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Ab initio study of the origin of the dead magnetic Ni layers at the Ni/Pt(1 1 1) interface

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Abstract

Two recent experimental works based on X-ray magnetic circular dichroism and superconducting quantum interference on Ni/Pt(1 1 1) superlattices have displayed very different magnetic behavior. One reports evidence of magnetically "dead" layers whereas in further work, no magnetically dead Ni layers were found. These magnetically different behavior can be explained by density functional calculations on various structural configurations at the interface. One Ni buried layer at the interface gives a good description of the magnetic profile reported experimentally on one hand, whereas two or three NiPt alloyed layers at the interface confirm the magnetic dead Ni atoms measured on the other hand.

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

1. Introduction

The study of magnetic thin films and multilayers is motivated mainly by their technological relevance for data storage devices and sensors. The multilayers prepared by alternate deposition of transition metal (Fe, Co, Ni, etc.) and nonmagnetic element (Pt, Ag, Au, etc.) have been extensively investigated. Ni/Pt multilayers in fcc(1 1 1) layered structure are characterized by very recent inconsistent experimental results reported in literature [1,2]. It is more or less clear that the existence (or not) of a magnetically Ni dead layer can be related directly to different sample preparation conditions. Indeed, using magnetometry techniques these authors report either a slightly enhanced [3] or strongly reduced magnetization [2] in Ni/Pt multilayers. These effects are attributed to the induced polarization [3] of Pt by Ni or to dead Ni layers at the Ni/Pt interface [2].

Through superconducting quantum interference device (SQUID), Wilhelm et al. [1] have deduced the magnetization of the sample prepared by e-beam grown and within X-ray magnetic circular dichroism (XMCD), they separate the magnetization arising from Ni and Pt, but the values obtained are not in good agreement with those predicted by their calculations with the tight-binding linearized

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