Microsc. Microanal. 21 (Suppl 3), 2015
doi:10.1017/S1431927615011174 Paper No. 1038

Study on the Atomic and Electronic Structure in CrN (VN, TiN) Films using C_S-Corrected TEM

Zaoli Zhang[1], Gerhard Dehm[2]

[1]. Erich Schmid Institute, Austrian Academy of Sciences, Leoben, Austria
[2]. Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
Email: zaoli.zhang@oeaw.ac.at

Transition metal nitrides have found wide-spread applications in the cutting- and machining-tool industry due to their extreme hardness, thermal stability and resistance to corrosion. The increasing demand of these nitrides requires an in-depth understanding of their structures at the atomic level. This has led to some experimental and theoretical researches [1-6]. The films used in this study were deposited by reactive direct current magnetron sputtering of a Cr/V/Ti metal target in an $Ar+N_2$ atmosphere at a constant total pressure of 1 Pa, a target power of 6 kW, and a temperature of 350°C. A TEM/STEM JEOL 2100F operated at 200 kV and equipped with an image-side C_S-corrector and a Gatan imaging filter (Tridiem) was utilized for characterizing the film structure.

In this paper, we will present some recent results on the atomic and electronic structures of metal nitride thin films (CrN, VN and TiN) on MgO and Al_2O_3 substrate (Fig.1 and Fig. 2) using advanced TEM techniques, such as C_S-corrected HRTEM/STEM, EELS/EDXS, quantitative atomic measurement and electron diffraction analysis as well as theoretical calculations. Interfacial detailed atomic and electronic structures are revealed and compared. Interface induced phenomena between nitride films and substrates are unveiled [2,3].

Particular study on the effect of N defects in the metal nitride (CrN) film has led to some interesting conclusions. Ordered nitrogen (N) vacancies were often found to well distribute at the {111} planes. Combining independent image analysis, such as atomic displacement/strain measurement using geometrical phase analysis, and spectrum analysis by examining the low loss and core loss, fine structure analysis, some generalized conclusions are drawn, which are: (i) a relationship between the lattice constant and N vacancy concentration in CrN is established [5], (ii) the change of ionicity in CrN crystal with the N vacancy concentration is shown; (iii) Particularly, a direct relationship between electronic structure change (L_3/L_2 ratio) and elastic deformation (lattice constants) in CrN films has been experimentally derived, revealing that the elastic deformation may lead to a noticeable change in the fine structure of Cr-$L_{2,3}$ edge, i.e. L_3/L_2 ratio [1]. Such experiments point out an indirect approach to acquire electronic structure changes during the elastic deformation.

The effect of randomly distributed defects in the films has been explored in a quantitative way using quantitative electron diffraction, combined with HRTEM and EELS analysis. Some quantitative relations are established.

References

[1]. R. Daniel *et al*, Acta Materialia **58** (2010), p. 2621.
[2]. Z. L. Zhang, *et al* Physical. Review B **82(**R) (2010) p060103-4
[3]. Z. L. Zhang, *et al* Journal of Applied Physics, 110 (2011) p043524-4
[4]. Z.L. Zhang *et al* Physical Review B **87** (2013) p014104.

[5]. T.P. Harzer, *et al* Thin Solid Films 545 (2013) p154–160
[6]. A.S. Botana *et al* Physical Review B **85** (2012), p. 235118
[7]. Acknowledgement: Gabriele Moser and Herwig Felber are gratefully acknowledged for their help with sample preparation, thanks are given to Dr.Hong Li for *ab-initio* calculations. Thank Dr. Rostislav Daniel and Christian Mitterer in Montanuniversität Leoben, Leoben, Austria for delivering the materials.

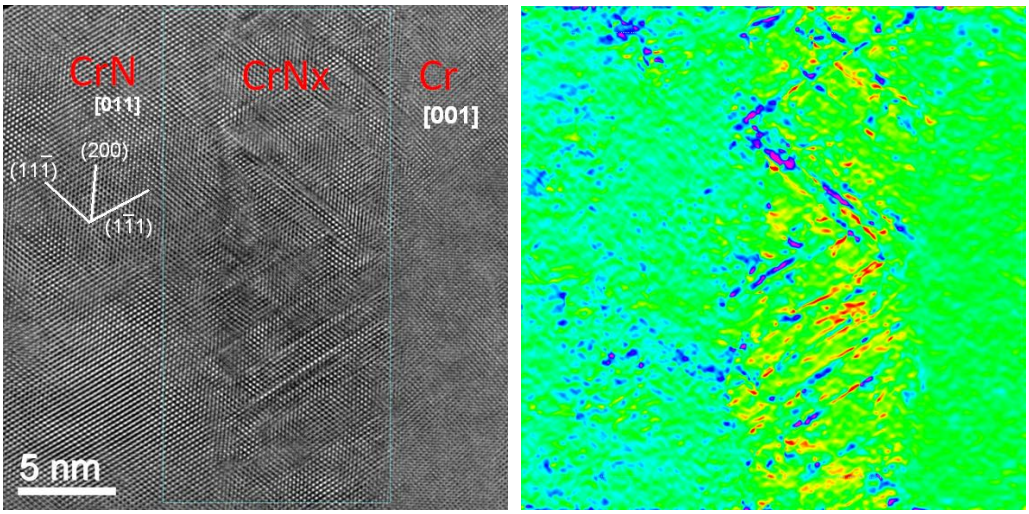

Figure 1. Left: HRTEM image of the CrN/Cr interface, a defective layer between Cr and CrN originated from the ordered N vacancy. Right: the anisotropic distribution of strain in the defective layer (e_{xx}).

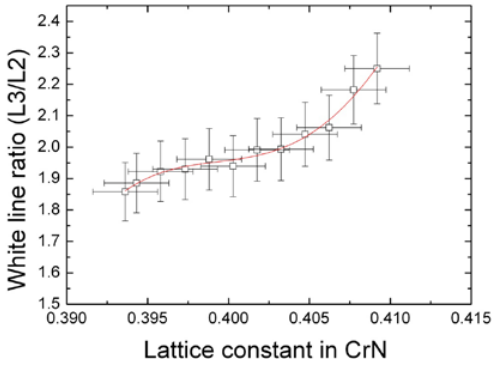

Figure 2. The change of white – line ratio with the lattice constant variations.