Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Journal of Magnetism and Magnetic Materials 300 (2006) 351–357
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

A drop of hyperfine field at Sn in Fe/Cr/Sn/Cr multilayers

A.K. Arzhnikov[a,*], L.V. Dobysheva[a], D.V. Fedorov[a], V.M. Uzdin[b]

[a]*Physical-Technical Institute, Ural Branch of Russian Academy of Sciences, Kirov str. 132, Izhevsk 426001, Russian Federation*
[b]*St.-Petersburg State University, ICAPE, 199178 St. Petersburg, Russian Federation*

Received 31 March 2005; received in revised form 6 May 2005
Available online 15 June 2005

Abstract

The magnetism of the Fe/Cr/Sn/Cr multilayers was studied by the first-principle density functional theory. Possible reasons for an experimentally well-known drop of the hyperfine field (HFF) at Sn with a decrease of the Cr width (at 3 nm) are considered. The calculations by LAPW and SKKR methods showed that two solutions exist in the $Fe_9/Cr_{14}/Sn/Cr_2$ system. One of them originates from the antiferromagnetic order in the bulk Cr, and the other is connected to the incommensurate spin density wave (ISDW) in Cr, which is realized in our case in a Cr film thinner than the half-length period of commonly observed ISDW. The ISDW solution is investigated in more detail with respect to its dependence on temperature and the accuracy of the Fermi-surface description. In the Cr layers with width lower than a quarter of the wave (3 nm), the ISDW cannot exist and thus cannot be a cause of the sharp drop of the Sn HFF. It is shown by the calculation of the $Fe_3/Cr_8/Sn/Cr_8$ system that another possible reason for the HFF drop, connected to imperfections at the Fe/Cr interface, may cause a significant decrease in the HFF at Sn. This is shown for an interfacial Fe/Cr mixing.

PACS: 73.20.Dx; 75.70.Cn; 71.15.Ap; 71.15.Cr

Keywords: Hyperfine field; Multilayer systems; Electronic structure

1. Introduction

Since the discovery of antiferromagnetic coupling between Fe layers [1] and giant magnetoresistance [2] in Fe/Cr multilayers several studies have paid great attention to the Cr magnetic properties in these systems. To date, however, the discussion on the magnetic order in thin Cr films continues; there is no clarity in the understanding of the interconnection between the Cr magnetic state and the magnetic coupling of Fe layers. Recently, the authors of Ref. [3] succeeded in obtaining the Fe/Cr multilayer systems with a Sn monolayer inserted. Multilayer systems $Fe_{d_1}/Cr_{d_2}/Sn/Cr_{d_3}$ with different widths

*Corresponding author. Tel.: +7 3412 218988; fax: +7 3412 250614.
E-mail address: arzhnikov@otf.pti.udm.ru (A.K. Arzhnikov).

0304-8853/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.jmmm.2005.05.021

d_1, d_2 and d_3 were investigated by various physical methods including the Mössbauer spectroscopy. One of the most important results was the established dependence of the hyperfine magnetic field (HFF) at Sn nuclei on the width of the Cr layer. This dependence is characterized by a sharp drop of the HFF magnitude at a Cr width less than 3 nm ($d_2 + d_3 < 3$ nm) [4]. Mössbauer experiments cannot provide a direct answer to the magnetization of Cr atoms, but if the HFF at Sn is assumed to be proportional to the local magnetic moments of the nearest Cr atoms, one should inevitably conclude that at a width of the Cr layer less than 3 nm, the Cr magnetic moments in these systems are close to zero.

As soon as the experimental data became available, theoretical first-principle calculations of the electron structure and the magnetic characteristics of Fe/Cr/Sn/Cr were conducted [5–8.] The calculations were performed by both linear methods [5–7] and the Green function formalism [7] with different approximations of the exchange-correlation potential. As a whole, the results obtained by different methods and authors agree well with each other and do confirm the possibility of estimation of the Cr magnetization from Mössbauer experiments at Sn [7]. Some differences between the results have, however, led to difficulties in the explanation of the peculiarities of the HFF variation and have elicited a number of unsolved questions.

In this paper, we focus our attention on the discussion of two hypotheses advanced earlier in Refs. [3,7] for explanation of the Sn HFF behavior. The first one is connected to the existence of the high- and low-spin states and a transition between them with a change in the Cr width. Such solutions were obtained for the $Fe_9/Cr_{14}/Sn/Cr_2$ system in Ref. [7]. The second hypothesis is connected to the effect of the Fe/Cr boundary quality on the Cr magnetization.

We have performed additional calculations of the periodical systems $Fe_9/Cr_{14}/Sn/Cr_2$ and $Fe_3/Cr_8/Sn/Cr_8$ (the latter being calculated with and without taking account of the imperfection of the Fe/Cr boundary). The calculations were conducted by the following methods: the full-potential linearized augmented plane wave method (FP LAPW) realized in the program package WIEN2k [9], and a screened Korringa–Kohn–Rostoker method developed in Jülich [10] in the atomic sphere approximation (ASA SKKR) and in a full-potential scheme (FP SKKR). The calculations employed the exchange-correlation potential in the local density approximation (LDA) in the formalism of Refs. [11,12]. As shown in Ref. [13], if scaled to the moment, the LDA and the generalized gradient approximation (GGA) yield the same behavior. The HFF is calculated by integration of the spin density over Thomson's sphere. This method, which is standard for the first-principle calculations, gives the HFF whose values may slightly deviate from the experimental ones due to an inconsistency in the exchange-correlation potential, but the discrepancy with the experiment is a typical character and may be taken into account.

For our calculations we have used the following models. The multilayer systems were presented as

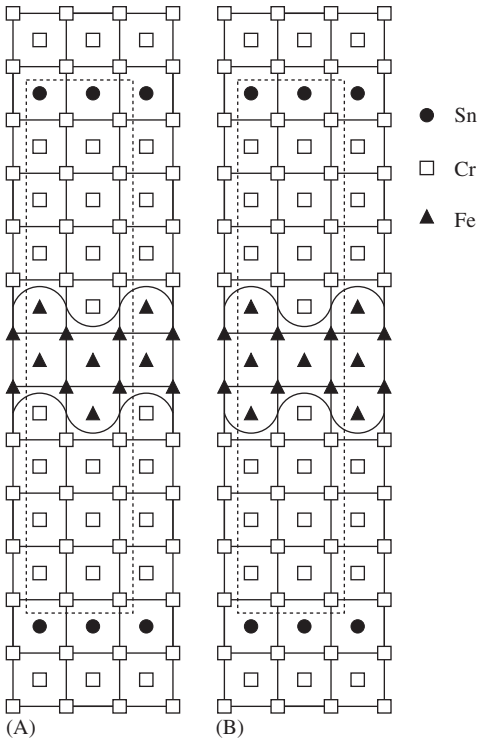

Fig. 1. Two types of mixing at the Fe/Cr boundaries (solid lines). Dashed lines show the unit cells.