COMBINING HIGH STRENGTH AND MODERATE DUCTILITY IN WEAR RESISTANT COATINGS: A MO_2BC STUDY

Rafael Soler, Max-Planck-Institut für Eisenforschung GmbH
r.soler@mpie.de
Stephan Gleich, Max-Planck-Institut für Eisenforschung GmbH
Hamid Bolvardi, RWTH Aachen University
Christoph Kirchlechner, Max-Planck-Institut für Eisenforschung GmbH
Jochen M. Schneider, RWTH Aachen University
Christina Scheu, Max-Planck-Institut für Eisenforschung GmbH
Gerhard Dehm, Max-Planck-Institut für Eisenforschung GmbH

Key Words: hard coatings, fracture toughness, crystallinity, single beam cantilevers, density functional theory

Wear resistant coatings employed in cutting and forming applications usually require the combination of high stiffness and high hardness, as these properties often enable low wear rates. Moreover, moderate ductility is often desirable as crack formation can lead to early service failure. Traditionally, the combination of high stiffness and high ductility has been considered as self-excluding. However, recent investigations based on correlative experimental and theoretical research suggest that this empirical relationship can be overcome by a new generation of hard coating materials.

For example, *ab initio* calculations have predicted Mo_2BC to exhibit a high stiffness in combination with moderate ductility [1]. The material crystallizes in an orthorhombic structure (space group *Cmcm*), in which B atoms are positioned in Mo_6B trigonal prisms and C atoms are at Mo_6C octahedral sites in alternating sequence (unit cell is shown in Fig. 1a). The calculated bulk modulus of 324 GPa for Mo_2BC surpasses the one of $Ti_{0.75}Al_{0.25}N$ (178 GPa) [2], often referred as benchmark coating, by more than 50%. In addition, Mo_2BC has been also predicted to be moderately ductile based on its ratio of bulk to shear moduli (B/G) and the calculated positive Cauchy pressure [3].

In this work we will present our most recent developments on this unique material. We will provide insight into the mechanical properties, in terms of: elastic modulus, E, and hardness, H; and fracture toughness, K_{IC}. The mechanical experiments are conducted by means of nanoindentation experiments and single beam cantilever testing, respectively. Correlation with extensive microstructural and chemical analysis, i.e. X-ray diffraction, transmission electron microscopy and atom probe tomography, will be shown. The influence of deposition conditions, namely substrate temperature, on the mechanical properties will be also discussed with respect to the resulting film microstructure, i.e. degree of crystallinity, average grain size, chemical homogeneity, etc.

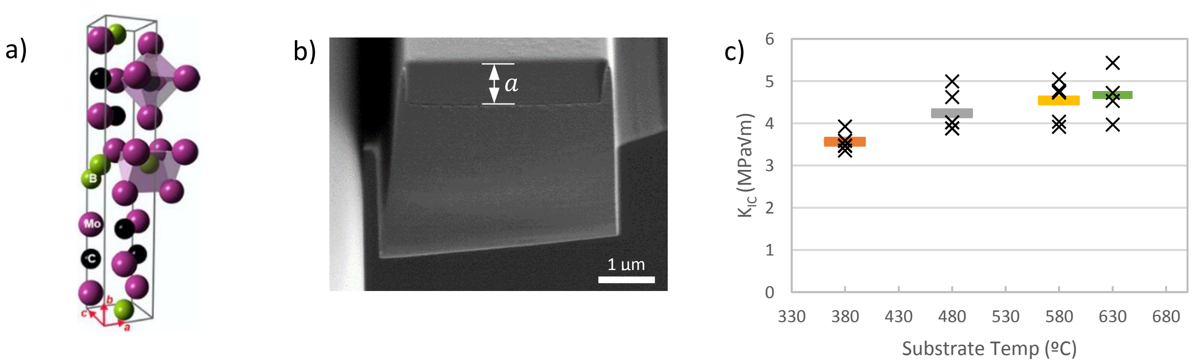

Fig. 1.: a) Unit cell of the Mo_2BC structure [3]; b) Representative fracture surface of a single beam cantilever; c) Fracture toughness dependency on substrate temperature.

[1] J. Emmerlich et al., Jour. Phys. D: Appl. Phys. (2009).
[2] C. Kuiying et al., Jour. Phys. D: Appl. Phys (2003).
[3] H. Bolvardi et al., Jour. Phys. Conden. Matter (2013).