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Application Note

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Interface Chemistry and Thermal Boundary Resistance in Ru/TaN/SiO_2 Interconnects Revealed Using Ga-Kα Laboratory HAXPES

Objective & Motivation

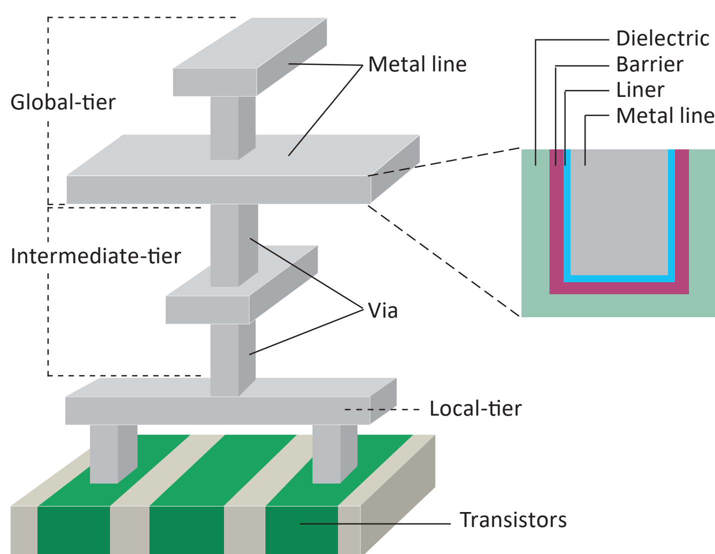

Figure 1: Multilevel interconnect structure and metal/adhesion/dielectric film stack schematics. As dimensions shrink, Cu requires thick diffusion barriers that increase resistivity and thermal resistance, motivating the transition to Ru/TaN stacks.

As semiconductor devices continue to scale next-generation very-large-scale integration (VLSI) circuits, copper interconnects face fundamental barriers to further miniaturisation. Copper requires a diffusion barrier to prevent contamination of surrounding dielectrics, but this barrier thickness cannot scale proportionally with line width. As a result, at advanced nodes the barrier occupies a significant fraction of the conductor volume, reducing conductivity and increasing resistivity. Additionally, as Cu linewidths shrink, resistivity increases sharply due to enhanced surface and grain-boundary scattering. Electromigration reliability also deteriorates because current densities rise dramatically in narrow lines, creating voids and failures.

These limitations have motivated the search for advanced VLSI interconnect architectures, and ruthenium has emerged as a leading candidate. Ru can be deposited with minimal barrier thickness, exhibits more stable resistivity at small dimensions, and offers improved interfacial adhesion to nitride layers such as TaN. However, Ru-based performance still depends critically on the buried interfaces beneath the metal. The composition and bonding of the TaN barrier – particularly nitrogen content and the presence of ultrathin oxides – have a direct impact on the thermal boundary resistance (TBR), which governs heat transfer and local device temperature.

The objective of this study is therefore to determine how TaN stoichiometry and interfacial chemistry influence TBR in Ru/TaN/SiO_2 interconnect structures relevant to next-generation VLSI circuits, and to identify the key chemical features that enable low-resistance, thermally stable interfaces. Because these interfaces lie tens of nanometers below the surface, conventional XPS cannot access them without sputtering, which would alter the chemical state. Ga-Kα HAXPES is used here as a nondestructive depth-sensitive tool to probe the true chemical environment of these buried layers and directly correlate chemical changes with thermal performance.

Technical Background

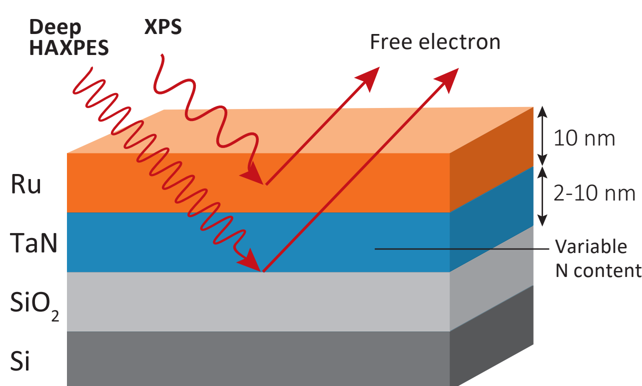

Figure 2: Ru/TaN/SiO_2 interconnect stack studied in this work. Ga-Kα HAXPES provides sufficient probing depth and intensity to analyze buried TaN and Ru interfaces nondestructively.

At nanoscale thicknesses, interconnect performance is governed less by the bulk conductivity of the conductor and more by the behavior of the interfaces between metal, barrier, and dielectric. The thermal boundary resistance at these interfaces determines how effectively heat can be extracted from the interconnect line. Even small deviations in TaN stoichiometry or thin interfacial oxide layers can substantially increase TBR, contributing to local heating and reducing device lifetime.

However, probing these buried interfaces is challenging. The Ru/TaN layer stack is typically 10–50 nm thick, which is beyond the practical probing depth of conventional XPS. Depth profiling by sputtering is unsuitable because it damages the interfacial bonding that controls heat transport.

Ga-Kα HAXPES overcomes these challenges by using 9.25 keV photons to generate high-kinetic-energy photoelectrons with long inelastic mean-free-paths. This allows direct measurement of Ta 3d, Ta 4f and Ru 3d core levels beneath intact overlayers, without sputtering or disturbing the interface. The technique is sensitive enough to distinguish between Ta_2N-rich phases, stoichiometric TaN, and ultrathin oxides such as Ta_2O_5 or RuO_2.

By combining these nondestructive chemical-state measurements with time-domain thermoreflectance (TDTR) and thermal modeling, the study reveals how nitrogen incorporation, bonding strength, and interfacial oxidation influence TBR and identifies clear trends that can be used to optimize Ru-based interconnect integration.

Methods

To study the influence of nitrogen incorporation, $Ru/TaN/SiO_2/Si$ stacks were fabricated with TaN deposited at four different Ar/N_2 sputter ratios (19:1, 17:3, 16:4, and 15:5). Additional samples with reduced TaN thickness (2, 5, and 10 nm) were prepared to evaluate the effect of barrier thickness independently of stoichiometry. Reference structures, including Ru/SiO_2 and $Cu/Ta/TaN/SiO_2$ stacks, were also examined for comparison.

HAXPES measurements were carried out with a Scienta Omicron HAXPES Lab using a monochromated Ga-Kα source (9.25 keV), which enables probing of deep core levels and information depths up to 50 nm, making it suitable for analysing buried layers. Ta 3d, Ta 4f, and Ru 3d core levels were measured without any sputter cleaning or depth profiling. Peak fitting was used to distinguish metallic Ta, Ta-nitride, and Ta-oxide components, as well as metallic Ru and RuO_2 contributions.

Thermal boundary resistance was determined using time-domain thermoreflectance (TDTR), with finite-element modeling used to validate the observed trends and separate the influence of material properties from measurement artifacts.

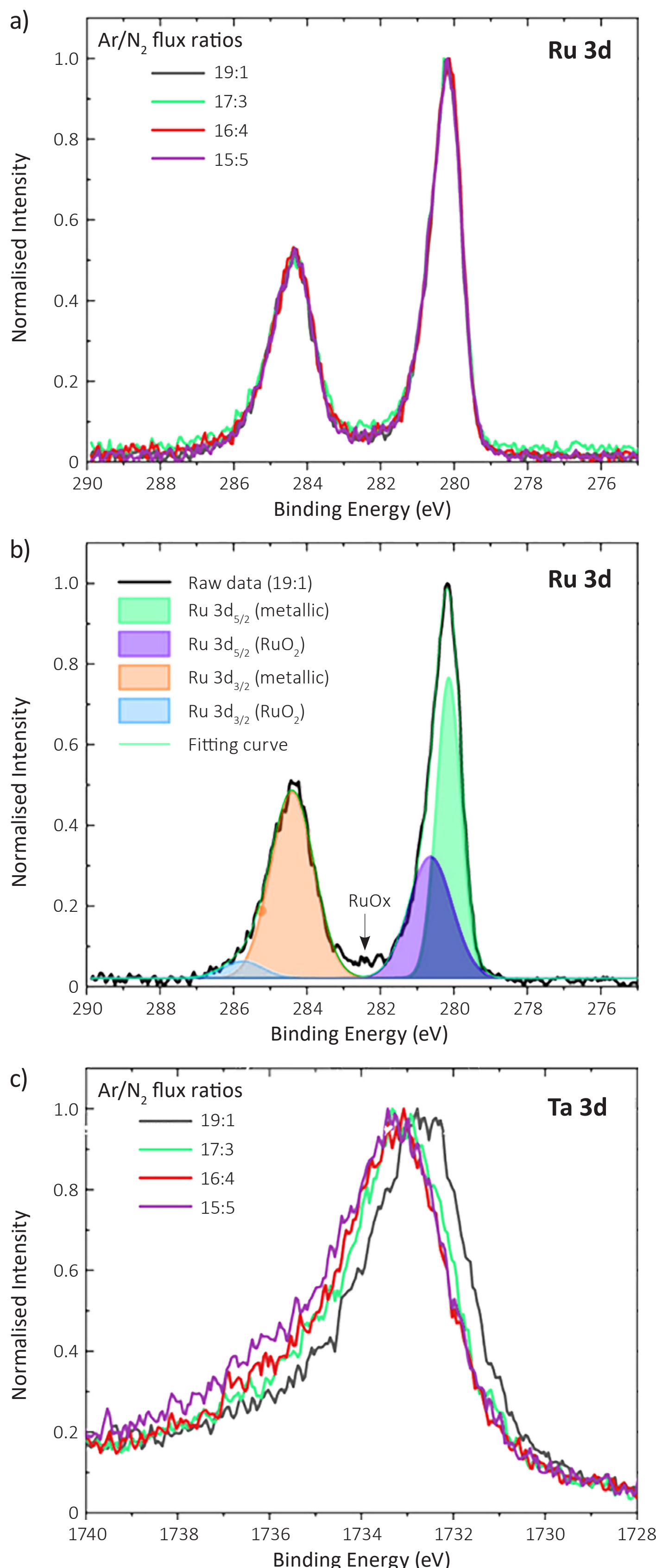

Figure 3. HAXPES core-level spectra from buried layers. Increasing nitrogen incorporation shifts Ta core levels to higher binding energy (c), indicating stronger Ta–N bonding, while Ru remains chemically stable across all TaN compositions (a).

Results

TaN stoichiometry and bonding evolution

The HAXPES results show a clear shift in Ta 3d and Ta 4f binding energies as nitrogen content increases. Low-nitrogen films display a larger metallic Ta contribution and lower binding-energy position, consistent with Ta_2N-rich compositions. As the N_2 flow increases during sputtering, the Ta core levels move to higher binding energy, indicating stronger Ta–N bonding and a corresponding increase in stoichiometric TaN.

This transition is not easily observed with conventional XPS, as the TaN layer lies beneath a continuous Ru film. HAXPES enables direct observation of the chemical state of TaN without altering the stack.

Stability of Ru and limited oxidation

The Ru 3d spectra exhibit a dominant metallic peak with a small and stable RuO_2 shoulder. Importantly, the Ru chemical state does not change significantly across the range of TaN stoichiometries. This indicates that the differences observed in TBR originate from changes within the TaN layer and its interface with the underlying SiO_2, rather than from variations in the Ru itself.

Detection of thin oxides

Even ultrathin oxide layers are clearly identified. Ta_2O_5 components appear at the TaN/SiO_2 interface, while RuO_2 forms only weakly at the Ru/TaN interface. Although these oxides are thin, their presence correlates with increased thermal resistance. The ability of HAXPES to detect these subtle features nondestructively is critical, as oxidation behavior often cannot be inferred from process conditions alone.

Correlation with thermal boundary resistance

The measured thermal boundary resistance shows a clear monotonic dependence on nitrogen incorporation in the TaN layer. As TaN becomes more nitrogen-rich and approaches stoichiometric composition, the TBR consistently decreases. This trend indicates that the evolution of TaN chemical bonding and lattice properties plays a key role in governing heat transport across the Ru/TaN/SiO_2 stack.

In contrast, Ta_2N-rich films deposited at lower nitrogen flow exhibit higher TBR. These results demonstrate that TaN stoichiometry, rather than layer thickness or changes in the Ru layer, dominates the observed thermal behavior.
The robustness of this trend across multiple samples and thicknesses highlights the critical influence of TaN composition on interfacial thermal transport.

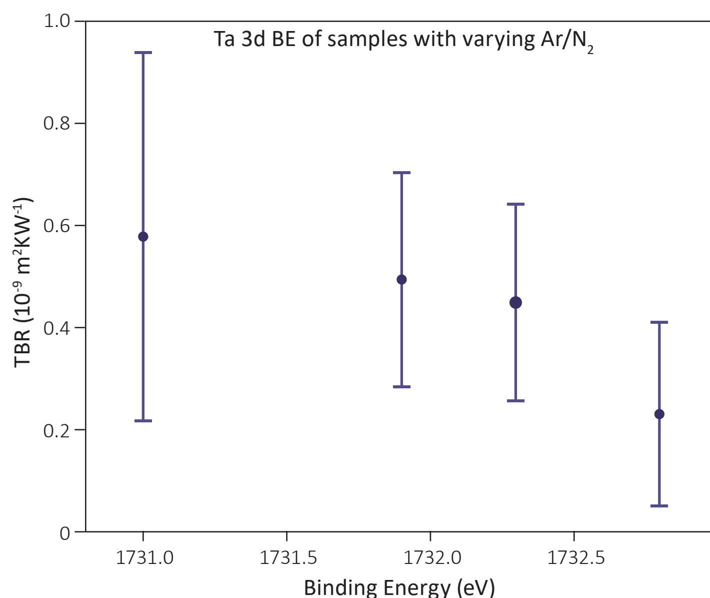

Figure 4. Measured Thermal boundary resistance of samples made with varying Ar/N2 flux ratios as a function of the Ta 3d metallic peak binding energy. TBR decreases systematically with increasing nitrogen content in TaN. The evolution of TaN chemical bonding correlates directly with improved heat transport across the Ru/TaN/SiO_2 stack.

Conclusions

This study demonstrates that the thermal performance of Ru/TaN/SiO_2 interconnect structures is strongly influenced by the chemical state of the buried TaN layer. Increasing nitrogen incorporation during deposition drives TaN toward a more stoichiometric composition, which correlates with a systematic reduction in thermal boundary resistance.
These results indicate that changes in TaN chemical bonding and associated lattice properties play a central role in determining thermal coupling across the Ru/TaN/SiO_2 interfaces.

Throughout the investigated parameter range, the Ru layer remains chemically stable, confirming that optimisation efforts should focus on controlling TaN stoichiometry and minimising interfacial oxidation. Ga-Kα HAXPES uniquely enables nondestructive access to these buried chemical states with sufficient depth sensitivity and chemical specificity.
For process engineers and materials developers, this provides a practical and reliable approach for evaluating interfacial chemistry in device-like stacks and for guiding the optimisation of barrier layers in next-generation interconnect technologies.

Further details and results are found in:
Zhan, T., Watanabe, T. et. al, 2022. ACS Appl. Mater. Interfaces 14, 7392–7404.
https://pubs.acs.org/doi/10.1021/acsami.1c20366

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