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High Resolution and Thermodynamic Analysis of Interconnect Metals and Diffusion Barriers.

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We have been engaged in a number of studies of the formation and stability of metallization contacts and diffusion barriers associated with integrated circuit manufacturing. Because of the dimensions involved, our primary characterization technique has been high resolution transmission electron microscopy (TEM), generally in the cross-section view. In order to interpret the behavior we rely on thermodynamic analysis by the application of ternary and quaternary phase diagrams.

This approach was first realized in the classical work by R. Beyers et al. [1] during an investigation of the formation of titanium disilicide (C54 versus C49). He showed that silica is the stable oxide in contact with the silicide and silicon, even though the free energy of formation of titania is larger. A. Bhansali et al. [2] extended this work using quaternary phase diagrams to clarify the behavior of more complex systems.

K. Holloway et al. [3] showed using high resolution TEM that many silicides were preceded by an amorphous interface phase comprising a mixture of the metal and silicon, including Ti, Zr, Ni, Co, Pt etc. Ogawa et al. [4] demonstrated that this occurs also during semiconductor manufacturing in titanium disilicde contact metallization, and should be avoided for good contacts. Later, H. J. Lee, K. W. Kwon et al. [5] revealed that an amorphous interface is present at the tantalum-copper interface for copper metallization, which is quite unexpected thermodynamically.

Throughout this period, we have used in parallel in situ high resolution TEM as a means of deducing reaction behavior at the atomic level. Konno et al. [6, 7] studied metallic-silicon systems which do not exhibit silicide formation (e.g. Al-Si, Ag-Si), obtaining real-time movies of metal-induced crystallization processes. More recently we have recorded the formation of NiSi as a possible future gate metal and have examined the transformations of a number of high-k gate oxides by this technique. (e.g. [8])

In summary, high resolution TEM combined with thermodynamic analysis is a powerful method to understand metallization behavior in integrated circuit manufacturing.

References

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