

# Verification of interfacial layers in doped WC-Co regarding their structure and chemistry by STEM imaging, simulation and analytical STEM

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WC-Co are used in a variety of applications such as in mining and in metal forming. Their mechanical properties are tailored to the application by altering the microstructure with respect to, e.g. WC grain size, WC grain morphology and metal binder content. WC grain size can be controlled by the addition of carbide forming elements, such as Cr, Ti and V [1]. Some of these elements have been observed to segregate to certain crystallographic surfaces of the WC grains forming ultrathin layers, at the interface between the WC grains and the Co binder, only a couple of monolayers in thickness [2].

C<sub>s</sub>-corrected STEM using a FEI Titan<sup>3</sup> G2 60-300kV has been applied to acquire ADF-/HAADF-STEM images and to chemically characterize the interface between WC and Co. For WC-Co with Ti addition, HAADF-STEM images revealed two monolayers at the WC basal facets with significantly different contrast indicating a significant mass density difference. EDXS-STEM and HAADF-STEM images revealed that these monolayers consist of Ti and W, respectively. This is in accordance with DFT calculations predicting the inner monolayer to contain essentially only Ti whereas the outer monolayer contains mainly W atoms. From DFT calculations it cannot be predicted whether the W monolayer is pure or contains Ti atoms. The calculated interatomic distances are in agreement with the experimentally measured ones [3].

STEM image simulations applying software packages QSTEM [4] and Dr. Probe [5] were performed using the structure proposed from the DFT calculations and these simulated ADF-/HAADF-STEM images were compared to the acquired STEM images.

In addition, in the STEM image simulations W atoms in one of the atom columns in the outer monolayer were successively replaced by Ti atoms to assess the change in the intensity.

Change in intensity due to mass loss or contamination was not taken into account in the ADF-/HAADF-STEM image simulations. However, by STEM image simulations the uncertainty due to delocalization of spectroscopic signals can be ruled out.

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## References

1. K. Hayashi, Y. Fuke, H. Suzuki *J. Jpn. Soc. Powder Powder Metallurgy* 19 [2], 67-71, (1972)
2. M. Kawakami, O. Terada, K. Hayashi, *J. Jpn. Soc. Powder Powder Metallurgy*, 53 [2], 166-171, (2006)
3. A. Meingast, E. Coronel, A. Blomqvist, S. Norgren, G. Wahnström, M. Lattemann, *International Journal of Refractory Metals and Hard Materials*, 72, 135-140, (2018)
4. C. Koch, Dissertation, Arizona State University, USA, (2002)
5. Barthel, J. (2017) *Dr. Probe - High-resolution (S)TEM image simulation software*. <http://www.er-c.org/barthel/drprobe/>