Material screening for future diffusion barriers: modelling of binary and ternary metal alloys and detailed experimental analysis of their barrier performance

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The exponential resistance increase in copper (Cu) interconnects due to densification and down scaling is a major challenge for future integrated circuits (ICs) [1]. Hence alternative copper diffusion barrier materials are necessary that replace the current TaN/Ta(Co) system [2,3].
In our work the diffusion behaviour of Cu into 7 binary and 3 ternary metal alloys with various compositions were investigated and compared. In order to achieve good diffusion barrier performance, the barrier material ideally has an amorphous structure, without grain boundaries that act as fast diffusion paths [4]. Therefore, the formation enthalpies of the alloys with various compositions were modelled using the Miedema model. With this semi-empirical model the stable amorphous composition range can be predicted [5,6]. Furthermore selected metal alloys were deposited via physical vapour deposition (PVD) on 300 mm wafers and their crystal structure, which was analysed by X-ray diffraction (XRD) analysis, was compared to the modelled data. Fig. 1 shows the results for one binary metal alloy (a) RuTa) and one ternary alloy (b) CoRuTa). The turquoise areas represent the theoretical amorphous composition range and the black dots and grids show the experimental XRD results. We can see that the black dots, which represent an amorphous structure lie all within those turquoise areas. Hence our model prediction works accurately. In addition to XRD analysis, the resistivity of the deposited alloys was measured via 4-point technique and the results are included in Fig. 1 in blue.

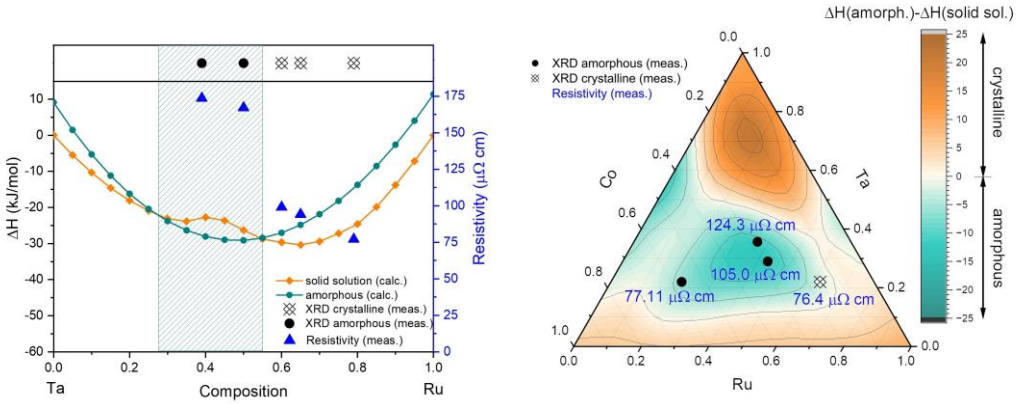

Fig. 1 Formation enthalpy for the solid solution and the amorphous phase calculated with the Miedema model, as well as crystallinity analyzed by XRD and resistivity (blue) for one binary metal alloy a) RuTa and one ternary metal alloy b) CoRuTa

After the theoretical and experimental evaluation, promising metal alloys were selected for the diffusion evaluation, which was performed by X-ray photoelectron spectroscopy (XPS) depth profiling. Therefore specifically designed material stacks were annealed at various temperatures for 10 minutes to induce copper diffusion. The XPS concentration profiles gave then insight into the diffusion mechanisms of Cu into those alloys. With this analysis we were able to categorize the diffusion behaviour and we found metal alloys with excellent barrier performance that could be alternatives to the currently used TaN.

References

1. IEEE, “International roadmap for devices and systems: More moore” Update (2022)
2. R. Clark, K. Tapily, K.-H. Yu, T. Hakamata, S. Consiglio, D. O’Meara, C. Wajda, J. Smith, and G. Leusink, APL Materials 6, 058203 (2018).
3. M. Naik, IEDM, 18-125 (2018).
4. T. Gupta, Copper Interconnect Technology, vol. 1. New York, NY: Springer, (2009), p.126
5. A.R. Miedema and A.K. Niessen, Calphad 7, 27–36 (1983).
6. Hans Bakker, Enthalpies in alloys: Miedemas semi-empirical model (1998).

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