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Ultra-thin transition-metal silicide films on Si: trends with chemical composition and substrate orientation HUA WU, M. HORTAMANI, P. KRATZER, M. SCHEFFLER, Fritz-Haber-Institut der MPG — Ferromagnetic films of monosilicides, if grown epitaxially on Si, could be an interesting materials system for spin injection into silicon. While the natural $P2_13$ structure of the compounds MSi (M=Mn,Fe,Co,Ni) is incompatible with Si surfaces, silicides with a CsCl-like crystal structure could be grown epitaxially. We study such films on Si(001) systematically by varying the transition metal species, and find ultrathin (2 or 3 monolayer) MnSi and CoSi films to be ferromagnetic, while FeSi and NiSi films turn out to be non-magnetic. For all films, capping by a Si layer is found to be energetically favorable. While MnSi shows a layered magnetic structure with sizable magnetic moments ($\sim 2\mu_B$) in the surface and interface layers, the CoSi films show homogeneous magnetization with magnetic moments of Co $\sim 0.5\mu_B$. Both findings are interpreted in terms of the electronic structure of the films. Comparing CsCl-like MnSi films on either Si(001) or Si(111), we find both to be thermodynamically stable with respect to bulk Mn, but metastable with respect to bulk $P2_13$-MnSi. The increase in stability with film thickness is monotonic for Si(111), but passes through less stable intermediate structures at < 1 ML Mn for Si(001). Hexagonal phases of Mn-silicides, which could conceivably be grown on Si(111) as well, are found to be energetically less favorable than the CsCl-like MnSi films proposed by us.

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