Complex magnetic behaviour of MnSi thin films on the Si(111) surface

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One of the challenges in the field of spintronics is the injection of a spin-polarized electric current into a semiconductor. This can be achieved by combining the semiconducting material with a ferromagnetic one, e. g., by epitaxially growing thin films of a transition metal silicide like MnSi on top of a Si(111) surface.
We perform density functional theory calculations for thin films of MnSi on Si(111) in their ground state crystal structure, the B20 structure.
The missing inversion symmetry of this material and its complex stacking sequence lead to a wide range of possibilities to grow the thin films on the substrate. We focus on the most probable ones and discuss their thermodynamic and magnetic properties, varying thickness, termination and orientation of the layer stack. Although bulk calculations of MnSi indicate a strengthening of ferromagnetism due to the substrate-induced lattice deformations and the resulting lowering of symmetry, antiferromagnetic tendencies can be observed in some of the thin films, which seem to depend on the chosen stacking sequence. In either case, the largest magnetic moments are found close to the interface and the surface. A dense Si termination leads to significantly reduced magnetic moments in the vicinity of the surface.
Furthermore, STM images are calculated to shed some light on the atomic structure behind recently observed experimental STM images.

9.7 cm

13.4 cm

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