

Nanoscale Thermal Resistance Mapping of Nanocrystalline Cu Thin Films Using Scanning Thermal Microscopy with Hertzian Contact Geometric Correction

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Introduction

As semiconductor interconnect dimensions scale below 100 nm, thermal management at grain boundaries becomes a critical bottleneck for device reliability [1]. Nanocrystalline Cu thin films, widely used in back-end-of-line (BEOL) metallization, exhibit grain-boundary thermal resistance that is inaccessible to conventional bulk measurement techniques. Scanning thermal microscopy (SThM) offers the spatial resolution needed to probe nanoscale thermal transport [2], but the measured thermal signal is inherently convolved with tip-sample contact geometry effects—particularly on rough, polycrystalline surfaces where local curvature varies at the scale of individual grains. In this work, we present a SThM-based method for quantitative thermal resistance (R_{th}) mapping of nanocrystalline Cu thin films, incorporating a newly developed Hertzian contact geometric correction algorithm.

Experimental Details

Cu thin films (50 nm, as measured by ellipsometry) were sputter-deposited on Ti(20 nm)/SiO₂/Si substrates and studied in two conditions: as-deposited and annealed at 250 °C for 3 min in Ar ambient. Field-emission SEM imaging (Fig. 2 a,b) confirmed nanocrystalline microstructure. XPS depth profiling (Fig. 5) confirmed that the as-deposited film maintained a predominantly metallic composition (~98 at.% Cu within the bulk), whereas the annealed film exhibited complete through-thickness oxidation, attributed to oxygen gettering effect of Ti [4] in the presence of residual oxygen in the annealing chamber. Four-point probe measurements yielded electrical resistivities of $7.6 \times 10^{-8} \Omega \cdot m$ for the as-deposited film and $3.45 \Omega \cdot m$ for the annealed sample (Fig. 6 b), consistent with the oxidation of copper. SThM measurements were performed using a Wheatstone bridge configuration ($V_{in} = 0.7$ V, $R_{var} = 347 \Omega$, amplifier gain $G = 1000$) with a 50 nm radius thermo-resistive probe. Approach-retract curves (Fig. 6(a)) were acquired to extract the non-contact voltage (V_{nc}) and contact voltage (V_c) for each sample.

Geometric Correction Algorithm

A key contribution of this work is the Hertzian contact geometric correction [3]. On a polycrystalline surface with higher surface roughness (RMS > 1 nm), convex grain peaks produce a smaller tip-sample contact area, artificially enhancing the thermal signal, while concave grain boundaries produce a larger contact area, suppressing it (Fig. 3). We compute the mean curvature H of the topography from the full differential-geometry expression for $z = f(x, y)$ [5] after Gaussian smoothing ($\sigma = 2$ px), de-

rive the local radius of curvature $R = 1/H$, and apply a correction factor $G = R/(R + r_{tip})$.

Thermal Resistance Mapping

Quantitative R_{th} maps were computed from the corrected thermal signal using the relation

$$R_{th} = R_{nc} \times \frac{(V_{pixel}/G) + K}{(V_{pixel,nc} - V_{pixel})/G},$$

where $K = V_{in}R_{var}/(R_o + R_{var})$ and $R_{nc} = 5.87 \times 10^4$ K/W. A more detailed discussion of this formulation can be found in our previous study [2].

Results and Discussion

The as-deposited metallic Cu film exhibited a mean R_{th} of 5.40×10^6 K/W with a narrow distribution ($\sigma = 0.03 \times 10^6$ K/W), reflecting the dense, fine-grained nanocrystalline structure. After annealing at 250 °C, the mean R_{th} increased to 6.41×10^6 K/W with a significantly broader distribution ($\sigma = 0.17 \times 10^6$ K/W). The 19% increase in mean R_{th} is attributed to the combined effects of grain growth, which concentrates thermal resistance at fewer but more prominent grain boundaries (Fig. 4 a,b), and the complete oxidation of the Cu film to resistive copper oxide, as confirmed by the XPS measurements (Fig. 5). The broadened R_{th} distribution reflects the heterogeneous microstructure of the annealed oxidized Cu film. Although oxidation increases electrical resistivity by ~8 orders of magnitude (Fig. 6 b), the corresponding rise in thermal resistance (19%) is modest, since phonon-mediated heat transport and interfacial resistances of system stack dominate R_{th} over electron conduction. The geometrically corrected R_{th} maps clearly resolve grain-boundary-scale thermal contrast that was previously obscured by topographic cross-talk. This demonstrates that SThM, combined with the proposed correction approach, can differentiate intrinsic thermal resistance variations at sub-100 nm length scales.

Conclusion

We have demonstrated a quantitative SThM methodology for nanoscale thermal resistance mapping of nanocrystalline thin films, enabled by a Hertzian contact geometric correction that reduces topographic coupling by over 85%.

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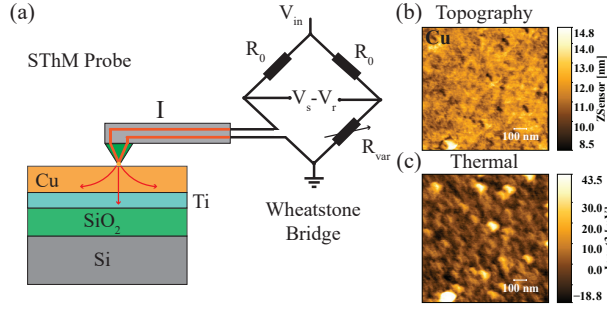


Fig. 1: (a) Schematic of the SThM measurement configuration: a resistive probe contacts the 50 nm Cu thin film deposited on Si/SiO₂ with a 20 nm Ti adhesion layer, with the probe integrated into a Wheatstone bridge circuit. (b) Topography and (c) thermal signal maps simultaneously acquired over a 1 μm × 1 μm scan area at 512 × 512px resolution. A detailed description of the SThM setup and calibration procedure is provided in [2].

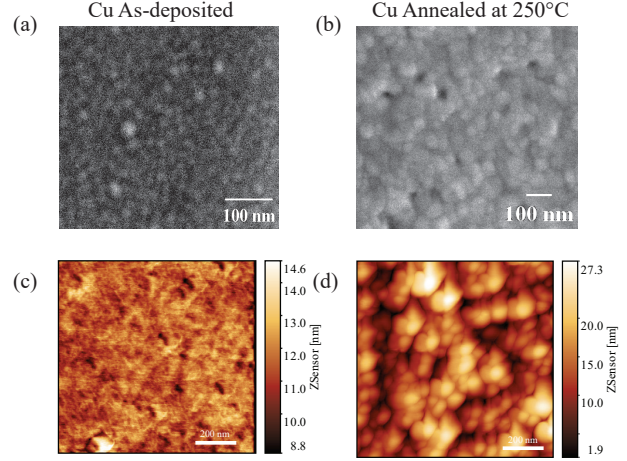


Fig. 2: (a) SEM micrograph of the as-deposited Cu film. (b) SEM micrograph after annealing at 250 °C. SThM topography maps: (c) as-deposited and (d) annealed samples, showing a uniform surface morphology for the as-deposited film (RMS roughness ~ 0.9 nm) and increased surface roughness after annealing (RMS roughness ~ 4.5 nm).

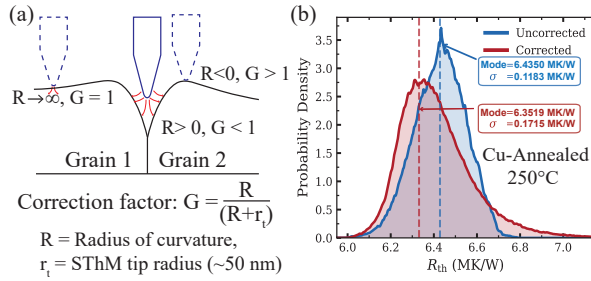


Fig. 3: (a) Schematic of the Hertzian contact geometric correction, where surface curvature modulates the effective tip-sample contact area. (b) R_{th} probability density distributions before and after geometric correction for the 250 °C annealed sample.

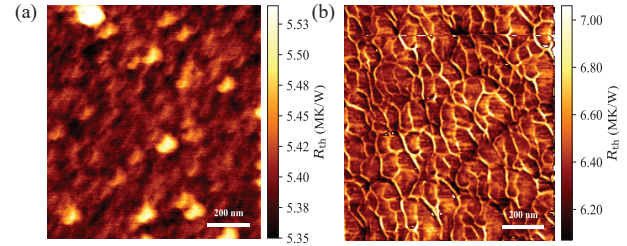


Fig. 4: SThM R_{th} maps after geometric correction: (a) as-deposited and (b) annealed, showing higher thermal resistance due to enhanced phonon scattering at grain boundaries.

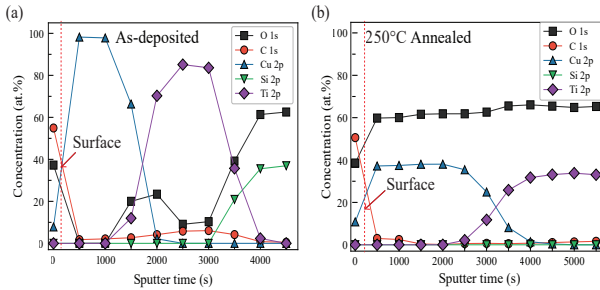


Fig. 5: XPS depth profiles of: (a) as-deposited, showing ~98 at.% metallic Cu in the bulk, and (b) after annealing at 250 °C for 3 min in Ar, revealing oxidation of the Cu and Ti layer (O 1s > 60 at.%, Cu 2p < 40 at.%).

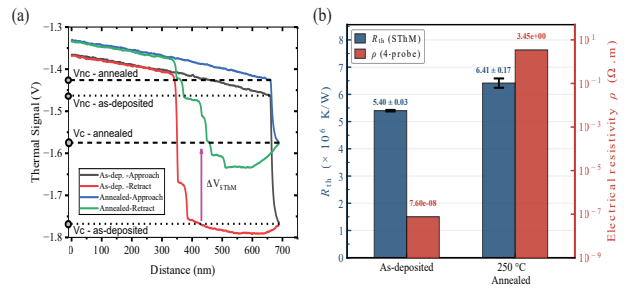


Fig. 6: (a) SThM approach-retract curves showing a larger thermal voltage drop for the as-deposited film, consistent with lower thermal resistance. (b) Mean R_{th} (SThM) and electrical resistivity ρ (4-point probe) for both samples.