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Quantum-well states in magnetic multilayers and non-Poisson islands formation during epitaxial growth

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Abstract

Mechanism, responsible for the non-Poisson growth of islands of metal on metal substrate is suggested. It is connected with confinement of the electrons with one spin projection inside of the quantum wells (QW) formed by islands. Oscillations of the energy of these electrons with width of the wells lead to the suppression of the formation of islands with definite thickness. This effect is especially important for the submonolayer coverage and for the initial phase of epitaxial process. Analogy between QW-theory for the oscillations of exchange coupling in metallic magnetic multilayers and the theory of non-Poisson islands formation is discussed. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Quantum-wells; Electron confinement; Three-dimensional island's growth

The physical nature of the epitaxial growth of metals on metal surfaces is a key point of modern technology of multilayered structure formation. Recent experiments show that the islands of magnetic metals on nonmagnetic substrate and nonmagnetic metals on magnetic substrates very often grow so that a Poisson distribution on the thickness does not hold. In particular, the Cr overlayer on an Fe surface has been investigated intensively [1–5]. Unusual behaviour during the evaporation of the first few monolayers of Cr on Fe substrate, even if the interface is smooth, has been reported in many experimental studies. Unguris et al. [1], using scanning electron microscopy with polarisation analysis, founded that there is a 'defect' in the antiferromagnetic ordering of a Cr overlayer on an Fe whisker between 1 and 4 monolayers (ML) which give a phase change in electron–spin polarisation P(Cr), although for the thicker coverage they observed oscillations of P(Cr) as a function of Cr thickness with a period in two atomic layers. Idzerda et al. [2] found a monotonic decrease of circular magnetic dichroism (CMD) signal from Cr atoms as function of Cr thickness. They connected it with interface roughness, but the experimental dependence shows a more rapid decrease than is consistent with a Poisson distribution on island thickness, Boske et al. [3] revealed that CMD signal for 2 MLs of Cr on Fe(1 0 0) has the same sign as for 1 ML contrary to the simple model of layer by layer growth. In contrast, Knabben et al. [4] found oscillations of the linear dichroism signal with Cr coverage. However, instead of a minimum for 2 MLs coverage, which would be natural for layer by layer growth, they detected the maximum whereas the minimum occurred at a coverage of 1.5 MLs. To explain the huge decrease of the total magnetic moment of an Fe sample with Cr overlayer which was detected in magnetometer experiments, Turtur and Bayreuther [5] suggested that the first two Cr layers on Fe have the magnetic moments ordered in the same direction, opposite to the magnetic moment of Fe substrate.

For an explanation of these results, where non-Poisson three-dimensional growth of Cr islands on Fe substrate was clearly revealed, we suggest a simple theory based on the idea of confinement of itinerant electrons within the Cr islands on Fe surface. The existence of the confined quantum-well (QW) states for the electrons in highly perfect layered structures has been well established both

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experimentally and theoretically. for Fe/Cr multilayers spin-polarised QW-like states were analysed within the framework of *ab initio* calculations [6]. It was proved, in particular, that QW-model more correctly describes the oscillations of exchange coupling in iron–chromium systems than RKKY-like models.

Let us consider a Cr island with thickness L on the ideal Fe surface and suppose that electrons at least with one spin projection are fully confined within the island. If L is much less then the lateral size of the island, we can use the infinite QW model for a description of the transverse movement of confined electrons and the free-electrons approach for the electron movement in the plane.

We assume that the Fermi energy of the system is fixed by a large number of electrons in the Fe substrate. In this case the total number of d-electrons is not fixed, and to compare the states with different distributions of the island thickness we have to consider the thermodynamic potentials $\Omega = E - \varepsilon_F N$ of the electrons in all QW. For the single well we have [7]

$$\Omega_L = \frac{Sm\varepsilon_F^2 n_L}{4\pi\hbar^2}\left\{ -1 + \frac{1}{3}\left(\frac{\pi^2\hbar^2}{2m\varepsilon_F L^2}\right)(n_L+1)(2n_L+1) \times\left[1 - \left(\frac{\pi^2\hbar^2}{2m\varepsilon_F L^2}\right)\frac{3n_L^2+3n_L-1}{10}\right]\right\}.$$

Here n_L is the number of quantum levels below Fermi-energy, S is the area of island. Analysis of the problem can be essentially simplified if we consider instead of Ω_L the value $\Delta\Omega_L = \Omega_L - \Omega_L^{cl}$, where Ω_L^{cl} is the quasiclassical contribution, which can be obtain from Ω_L by substitution of the integer number n_L by the quasiclassical value α:

$$n_L \to \alpha = \frac{\sqrt{2m\varepsilon_F}}{\hbar\pi}L.$$

The straight calculation shows that Ω_L^{cl} contains only contributions proportional to the L^1, L^0, L^{-3}:

$$\Omega_L^{cl} = \frac{Sm\varepsilon_F^2}{4\pi\hbar^2}\left[-\frac{8}{15}\alpha + \frac{1}{2} + \frac{1}{30}\alpha^{-3}\right].$$

After summation of the contributions to Ω^{cl} from all QW on the sample surface, we will obtain a term proportional to the total volume of all islands (which is constant for the given coverage), and a term proportional to the total area of the islands (also constant for the coverage exceeding 1 ML). The third contribution appears to be small even for monolayer islands and can be omitted. As a result, when the coverage is fixed, for the determination of the distribution of islands on thickness it is enough to compare $\sum_{L_i}\Delta\Omega_{L_i}$ instead of $\sum_{L_i}\Omega_{L_i}$.

Fig. 1 shows the dependence $\Delta\Omega_L$ for the single QW and the number of quantum levels in the well versus width L. $\Delta\Omega_L$ oscillate with L and decrease as L^{-2}. It means that the main contribution to the $\sum_{L_i}\Delta\Omega_{L_i}$ arises from the electrons, localised in the narrowest QW. Similarly, the electrons in the narrowest QW determine the oscillations of exchange coupling in metallic magnetic superlattices and sandwich systems [7].

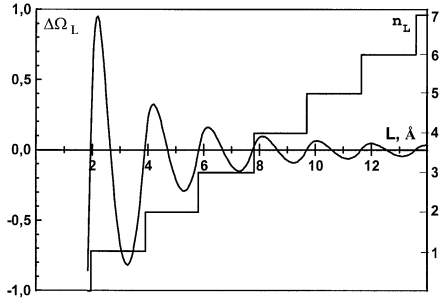

Fig. 1. $\Delta\Omega_L$ (arb.un.) and a number of quantum levels in the well versus well thickness L.

Note, that the thickness of the QW can be changed only discretely by the half of the a lattice constant in the case of Cr islands on Fe(1 0 0) surface. Period of oscillation in Fig. 1 is about 2A which is of the same order as the lattice constant. So, if for the islands with a thickness of 2 MLs $\Delta\Omega_L$ is larger then for 1 ML and 3MLs, then the formation of 2MLs islands will be suppressed.

It should be stressed that our model of an infinite QW simplifies the detailed behaviour of a real system. The finite depth and the shape of the QW influence the phase and the period of the $\Delta\Omega_L$ oscillation. Alloying in the interface region leads to an erosion of the islands, so that only for the part of the sample surface this picture can be applied. Despite this, the confinement of an electron in the QW definitely leads to the non-Poisson distribution of the islands on thickness and can be one of the reasons for the behaviour obtained in the experiments. The growth of three-dimensional islands for higher thicknesses has to shrink the dependence of polarisation on the coverage and leads to the same effect as alloying in the interface region. Suppression of 2MLs islands can be one reason for the MCD-signal oscillations which were obtained in the experiments [4] as well as the apparent FM ordering of the first and the second Cr monolayer [5]. Similar mechanism can be responsible for the initial nucleation and subsequent growth of Co on Au(1 1 1). In this system, using scanning tunneling microscopy, it was discovered that the islands are two atomic layer high and grow laterally with increasing coverage [8].

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