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Effects of Alloying Elements on Cobalt Silicide Formation

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Beamline(s): X20C

Introduction: Alloying elements can substantially affect the formation of cobalt silicide, which is an important alternative to Ti silicide for contacts to Si in CMOS devices. Co silicide is much more sensitive to impurities and to the preparation of the Si surface before deposition and typically leads to rougher interfaces and higher leakage currents. The successful formation of Co silicide now relies on a thin suboxide at the Si/Co interface that affects the diffusion during annealing sufficiently to limit the surface roughness and the epitaxial faceting between the silicon and the disilicide. The goal of the present work is to achieve better control over the formation of the silicide phases and the final roughness of the film.

Methods and Materials: A comprehensive study of phase transformation was performed on 23 Co alloys with a range of alloying element concentrations.¹ Films were deposited in a UHV multisource sputtering system, each film containing the same amount (8nm) of Co and varying amounts of one of 23 alloying elements. Films were capped with 20nm of TiN. In a first study, films were grown at 2 and 5.6 at.% alloying element concentration, and there was an air break before TiN deposition. In the second study, a subset of 10 alloying elements was chosen, and films were grown with alloying element concentrations ranging from 1 up to 20 atomic %, without an air break. Additionally, a set of pure Co samples was grown on Si wafers subjected to varying amounts of oxidation before deposition. Using *in-situ* characterization techniques in which x-ray diffraction and elastic light scattering are monitored simultaneously, we followed the formation of the silicide phases and the associated variation in surface roughness in real time during rapid thermal annealing up to 920 C. The roughness of the interface was also measured using grazing-incidence x-ray reflectivity.

Results: For pure Co silicide, we detected the formation of all stable silicide phases (Co_2Si , CoSi , and CoSi_2) as well as abnormal (001) grain growth in the Co film and thermal degradation of the silicide layer at high temperatures. For Co silicide in samples exposed to increasing amounts of deionized water before deposition, the $\text{Co}(002)$ and Co_2Si peaks both decrease, while the final CoSi_2 peak intensity is the same for all of the samples.

For the transition elements in the first set of Co alloy samples, none of the elements leads to a significant decrease in the formation temperature of CoSi , and variations in formation temperature with concentration do not follow a definite tendency. While most elements lead to an increase in the formation temperature of the disilicide that is more significant with a larger concentration of the additive, Ni, Cu and Pd lead to a decrease. Resistivities of the disilicides varied from about 17 to 46 $\mu\Omega\text{-cm}$, with some samples with 2 at.% alloy additions showing resistivities comparable to that of pure CoSi_2 (15-20 $\mu\Omega\text{-cm}$), and most showing an increase in resistivity with increasing alloy concentration. For the addition of 2 at.% most alloys are within 20% of the resistivity of pure CoSi_2 . (The maximum resistivity for device applications should be $\sim 25 \mu\Omega\text{-cm}$).

Reflectivity scans showed that, relative to pure Co, alloying with Cr improves the monosilicide interface roughness, while alloying with Nb makes it worse. For the disilicides, Ge, V, Ti, Cr, Re, Nb, Ni, Ir, Ta, Rh, Fe alloys resulted in smoother interfaces (on a decreasing scale) than pure Co.

Conclusions: We show that by selecting an alloy with a specific composition, we can change the phase formation temperatures and modify the final CoSi_2 film texture and roughness. Not surprisingly, the effects of alloying can vary drastically. Differences in phase formation temperatures, surface and interface roughness, sensitivity to impurities, and morphological stability of the silicide have been observed. The large variations in formation temperature for the disilicide can be explained from multiple factors depending on the additive element selected. For example, miscibility and entropy of mixing are critical in understanding the nucleation. Surface energy arguments can be dominant in some cases and be influenced by slight amounts of oxygen at the surface or interface. The comparison of roughness, resistivity, and formation temperatures of silicide phases in this extensive study allows us to select candidate alloys for implementation in device development and permits the tailoring of material properties.

References:

1. C. Lavoie, C. Cabral Jr., F.M. d'Heurle, J.L. Jordan-Sweet, and J.M.E. Harper, "Effects of Alloying Elements on Cobalt Silicide Formation," submitted to J. Electronic Mater.