# An Interface Study using ElectronEnergy-Loss Near-Edge Structure

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The importance of interface studies cannot be over-emphasized in materials analysis as the interfacial structure and chemistry can often determine the overall properties on the macroscopic scale. EELS (electron energy-loss spectroscopy) and, in particular, ELNES (energy-loss near-edge structure) are commonly used to elucidate the bonding and localized electronic structure at interfaces. However, when an ELNES spectrum is taken on the interface, it actually consists of independent localized signals from both interfacial atoms as well as those in the bulk matrix due to the finite analysis volume caused by beam spreading. A spatial difference method has been developed to isolate the contribution from the interface with spectra recorded both on the nearby matrix and on the interface [1, 2]. The spatial difference determined by subtracting the scaled matrix spectrum from the interface spectrum is assumed to reflect the structural and chemical information at the interface. However, both thickness variation and phase difference across the interface make the scaling in a pre-edge region difficult. An alternative approach is to take an EELS linescan using a fine focused probe, that is, a set of spectra obtained by progressively moving the probe across the interface. The dataset is then analyzed by investigating the ELNES variation of the atomic species of interest across the interface. In this paper, a Cu-TiN interface was studied using this technique.

Fig. 1 shows a high resolution TEM (HRTEM) image of a Cu-TiN interface. The absence of any interfacial layer in the projected atomic structure indicates that Cu-N bonds and/or Cu-Ti bonds have been established at this atomically abrupt interface. Discrimination between the two bonding mechanisms is difficult based on either HRTEM imaging or Z-contrast STEM (scanning transmission electron microscopy) imaging. The EELS experiments were performed by taking a linescan across the interface in STEM mode using probe size of 2Å and spectrum energy resolution of 0.8eV. The spectra obtained were then analyzed using an EELS model which incorporates both the ELNES and the specimen thickness effect [3]. Using the maximum likelihood method, the model provides the best fit to an experimental spectrum by estimating the required physical parameters which include those describing the ELNES. Fig.2 shows the experimental excitation edges (black curves) of $Cu-L_{23}$, $Ti-L_{23}$ and N-K taken from the matrix and at the interface. The simulated edges (red curves) were also shown for comparison, which were obtained using the model with the ELNES determined from the bulk matrix. While all matrix spectra were fitted well, the difference is clearly seen for the $Cu-L_{2,3}$ and N-K edges in the few spectra near the interface (denoted by arrows). This difference is not visible for the $Ti-L_{2,3}$ edge across the interface. The ELNES fingerprints the chemical bonding, changes of the valence states of the atomic species and changes in the structural arrangements of neighboring atoms in a solid. This result implies that there exists Cu-N bonding at the interface and the local coordination of Ti near the interface remains same as in bulk TiN. Clearly, the linescan method combined with the EELS model provides a powerful tool for interface studies.

References
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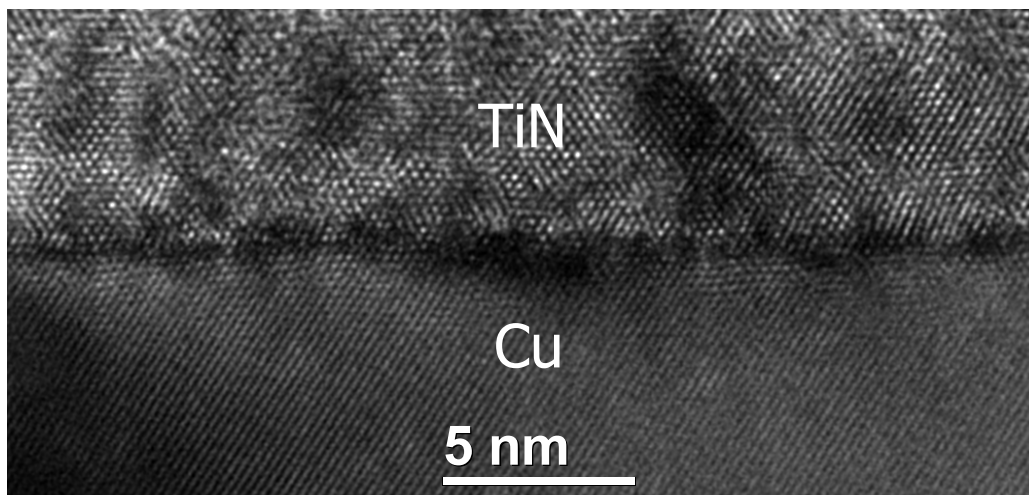[3] J. Verbeeck, S. Van Avert, G. Bertoni, Ultramicroscopy 106 (2006) 976.

Fig.1 HRTEM image of an atomically abrupt Cu/TiN interface, showing the absence of any interfacial layer.
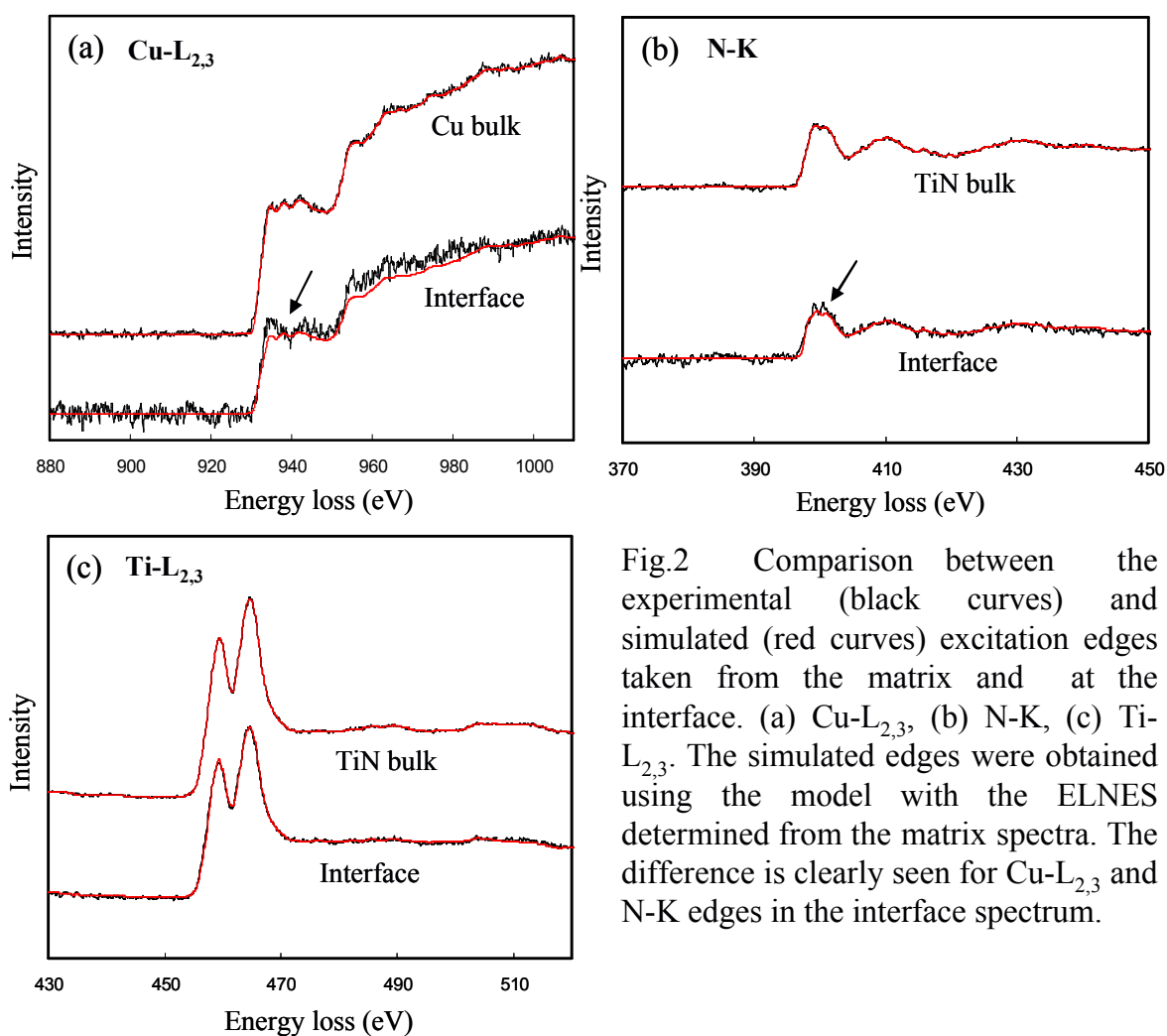


Fig.2 Comparison between the experimental (black curves) and simulated (red curves) excitation edges taken from the matrix and at the interface. (a) Cu-$L_{2,3}$, (b) N-K, (c) Ti-$L_{2,3}$. The simulated edges were obtained using the model with the ELNES determined from the matrix spectra. The difference is clearly seen for Cu-$L_{2,3}$ and N-K edges in the interface spectrum.