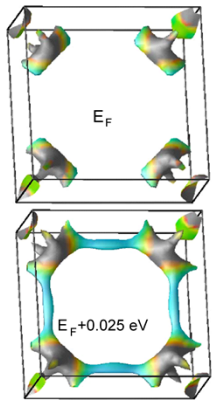
Control of composition and strain leads to useful properties in an environmentally friendly silicide



Topological changes near the electron Fermi surface lead to a dramatic transition in lattice, thermal expansion, electrical conductivity, and magnetization.

Scientific Achievement

Metastable α-$FeSi_2$, a phase with useful ferromagnetic and transport properties, was epitaxially stabilized as a thin film on silicon.

Significance and Impact

Environmentally friendly $FeSi_2$ in its natural form is either metallic or non-magnetic, depending on the temperature. The epitaxially stabilized form is a magnetic semiconductor at room temperature, as needed for spintronic and other applications.

Research Details

- Growth by pulsed laser deposition.
- Magnetization, electric conductance and thermal expansion, with a transition at 50 K.
- Density functional calculations and Boltzmann transport describe the unusual electronic structure with and without strain.

Work was performed as User Project at the Center for Nanophase Materials Sciences, and Materials Sciences and Engineering Division, ORNL

G.X. Cao, et. al., *Phys. Rev. Lett*. 114, 147202 (2015)
DOI: 10.1103/PhysRevLett.114.147202

U.S. DEPARTMENT OF ENERGY | Office of Science

THE UNIVERSITY of TENNESSEE KNOXVILLE | OAK RIDGE National Laboratory

Narrative Highlight Text:
Transition-metal disilicides have been extensively investigated in bulk and thin film forms for their roles as constituents in microelectronic and optoelectronic devices. In contrast to other metallic disilicides, environmentally friendly iron disilicide (FeSi2) is particularly appealing as a material for thermoelectric or optoelectronic devices due to its semiconductor behavior. In this work, new electronic behavior of the α-FeSi2 (111) thin films, which is in between that of metals and semiconductors, as well as ferromagnetism, are tailored via pulsed laser deposition on silicon. An unusual transport property with a strong crossover at 50 K was found, accompanied by the onset of ferromagnetism with a first order transition, as well as a substantial magnetoresistance. Density functional theory (DFT) calculations were used to enable improved understanding of the transport property and to verify the ferromagnetism with a slight excess of Fe stoichiometry.

Reference

"Ferromagnetism and Nonmetallic Transport of Thin-Film α-FeSi2: A Stabilized Metastable Material"
G. Cao,[1] D. J. Singh,[2] X.-G. Zhang,[1] G. Samolyuk,[2] L. Qiao,[1] C. Parish,[2] K. Jin,[3] Y. Zhang,[3,2] H. Guo,[2] S. Tang,[1,3] W. Wang,[2] J. Yi,[1,3] C. Cantoni,[2] W. Siemons,[2] E. A. Payzant,[1] M. Biegalski,[1] T. Z. Ward,[2] D.Mandrus,[3,2] G. M. Stocks,[2] Z. Gai[1]
[1] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
[2] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6056, USA
[3] Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA
Physical Review Letters, 114, 147202 (2015). DOI: 10.1103/PhysRevLett.114.147202

Acknowledgment of Support
This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences (Z. G., G. C., X.-G. Z., L. Q., M. B., E. A. P.), U.S. Department of Energy. Part of this effort was supported by the U.S. DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division (D. J. S, G. M. S., T. Z. W., G. M. S., Y. Z., C. P.), and under U.S. DOE Grant No. DESC0002136 (H. G., W. W.).