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Phase field modeling of the morphology evolution of metal silicide thin films MATHIEU BOUVILLE, DONGZHI CHI, Institute of Materials Research and Engineering (Singapore), SHENYANG HU, LONG-QING CHEN, Pennsylvania State University (U.S.A.), DAVID J. SROLOVITZ, Princeton University (U.S.A.) — The formation and evolution of thin polycrystalline films formed from the reaction of metals on silicon (metal silicides) or germanium (germanides) is key to the performance in semiconductor devices. NiSi is a candidate for replacing $CoSi_2$ because of its lower resistivity and its lower Si consumption, but is less stable at high T. As the NiSi grains agglomerate into islands *via* grain boundary grooving the film may lose connectivity. At elevated temperature a higher resistivity disilicide phase, $NiSi_2$, will form. We use phase field simulations to predict the evolution of the microstructure and morphology of the silicide film to determine the controlling mechanisms and key physical parameters to aid in metal silicide optimization. Diffusion, phase transformation, elastic energy, and interfacial energy all play important roles in the evolution. Experiments suggest that alloying Ni with Pt or implanting BF_2 delays NiSi agglomeration and the formation of $NiSi_2$. We test two possible mechanisms: additives modify (i) the relative stability of the phases or (ii) the interface energies (which changes the wetting angles and hence the driving force for boundary grooving).

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