Available online at www.sciencedirect.com
SCIENCE DIRECT®
Surface Science 594 (2005) 148–155
SURFACE SCIENCE
www.elsevier.com/locate/susc

Magnetic map and interlayer exchange coupling in Fe/Ni(1 1 0) and Fe/Ni(1 1 1) superlattices

A. Hadj-Larbi [a,*], O. Adjaoud [a], S. Bouarab [a], C. Demangeat [b]

[a] Laboratoire de Physique et Chimie Quantique, Université Mouloud Mammeri de Tizi-Ouzou, 15000 Tizi-Ouzou, Algeria
[b] Institut de Physique et Chimie des Matériaux de Strasbourg, 23, rue du Loess, B.P. 43, F-67034 Strasbourg Cedex 2, France

Received 7 April 2005; accepted for publication 20 July 2005
Available online 11 August 2005

Abstract

The magnetic properties of Fe/Ni(1 1 0) and Fe/Ni(1 1 1) superlattices with face centered cubic structures are investigated through ab initio calculations. We determine the interlayer exchange coupling between the ferromagnetic Ni slabs versus the Fe spacer's thickness as well as the magnetic map. For both directions of polarization (ferromagnetic and antiferromagnetic) a strong ferromagnetic coupling between the Fe and Ni atoms is depicted at the Fe–Ni interfaces, whereas an oscillatory behavior of the magnetic moment is obtained inside the Fe films giving rise to an antiferromagnetic-like arrangement. The Fe interface mean magnetic moment has a tendency to stabilize around $2\mu_B$. A very different interlayer exchange coupling is obtained for the (1 1 0) direction as compared to (1 1 1).

Keywords: Density functional calculations; Magnetic interfaces; Metal–metal interfaces; Iron; Nickel

1. Introduction

Besides its base centered (bcc) ground state configuration [1] Fe can be stabilized in face centered (fcc) and hexagonal closed packed (hcp) bulk phases. The bcc ground state is clearly ferromagnetic whereas the fcc and hcp phases are respectively antiferromagnetic and non-magnetic. In fact experimental results and theoretical calculations show that Fe with fcc crystalline structure may form different magnetic phases, including low-spin antiferromagnetic, low and high-spin ferromagnetic, non-magnetic states as well as spin-spiral [2–7]. In contact with strong ferromagnet like Co or Ni, Fe atoms in fcc configuration present an induced magnetic configuration.

In Ni/Fe/Ni(1 1 1) trilayers, Fratucello et al. [8] measured, by Mössbauer spectroscopy, a high hyperfine field (≈28 T) assigned to Fe atoms close to Fe–Ni interface with a high-spin ferromagnetic

* Corresponding author. Tel./fax: +213 26214848.
E-mail address: hadjlarbi@yahoo.com (A. Hadj-Larbi).

0039-6028/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.susc.2005.07.020