Atomic and electronic structural studies of VN/MgO (001) interface by an image-side C_S-corrected electron microscope

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Transition metal nitrides are extremely hard materials, which are often used in multilayered coatings, where the coating hardness even exceeds the hardness of the constituent monophase nitrides [1-2]. Such coatings are promising for applications in which high hardness and wear resistances are needed. A model system of epitaxially grown VN film on MgO is particularly interesting to obtain a basic understanding of the interfacial atomic and electronic structure at the atomic scale, which is very crucial for reliable applications.

With the modern C_S-correction technique a tremendous progress in HRTEM made it possible to achieve ultra-high resolution in a 'mid-voltage' microscope through both hardware and software corrections [3-4], providing new opportunities for direct interpretation of image contrast, particularly, the contrast from light elements, and microanalysis with improved spatial resolution in materials science applications [4].

In this work, cross-sectional TEM specimens were prepared using Tripod polishing, and a short Ar^+ milling at 4.0 KV and 2 mA was followed. Using an image-side C_S–corrected microscope (JEOL 2100F, Gatan Tridiem), the atomic and electronic structures of the VN/MgO(100) interface are investigated. O and N atom columns at the interface can be clearly imaged and quantitative comparison with simulated images based on an atomic model obtained by *ab-initio* calculations are performed. By phase analysis, the atom displacements across the interface are revealed. Electronic structure at the VN/MgO interface is characterized by ELNES and DFT calculations.
Experimental HRTEM images were acquired under a small negative C_S and under-focus. Figure 1a shows the interface image recorded along [110] zone axis, which clearly displays O and N atoms in individual layers and at the interface. The intensity of O atom in MgO is slightly stronger than the intensity of N atom in the VN. The interface can be well located by combining the intensity profile of the image with a phase analysis. The atomic displacement analysis shows an increase in (002) lattice spacing across the interface from MgO to VN (Figure 1b, upper), and the unit cell dilation across the interface gives a gradient change across the interface (Figure 1b, lower). HRTEM image acquired along [100] zone axis (Figure 2a) provides a clear indication of the interface position due to a contrast difference across the interface when imaged under a certain thickness and defocus value. The image contrast is in agreement with the simulated image (Figure 2b) based on a calculated atomic model (Figure 2c).
High spatial EELS spectrum from the specific interface was acquired (Figure 2d, red curve), showing the fine structures of V-$L_{2,3}$ and O- K edges from VN/MgO interface. Comparison with the O-K edge in MgO reveals slight changes, which may originate from the differences

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in local coordination of the O atoms at the interface. This will be further studied by comparing with the results from DFT calculations.

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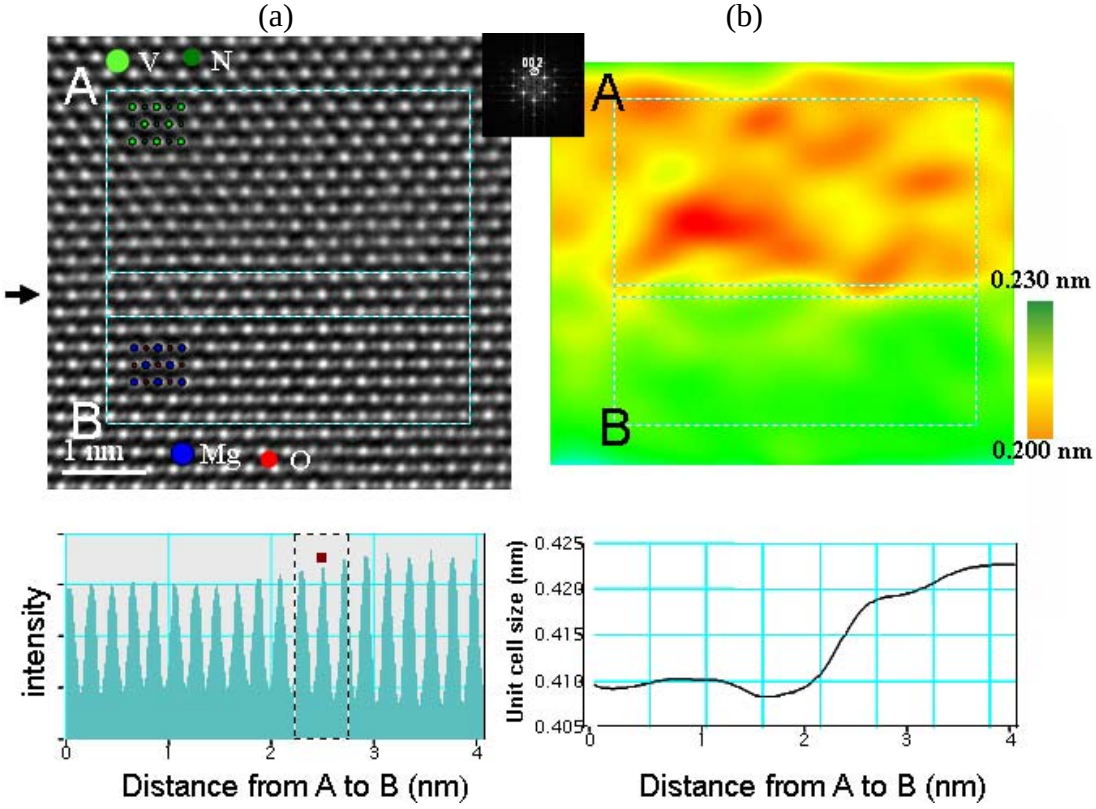

Figure 1. (a) HRTEM image of VN/MgO along [110] direction recorded with C_S (~ –3 µm). O and N atom columns are clearly visible (The interface is indicated by an arrow), intensity profile (below) over a rectangular area reveals the intensity difference across the interface. (b) Color map of modulation of the 002 spatial frequency, the twice of 1/|002| gives the dilation of the unit cell across the interface.

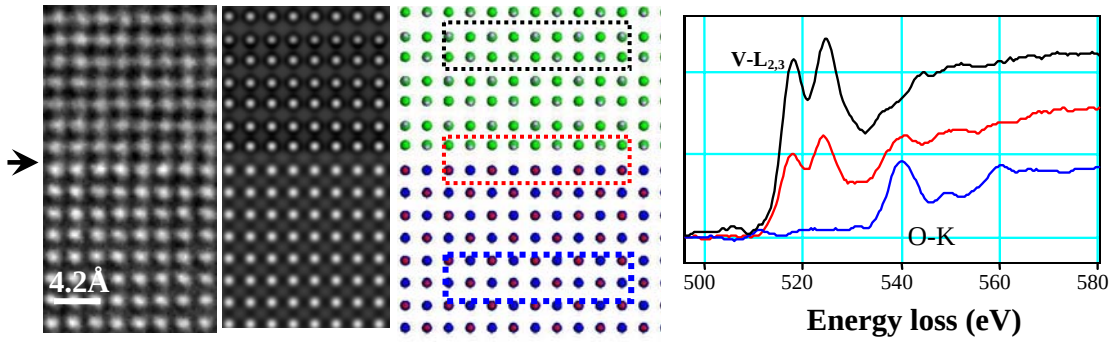

Figure 2. (a) HRTEM image along [100] direction, a simulated image (b) based on an atomic model (c) obtained from *ab-initio* calculation. (d) ELNES spectra from a region (indicated in the model) in VN, MgO and the interface, demonstrating small differences in the O-K and V-$L_{2,3}$ edge at the interface and in bulk.

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