Epitaxial Ferromagnet on Ge(111)

C. Zeng,[1] S.C. Erwin,[2] L.C. Feldman,[3,4] Y.W. Song[3], J.R. Thompson,[1,4] and Hanno H. Weitering[1,4]

[1]*Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37996,USA*
[2] *Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375 USA*
[3]*Department of Physics, Vanderbilt University, Nashville, TN 37235, USA*
[4]*Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

Abstract
High-quality, epitaxial Mn_5Ge_3 alloy films were grown on Ge(111) using molecular beam epitaxy. Low-energy electron diffraction, ion channelling, and X-ray diffraction experiments reveal the Mn_5Ge_3(100)//Ge(111) epitaxial relationship with $[100]_{Mn5Ge3}$ // $[1\bar{1}0]_{Ge}$. The alloy films are ferromagnetic below 295 K. The saturation magnetic moment per Mn atom at T = 5 K is 2.7μ_B, which is in good agreement with first-principles density functional theory calculations. These new alloy films are promising candidates for spin-injection into silicon-compatible materials and devices.

Keywords
Metal-semiconductor magnetic thin film structure, molecular beam epitaxy, magnetic measurements, scanning tunneling microscopy, x-ray photoelectron spectroscopy, Mn_5Ge_3.

Introduction
The difficulty of injecting spin-polarized electrons into a semiconductor is a major bottleneck in spintronics research. There are two ways to realize spin injection. One of these is to fabricate a ferromagnetic-metal/semiconductor heterostructure; the other is to use a dilute magnetic semiconductor as the spin aligner. The former method does not work well because chemical intermixing and/or lattice mismatch at the interface usually results in a significant loss of spin polarization. The large "conductivity mismatch" [1] between the ferromagnetic metal and semiconductor furthermore limits the spin injection efficiency. The latter method of using a dilute magnetic semiconductor is limited by the low Curie temperature, T_c. In this paper, we report on a novel, high-quality epitaxial interface with good potential for spin injection, namely a ferromagnetic Mn_5Ge_3 alloy on Ge(111). The films were characterized using a variety of surface- and thin film analysis techniques as well as first-principles density functional theory calculations.

Experimental and Computational details
The deposition experiments were carried out in a molecular beam epitaxy system. Mn_5Ge_3 films are fabricated by depositing 40 nm Mn onto Ge(111) and subsequent annealing at 150°C for several minutes. The films were characterized *in-situ* by x-ray photoelectron spectroscopy, low-energy electron diffraction, and scanning tunneling microscopy (STM). Magnetic properties were measured *ex-situ* using a superconducting quantum interference device or "SQUID" magnetometer. Structural information was obtained from x-ray diffraction θ-2θ scans, Rutherford Backscattering Spectrometry, and ion channelling experiments. The spin-resolved band structure and STM images were computed using the local-spin-density approximation (LSDA) to density-functional theory with projector-augmented-wave potentials and a plane-wave basis set.

Results and Discussion
The lattice mismatch between the (100) hexagonal basal plane of Mn_5Ge_3 and Ge(111) is 3.7%, so we expect Mn_5Ge_3(100)//Ge(111). X-ray diffraction θ-2θ scans show Mn_5Ge_3 (200) and (400) reflections besides the Ge (111) and (333) reflections, which confirms the Mn_5Ge_3(100)//Ge(111) epitaxial relationship. The (111) and (333) reflections of bulk Ge have a pronounced shoulder at lower θ-angles which is indicative of a tetragonal distortion of the substrate layers beneath the film. This is most likely due to an extended diffusion profile of the Mn into the bulk substrate. Rutherford Backscattering Spectrometry and ion-channeling experiments confirmed the stoichiometry and epitaxy of the films. STM images of the film surface display large terraces with a $(\sqrt{3}\times\sqrt{3})R30°$ honeycomb structure, which agrees perfectly with the simulated image of the Mn-terminated Mn_5Ge_3 (100) bulk-truncated surface

from the LSDA calculations; see Fig. 1(a). Magnetic properties were measured with a SQUID magnetometer. Fig. 1(b) shows the temperature-dependent remanent magnetization. It reveals a T_c of about 295 K [3]. Hysteresis loops at $T = 5$ K with in-plane and out-of-plane field orientations are shown in the inset. The easy axis is in-plane which is most likely due to the shape anisotropy [3]. The multiplet splitting of the Mn 3*s* core level in X-ray photoelectron spectroscopy [4,5] indicates an average magnetic moment of 2.7μ_B per Mn atom, which is in almost perfect agreement with the 2.6μ_B from the LSDA calculations and SQUID measurements.

Conclusions

We have grown and characterized a high-quality, epitaxial ferromagnet on Ge(111). The Curie temperature is 295 K and the average saturation magnetic moment per Mn atom at $T = 5$ K is 2.7 μ_B. The experimental findings are in good agreement with the LSDA calculations. This alloy interface is a promising candidate for spin injection into silicon-compatible materials and devices.

Acknowledgements

This research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725, and by the Office of Naval Research.

References

[1] G. Schmidt *et al.*, Phys. Rev. B **62**, R4790 (2000).
[2] N. Yamada, J. Phys. Soc. Jpn. **59**, 273 (1990)
[3] J. Shen, J. Kirschner, Surf. Sci. **500**, 300 (2002)
[4] S.-J. Oh, G.H. Gweon, J.G. Park, Phys. Rev. Lett. **68**, 2850 (1992)
[5] V.R. Galakhov et al., Phys. Rev. B **65**, 113102 (2002).

Figures

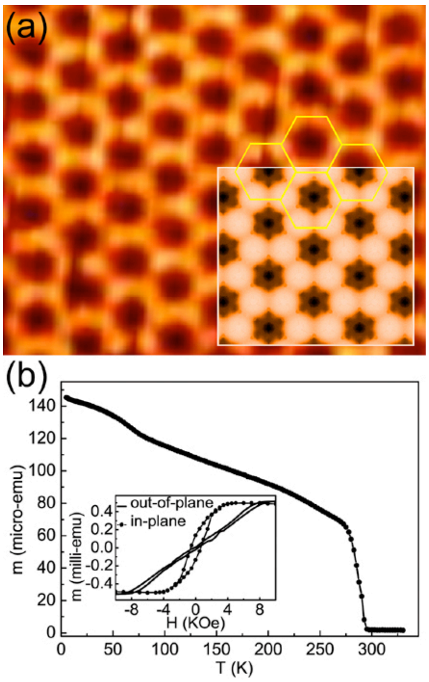

Fig 1: (a) Filled-state STM image of Mn_5Ge_3 films on Ge(111). The inset is the simulated result. (b) Magnetic measurements of the Mn_5Ge_3 films on Ge(111).