A structural characterization of a Cu/MgO (001) interface using C_s corrected HRTEM

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Materials containing ceramic and metal phases play a significant role in modern materials technology with applications ranging from catalysts, gas sensors, superconductors, hard coatings, to cell capacitors in memory devices. Their macroscopic mechanical, physical, and chemical properties are often controlled by the metal/ceramic interface. Thus, a fundamental understanding of the atomic scale structure and chemistry of those interfaces is necessary for the improvement of their macroscopic properties.

Due to their technological importance, metal/ceramic interfaces have been widely studied during the last two decades. Most of the structural studies present a combination of high resolution transmission electron microscopy and image simulation [1]. Information on the type of bonding and chemical chemistry were obtained by electron energy loss spectroscopy [2-4], Auger electron spectroscopy, or atom probe analysis [3, 4]. With the recent development of microscopy techniques, especially the improvement of the resolution by implementing a C_s corrector, HRTEM now provides the required resolution to study interfaces at the atomic scale and allows for ordered structures to discriminate between different elements, like Mg and O in MgO.

This paper presents a study of a model metal/ceramic interface by C_s corrected HRTEM: copper film on magnesium oxide substrate. 1µm thick Cu layers were grown on MgO (001) substrates by magnetron sputtering [5]. Cu exhibits a cube-on-cube epitaxial relationship with the MgO substrate, i.e. $(001)_{Cu}//(001)_{MgO}$ and $[001]_{Cu}//[001]_{MgO}$. The lattice misfit, δ, between the two lattices is $\delta = (a_{MgO}-a_{Cu})/a_{MgO} = 0.14$, where $a_{MgO}=0.4212$ nm and $a_{Cu}=0.3620$ nm are the lattice parameters of MgO and Cu. The aim of the present study is to characterize the atomic structure of this interface.

The samples were prepared using the conventional cross-sectional preparation technique [6]. Discs of 3mm in diameter were cut out of the cross-section, mechanically polished down to 100µm, and then thinned using a Gatan Dimpler down to a minimal thickness of 10µm, and finally Ar^+ ion milled using a Gatan Duo-mill operated at 6 kV. HRTEM was performed with an image-side C_s corrected Jeol 2100F operated at 200kV.

Figure 1 presents a bright field image of the Cu film on MgO (001) and the corresponding selected diffraction area pattern recorded along <110> zone axes. Images recorded under two beam conditions reveal the presence of dislocations in the Cu film compensating the mismatch of ~14%. The C_s corrected HRTEM image allows to discriminate between Mg and O columns as indicated by the simulated image in Figure 2. At the interface the intensity of the atomic columns indicated differences in the coordination and stoichiometry. This will be further analyzed by quantitative image simulation and comparison with EELS data based on the atomic structure model derived by density functional theory.

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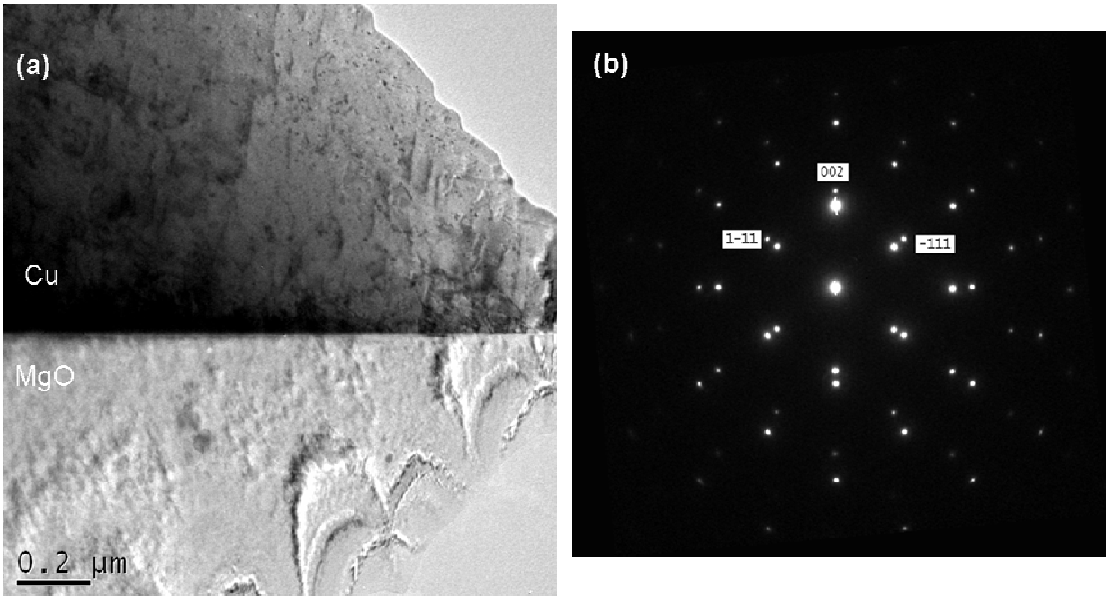

Figure 1. (a) Conventional TEM micrograph of edge-on Cu/MgO (001) interface viewed along <110> and (b) corresponding selected area diffraction pattern.

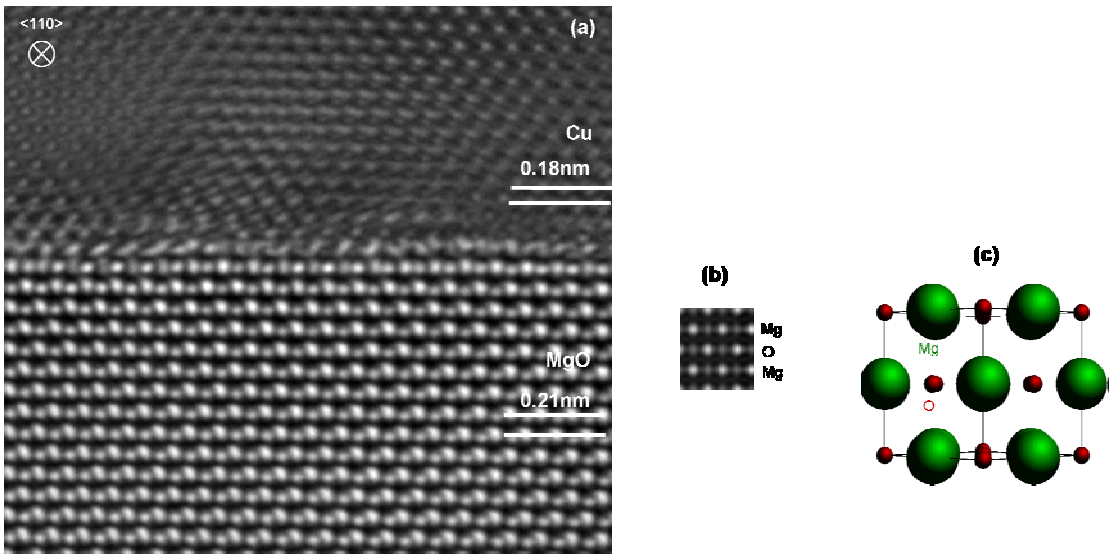

Figure 2. (a) HREM micrograph of the interface viewed along <110>, (b) simulation of a bulk MgO crystal and (c) corresponding schematic atomic model.

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