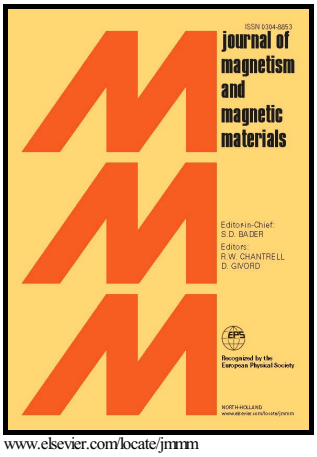
Substrate matters: Magnetic tuning of the Fe monolayer

A.A. Ramanathan, J.M. Khalifeh



www.elsevier.com/locate/jmmm

PII: S0304-8853(16)31438-X
DOI: http://dx.doi.org/10.1016/j.jmmm.2016.11.096
Reference: MAGMA62171

To appear in: *Journal of Magnetism and Magnetic Materials*

Received date: 14 July 2016
Revised date: 15 November 2016
Accepted date: 20 November 2016

Cite this article as: A.A. Ramanathan and J.M. Khalifeh, Substrate matters Magnetic tuning of the Fe monolayer, *Journal of Magnetism and Magneti Materials,* http://dx.doi.org/10.1016/j.jmmm.2016.11.096

Substrate matters: Magnetic tuning of the Fe monolayer

A.A. Ramanathan* and J.M. Khalifeh

Department of Physics, The University of Jordan, Amman-11942, Jordan

Abstract

The effect of substrate on the magnetism of the Fe monolayer (ML) is investigated using the total energy DFT calculations with the local spin density approximation (LSDA). The results show an in plane ferromagnetic coupling (FM) and a magnetic moment of $1.78\mu_B$ for the relaxed Fe ML in the presence of the vanadium substrate. In comparison, the surface Fe(001) magnetic moment ranges between $2.97\text{-}3.01\mu_B$. This difference in the Fe surface moment of more than $1\mu_B$ in the presence or absence of Vanadium allows tuning of the Fe magnetic moment and has great potential as a magnetic switch and in spintronic devices. The surface magnetic quenching of Fe with V is much more pronounced than with other transition metal substrates like Molybdenum or Tungsten. We have a reduction of 40.5% of the Fe (001) surface moment which is more than double the reduction obtained with the Fe/Mo(001) or the Fe/W(001) systems. The magnetic quenching is due to the strong hybridization between the Fe and V d bands. This is supported by the observed charge density redistribution and large inward relaxation of 18.37% for the Fe surface upon structural relaxation. The Fe ML is antiferromagnetically (AF) coupled with the V interfacial layer, which has an appreciable induced magnetic moment of $0.48\mu_B$.

Key words: DFT; surface magnetic quenching; Fe monolayer; electronic structure; relaxation

1. Introduction

Nowadays deposition techniques like Atomic Layer Deposition [1-3], and Molecular Beam Epitaxy have given rise to a whole new world of possibilities, since it is now possible to deposit in a uniform and controlled manner layers of atoms of different types on well-defined crystalline planes. Tailoring the magnetic properties of alloys, multilayers, superlattices, and other nano-structures using multi-element composition is now an attainable goal and the fabrication of novel materials with unique properties has