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Theoretical study of thin Fe films deposited on a Cr(001) substrate: step-induced extended defects

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Abstract

In this paper we present a theoretical study of the magnetic properties of a few Fe monolayers deposited on a Cr(001) substrate containing monatomic steps. We use the real space recursion method in a tight binding framework to determine the electronic structures of non-periodic systems involving large numbers of inequivalent atoms (up to 1130). We investigate the nature of the magnetic defects induced in the Cr spacer layer by interfacial steps in relation to recent experiments. We show that even if a multidomain magnetic configuration of the Fe overlayer is the most favoured one without an external applied field, defects can link two successive steps for thick Fe overlayers and rough interfaces.

The magnetic behaviour of Cr layers in Fe/Cr superlattices or sandwich structures has recently been shown to be particularly complex and strongly sensitive to the growth preparation [1–4]. For example, it has been shown that (i) the Cr layer can introduce a large decrease of the whole magnetization when deposited on Fe(001) [1]; (ii) the interlayer magnetic coupling – which is theoretically expected to oscillate with the parity of the number of Cr monolayers [5] – oscillates out of phase in Fe/Cr/Fe sandwiches [2]; and (iii) the long-range antiferromagnetic order is suppressed by magnetic defects due to the interfacial roughness [3]. All of these experimental studies suggest that magnetic defects induced in the Cr spacer layers by interfacial topological defects play an essential role.

The aim of this work is to investigate the competition between single and multidomain configurations of the Fe overlayer due to the step and related to the presence of magnetic defects. In this work, we assume that the moments are collinear. For such a study, we have to determine the magnetic moment map (MMM) in the vicinity of a single step. This is done here in the tight binding framework and with the real space recursion method as described previously [6].

If Fe is deposited on a Cr substrate containing terraces with monatomic steps (Fig. 1), the Fe magnetic moments are opposite to those of the Cr surface due to the strong Fe–Cr antiparallel coupling [6]. Consequently, the magnetic moments of Fe atoms deposited on different Cr terraces will be antiparallel and a defect line appears near the edge of the step in the Fe layer at the separation between the two magnetic domains: this situation corresponds to a multidomain (MD) Fe overlayer (Fig. 1a). In this case, the most stable MMM is obtained when the number of frustrated Fe–Fe ferromagnetic links is the lowest and when there is no frustration of the Fe–Cr antiparallel coupling. The perturbation due to this defect line is found to be strongly localized near the step as a consequence of the assumed collinear character of the MMM. If we take into account the finite magnetic anisotropy of the Fe overlayer, the ground state energy will

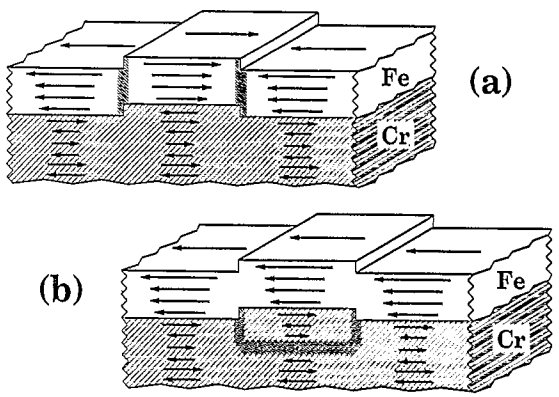

Fig. 1. Schematic representation of the two situations: (a) frustrations in the Fe overlayer, and (b) frustrations in the Cr layer due to a single-domain Fe overlayer. The magnetic 'walls' are also represented schematically (oblique shading).

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be lower than the energy we calculate from the collinear arrangement, and the thickness of the defect will be larger.

The domains in the Fe overlayer can be aligned by a strong external magnetic field; this situation corresponds to a single-domain (SD) Fe overlayer. Half of the Fe magnetic moments switch from a negative to a positive value and the strong Fe–Cr interfacial coupling introduces a frustration of the Cr antiferromagnetic order in the substrate (Fig. 1b). Fig. 2 shows the MMM near the step resulting from a self-consistent calculation over 1130 inequivalent atoms for such a situation. For this calculation, the starting MMM was obtained by changing the sign of all magnetic moments on the first 15 Cr monolayers in the left part of the step. The frozen levels of the atoms on the left part of the self-consistent domain have been obtained by calculating the wall in the Cr substrate covered by three Fe monolayers, the magnetic moments being oriented so that frustration occurs in the Cr antiferromagnetic order. During the self-consistent procedure, the angle α between the normal and the defect plane (see Fig. 2) has increased from 0° to 45°. In such a case the perturbation is very large and consequently the energy of this defect is also very large.

However, such defects can have much smaller extensions and smaller energies when two steps are separated by a small terrace. Consequently, the formation energy of this defect is much smaller and becomes comparable to that of a defect induced in the Fe overlayer. Therefore, a transition from the multidomain (MD) to the single-domain (SD) solution occurs without any external magnetic field when the Fe overlayer thickness (e_{Fe}) increases. Indeed, for the SD case, the defect is in the Cr substrate and its energy does not depend on e_{Fe}, whereas for the MD case, the lateral size of the negative magnetic Fe domain in-

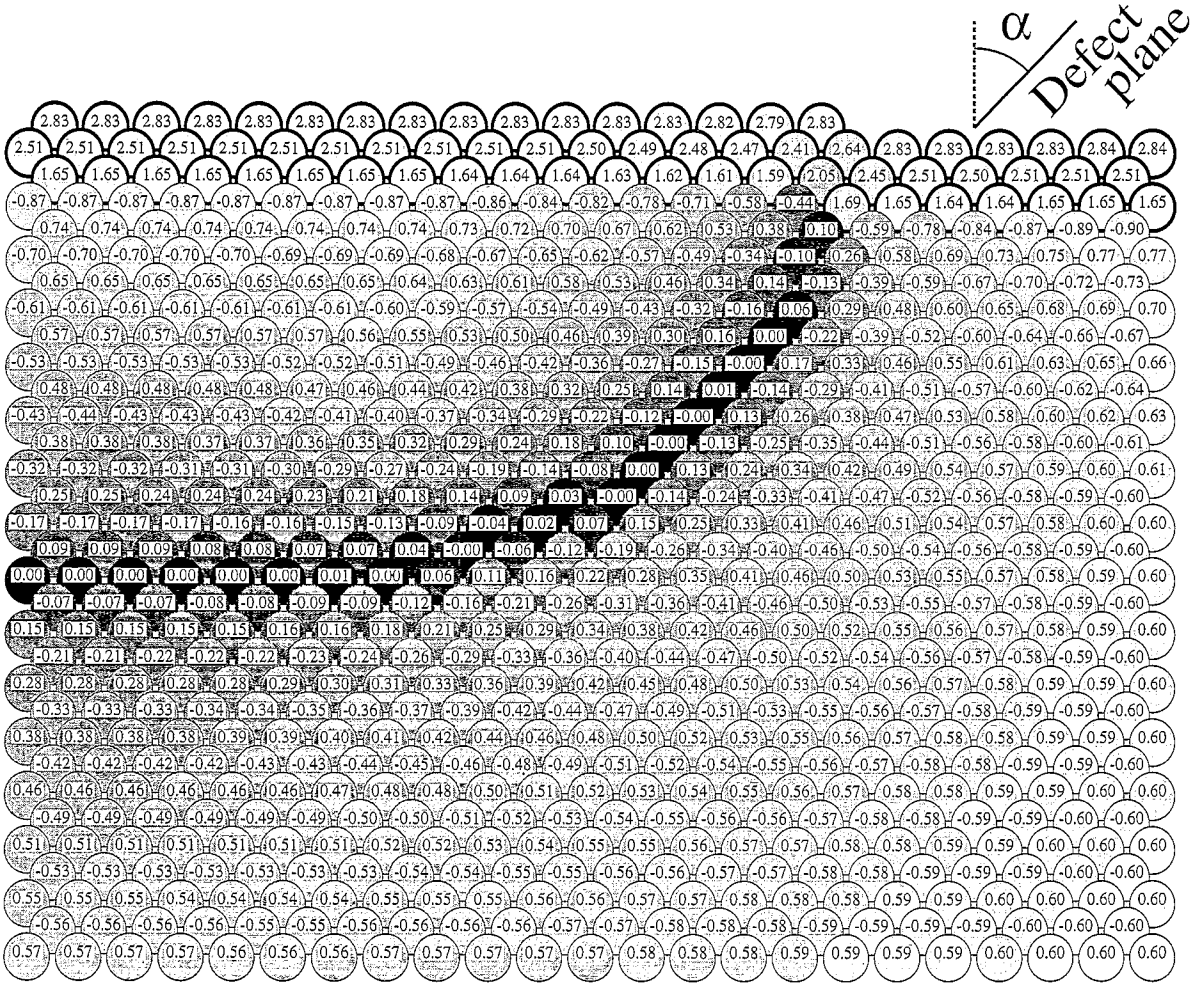

Fig. 2. Magnetic moment distributions of three Fe monolayers deposited onto the Cr(001) stepped substrate with the magnetic defects in the Cr substrate. The grey level $g(p)$, with $p = |M(x_i, z_i)/M(x \to \infty, z_i)|$, of the filled circles corresponds to the pertubation level of the magnetic moment at the position (x_i, z_i) relative to that of the non-perturbed value obtained for $x \to \infty$ with $x > 0$. $g(p)$ is equal to p when $p \leq 1$ and to $2 - p$ when $p > 1$. White corresponds to $g = 1$ and black to $g = 0$. The Fe atoms are shown with thicker outlines.

creases with e_{Fe} and the energy of the defect increases linearly with e_{Fe}. Our calculations show that the linear behaviour is reached for $e_{Fe} = 4$ and that the transition from a multidomain to a single-domain Fe overlayer occurs for an Fe thickness equal to the lateral size of the terrace.

In conclusion, when the growth mode approaches the layer-by-layer one for which the size of the terrace is large, the Fe overlayer is in a multidomain state with no net magnetization. However, it is possible to obtain a single-domain thick Fe overlayer when the Fe/Cr interface is rough, i.e. when the terrace size is small, but extended magnetic defects occur in the Cr layer linking successive steps.

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