Thin films of TiN have been applied widely for its good electrical property and chemical stability. High-quality TiN can make further understanding of its properties, particularly its relationship with oxides. Here we characterize the TiN/MgO interface using STEM annual dark field (ADF) and annual bright field (ABF) images and make a comparison of both imaging contrast for the different elements. Though ADF images can easily provide direct visualization of atomic column positions of heavy atoms, for light elements it is usually invisible even at high resolution. Recently, ABF imaging technique has been proved to be useful for observations of atomic positions of light elements in single crystals.

ADF/ABF imaging was performed in a Cs-corrected JEOL ARM200F with a Schottky gun at 200kV with 0.08nm probe. TiN thin films were grown on MgO substrate by pulsed laser deposition method. The full-width at half-maximum of X-ray rocking curve (002) is about 60 arcsec, implying that TiN films deposited on MgO are of good quality. Cross-sectional STEM specimens were prepared by tripod polishing method, followed by Ar-ion milling at 4⁰ and 3-4 kV.

In our observations, all ADF images show that atomic positions of Ti and Mg exhibit strong bright contrast, O in weak bright contrast, whereas the contrast of N atoms is hardly observed, as shown in Fig. 1. The contrast can be further improved as shown in the filtered images (the insets in Fig. 1) in which O positions are clearly visible while N ones are still barely seen. Also, it is difficult to see the contrast difference of O from N at the interfacial region. The ABF image in Fig. 2 clearly reveals that atomic columns of Ti, N, Mg, and O as dark spots where the darkness depends on their atomic number. Also the visibility of all atomic positions can be significantly increased in the filtered ABF images, but it remains difficult to identify exact atomic species at the interface because the difference in the intensity of light element atoms is too low. Interestingly, the ABF contrast shows additional dark spots in MgO where exist no atomic columns between Mg along <112>, and similar contrast is also seen in some TiN regions. The causes for such contrast may need further investigations. Both ADF and ABF images show that the TiN/MgO interface is almost fully coherent with epitaxial relationships of \((001)_{\text{TiN}}//(001)_{\text{MgO}}\) and \([1-10]_{\text{TiN}}/[1-10]_{\text{MgO}}\) because of a small lattice mismatch (δ=0.466%) between MgO and TiN. The arrangements of Mg, O, Ti and N atomic columns can be seen in order. Moreover, both images indicate that the ionic bonding sequences of cations and anions along [001] direction through the TiN/MgO interface is maintained without any interruption from MgO to TiN, i.e., Mg-O-Ti-N and O-Mg-N-Ti atomistic bonding.

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Fig. 1: ADF image of the TiN/MgO interface along [1-10] zone axis. Ti, Mg and O atomic positions as marked in TiN and MgO filtered images in the insets. (angle > 90 mrad)

Fig. 2: ABF image of the TiN/MgO interface along [1-10] zone axis. Ti, N, Mg and O atomic positions as marked in TiN and MgO filtered images in the insets. (angle ~ 11-22 mrad)