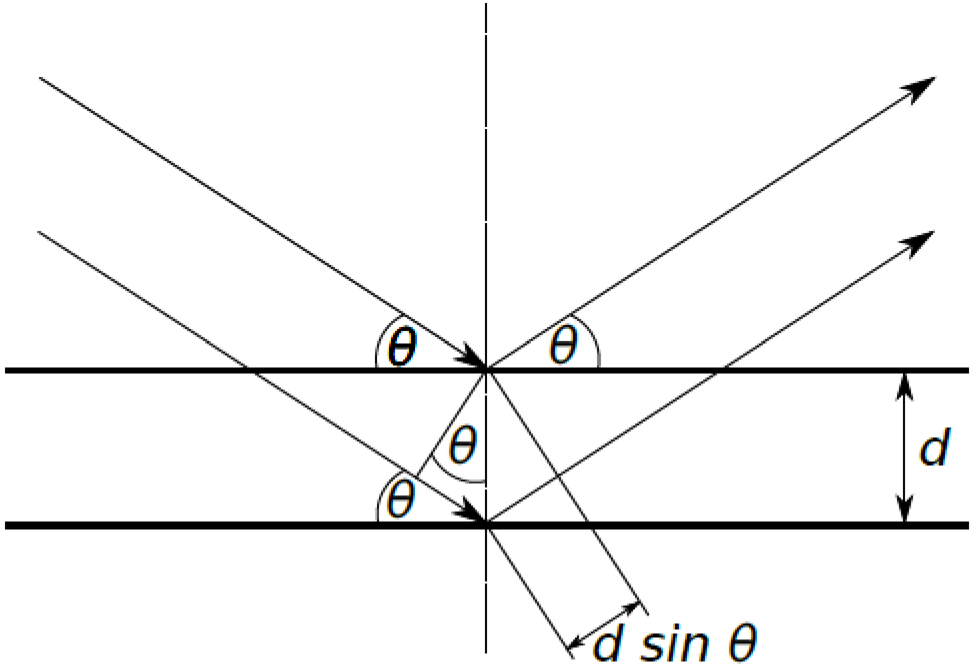
Used characterization methods

- X-ray diffraction
- Scanning electron microscopy
- Electron recoil detection analysis

X-ray diffraction (XRD)

- Information about the crystal structure
- Uses the scattering of photons on the atoms of the lattice
- The superposition of the scattered waves from individual atoms leads to classical reflection of light
- The incident rays are reflected from the atomic planes and interfere with each other
- Constructive interference occurs, when the Bragg condition is met

X-ray diffraction (XRD)

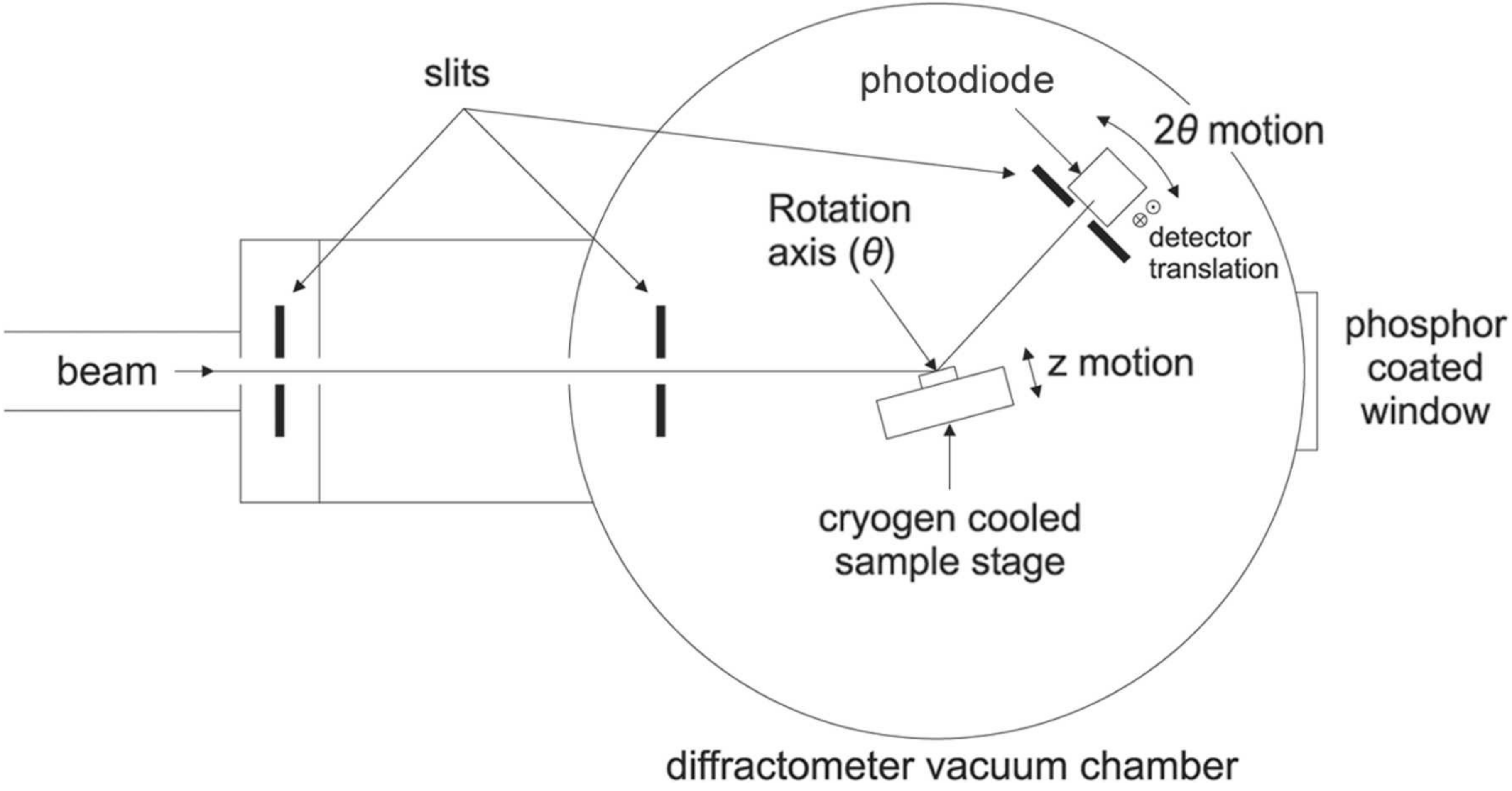


- The Bragg equation:

$$2d\sin\theta = n\lambda$$

- λ is the wavelength of the incident light,
  d is the distance between atomic planes,
  n is an integer and
  θ is the angle of incidence.

X-ray diffraction (XRD)



X-ray diffraction (XRD)

- Three methods of measuring:
  - Debye-Scherer – monochromatic light and polycrystaline material
  - Laue – polychromatic light and monocrystaline material
  - Monochromatic light and monocrystaline material

- The combination of polychromatic light and polycrystaline material creates too many diffractions

X-ray diffraction (XRD)

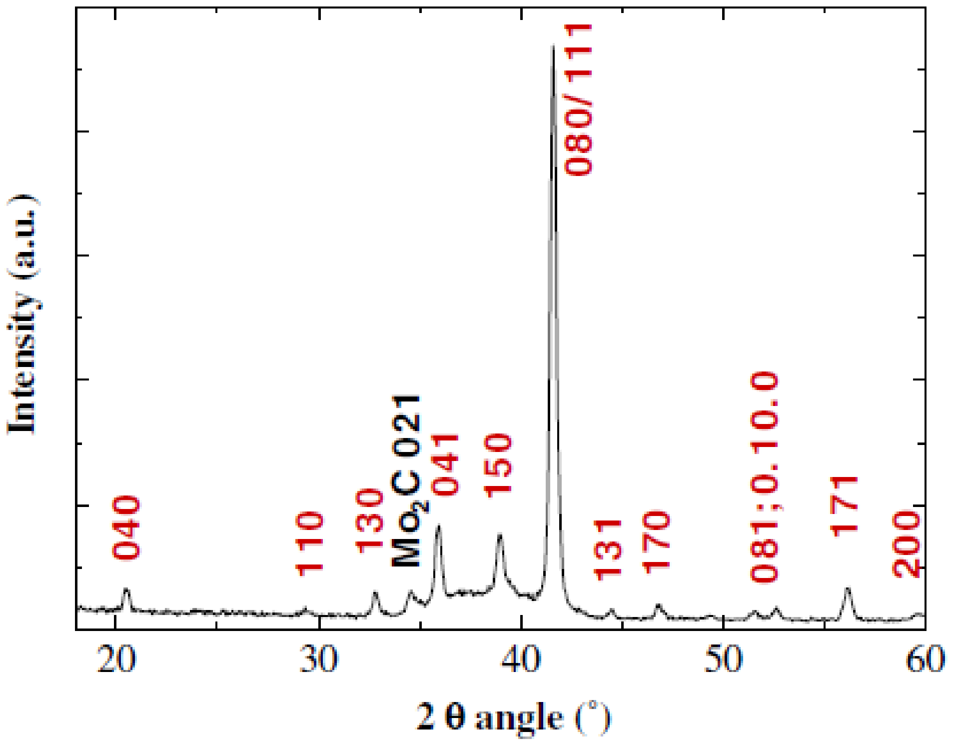


Figure 5. X-ray diffractogram of a Mo_2BC thin film deposited at ~900 °C on $Al_2O_3(0001)$ substrate.

- The sample consists predominantly of Mo_2BC
- There is a minor contribution detected, stemming from Mo_2C
- Good agreement between the measured peak positions and the reference values
- The relative intensities of the diffractogram do not match due to the sample being textured

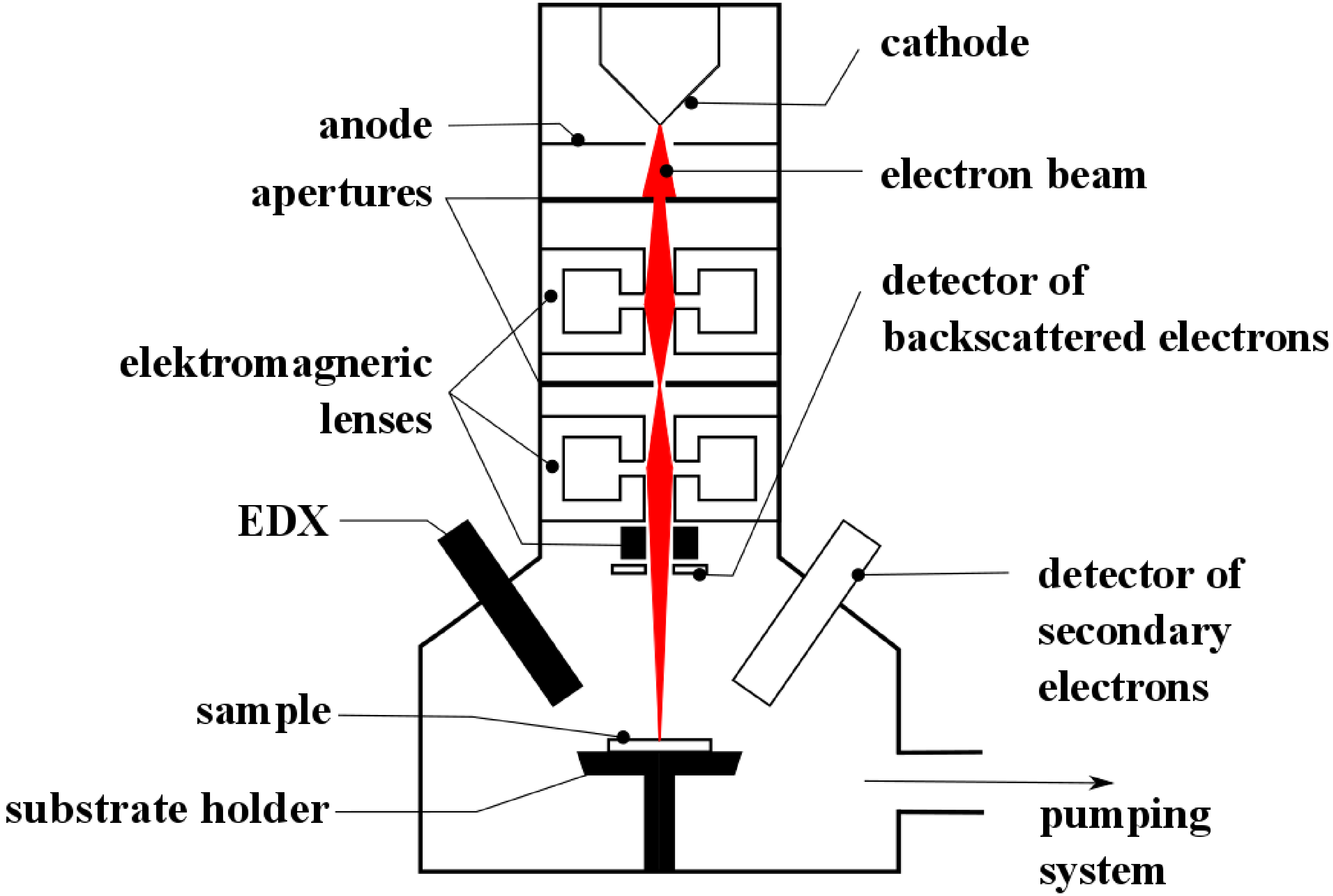
Scanning electron microscopy (SEM)

- Used for imaging of surfaces
- Focused beam of accelerated electrons
- The beam is focused and directed by electromagnetic lenses and scanns the surface
- High vacuum is necesary to prevent collisions of electrons with gas particles
- Possibility to use with EDX or WDX to determine composition

Scanning electron microscopy (SEM)

- Two basic kinds of signal:
- Backscaterred electrons
  - Electrons with high energy reflected from the surface
  - Greater penetration depth but worse spatial resolution
  - Number of reflected electrons depends on the atomic number of the particle – greater mass – more reflected electrons – brighter spot
- Secondary electrons
  - Electrons emitted from the surface due to inelastic scattering
  - Because of their low energy, only electrons created at the surface leave the sample
  - Mostly information about topography – electrons are emitted mostly from sharp edges

Scanning electron microscopy (SEM)



Scanning electron microscopy (SEM)

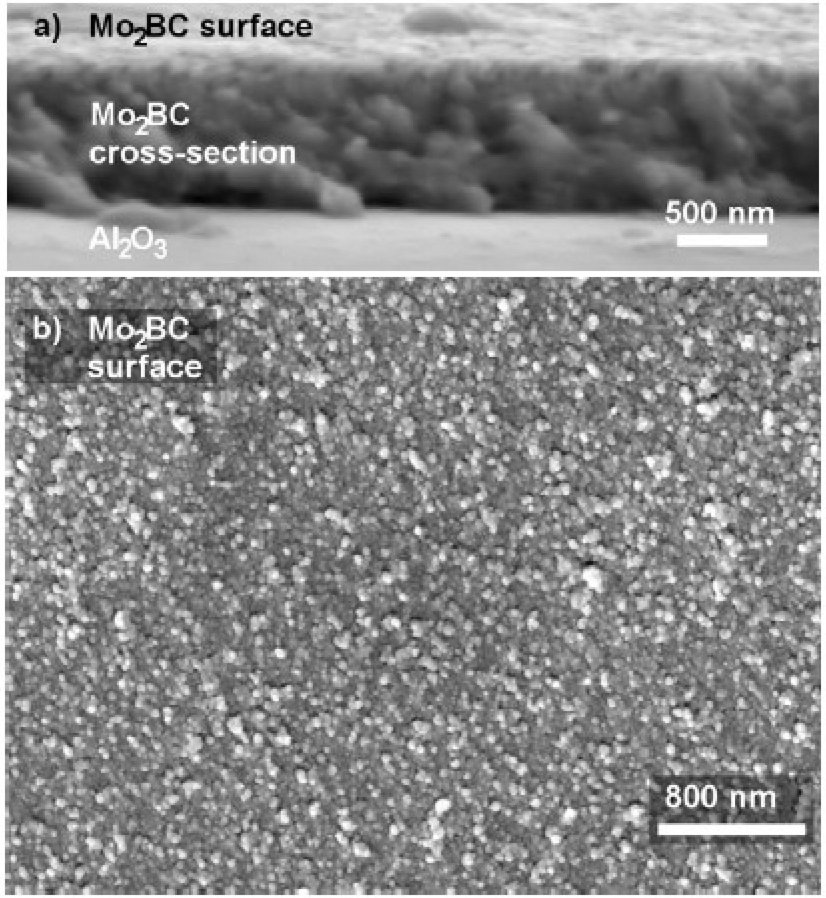
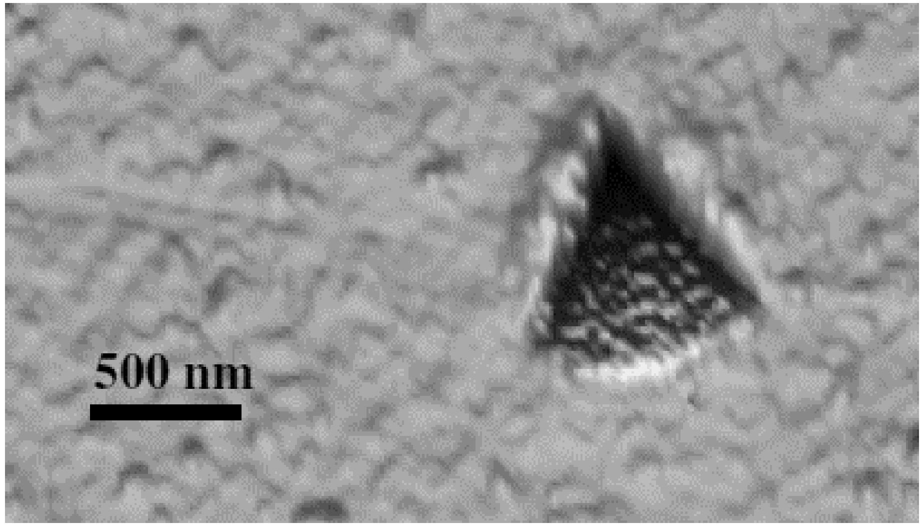


Figure 6. SEM image of (*a*) cross-section and (*b*) surface of a Mo_2BC thin film grown at ~900 °C on $Al_2O_3(0001)$.

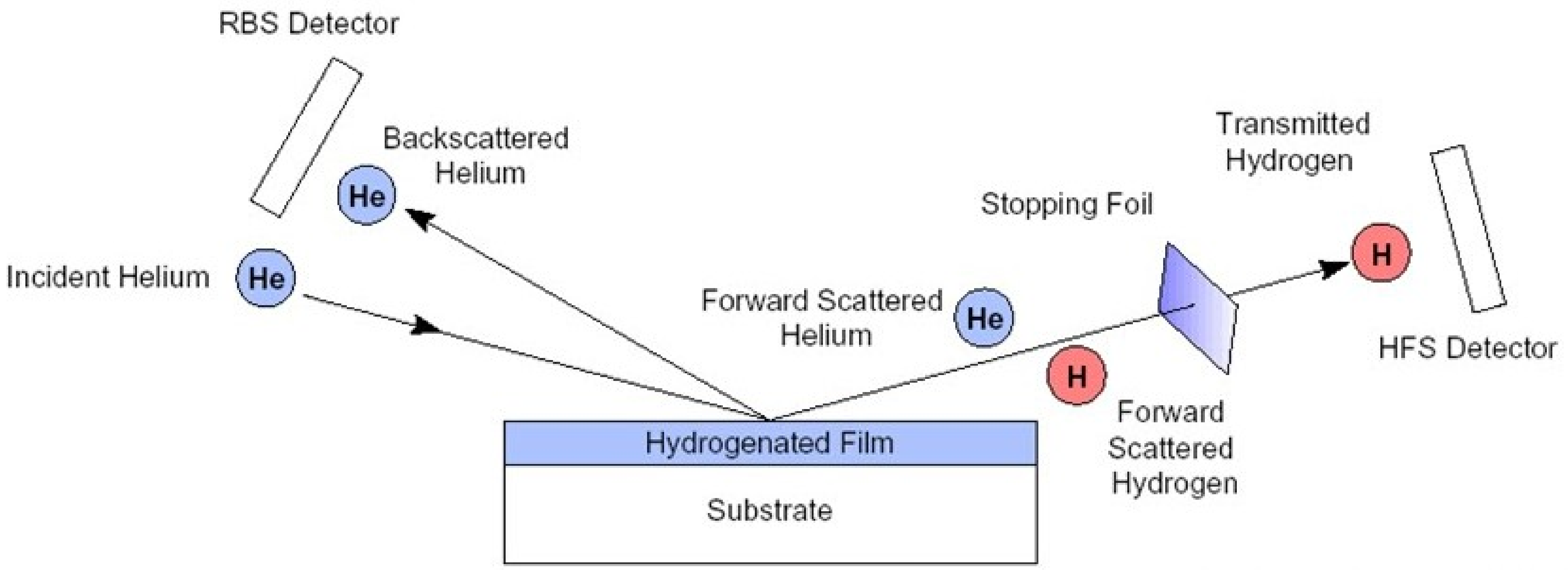
- No formation of pores or cavities
- Surface features with a diameter well below 100 nm
- No crack formation observed around the indent



Energy recoil detection analysis (ERDA)

- Detection of light elements in a heavy matrix
- Analysis of forward scattered ions or atoms
- A single collision
- Particles can by identified by their kinetic energy
- Analysis of particles: TOF, thin foil

Energy recoil detection analysis (ERDA)



Charles Evans and Assoc., RBS APPLICATION SERIES NO. 3

Energy recoil detection analysis (ERDA)

- The film consists of 49 at% Mo, 27 at% B and 24 at% C
- The chemical formula $Mo_2B_{1.1}C_1$, which is very close to the nominal stoichiometry of Mo2BC.
- O and H were not detected in the film.
- The variation of B from stoichiometric Mo_2BC composition is within the expected measurement error.

Conclusion

- Mo_2BC thin films were synthesized using DC magnetron sputtering on Al_2O_3 at a substrate temperature of ∼900 °C.
- XRD measurements and ERDA confirmed that the grown film is almost phase pure and of near-stoichiometric composition
- No formation of cracks was observed implying moderate ductility
- Deformation experiments carried out with nanoindentation confirmed the high stiffness of Mo_2BC

Thank you for your attention!

J. Emmerlich, D.Music,M. Braun, P. Fayek, F. Munnik, J.M. Schneider, J. Phys. D: Appl. Phys. 42 (2009) 185406

Peter E.J. Flewitt, R.K. Wild: *Physical Methods for Materials Characterisation*, Series in Materials Science and Engineering

https://sites.google.com/a/lbl.gov/rbs-lab/ion-beam-analysis/elastic-recoil-detection-analysis-erda

http://journals.iucr.org/s/issues/2005/04/00/kv5008/kv5008fig1.html