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First-principles calculation for spin-density wave in Fe/Cr multilayers

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Abstract

A first-principles electronic structure calculation for Fe/Cr multilayers is presented, where a spin-density-wave order in the Cr layer is taken into account in addition to an antiferromagnetic one. The interlayer magnetic coupling between ferromagnetic Fe layers is investigated, and oscillation of the coupling with a two-monolayer period of the spacer thickness of the Cr layer is illustrated. The appearance of the spin-density-wave order in the Cr layer is furthermore demonstrated.

Keywords: First-principles calculation; Multilayers; Spin-density wave

As an archetype of spin-density wave (SDW) in itinerant electron systems, Cr has been extensively investigated up to the present. An interest has recently focused on SDW in Fe/Cr multilayers, in connection with the interlayer magnetic coupling between ferromagnetic Fe layers. The coupling of magnetizations of the two successive Fe layers oscillates between parallel and antiparallel with a two-monolayer period of the spacer thickness of the Cr layer, and for thicker Cr layers the oscillation is followed by periodic phase slips, which are considered to be due to incommensurability of an SDW order in the Cr layer [1]. One of the points at issue is whether the SDW in Fe/Cr multilayers is attributed to the Fe proximity layers or to the Fermi-surface nesting, which is intrinsic in the bulk Cr and is closely related to its electronic structure [2]. The electronic structure calculation is therefore expected to supply significant knowledge for the discussion about the SDW in Fe/Cr multilayers; there have been some electronic structure calculations for Fe/Cr multilayers, but in these calculations Cr layers have been assumed to be antiferromagnetic (AF) and the SDW order has hardly been considered [3].

We here present a first-principles electronic structure calculation for Fe/Cr multilayers, which is performed by means of the Korringa–Kohn–Rostoker (KKR) Green function method within the framework of the local spin density (LSD) functional formalism. The calculation is carried out for periodic multilayers which consist of ferromagnetic Fe layers and AF or SDW Cr layers, with the magnetizations of the two successive Fe layers being aligned parallel or antiparallel, in other words, with the interlayer magnetic coupling being ferromagnetic or antiferromagnetic. The purpose of this work is to survey variation of the interlayer magnetic coupling with respect to the thickness of the Cr layer, together with an investigation for the possibility of the appearance of an SDW order in the Cr layer. It is to be added that the present author performed a first-principles calculation for bulk SDW Cr with results in good agreement with experiments; for example, the wave vector of SDW of the lowest total energy per atom is found to be $a^*(19/20, 0, 0)$, which is close to the observed one $a^*(0.952, 0, 0)$, where $a^* = 2\pi/a$ and a denotes a lattice constant of the chemical bcc lattice [4].

In the present calculation, we consider perfect multilayers without interfacial roughness, which usually leads

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the coupling of the local magnetic moments between Fe and Cr atoms across the interface to a strongly antiparallel one, in comparison with that between Cr atoms [3]. This antiparallel interfacial coupling between Fe and Cr layers may influence the magnetic order of the inner Cr layer to some extent, especially when Fe layers exist both sides of the Cr layer, as is the case of periodic Fe/Cr multilayers or Fe/Cr/Fe sandwiches. When the magnetizations of two successive Fe layers are aligned parallel, an AF order is commensurate with a Cr layer of an odd N_{Cr} and needs one defect layer for that of an even N_{Cr}, where N_{Cr} (N_{Fe}) denotes the number of monolayers of the Cr (Fe) layer. We do not consider such unfounded defect layers but instead consider an SDW order such that a Cr layer contains a half period of SDW (half SDW order), which is really commensurate with a Cr layer of an even N_{Cr}. On the contrary, when the magnetizations of two successive Fe layers are aligned antiparallel, an AF order is commensurate with a Cr layer of an even N_{Cr} and a half SDW order is commensurate with that of an odd N_{Cr}. Thus the magnetic order of the Cr layer may be governed by the parity of N_{Cr}, and the oscillation of the interlayer magnetic coupling with a two-monolayer period seems quite natural. It is to be emphasized that the wave vector of the SDW is not determined by the Fermi-surface nesting but by N_{Cr}; the half SDW order corresponds to an SDW order of a wave vector $a^*(q,0,0)$ with

$$q = \frac{N_{Cr} - 2}{N_{Cr} - 1} \tag{1}$$

and accordingly to that of bulk Cr when N_{Cr} is around 20. When N_{Cr} is not so large, it is not likely that a Cr layer of the multilayers admits a part of the SDW with a specific wave vector, which is determined by the Fermi-surface nesting and is usually incommensurate with the chemical lattice.

Let us discuss results of the calculation, which is carried out for the multilayers with $N_{Cr} \leqslant 21$ and with $N_{Fe} = 3$ for an odd N_{Cr} and $N_{Fe} = 4$ for an even N_{Cr}. We adopt the experimental lattice constant of bulk Cr (that is, $a = 5.45$ a.u.) to view variation of the interlayer magnetic coupling J_{Fe} with respect to N_{Cr}; J_{Fe} is defined as

$$J_{Fe} = E_{ap} - E_p, \tag{2}$$

where E_{ap} and E_p are the total energy per one atom when the magnetizations of the two successive Fe layers are aligned antiparallel and parallel, respectively. In Fig. 1, we show J_{Fe} for the case of $a = 5.45$ a.u., and it is found that J_{Fe} is positive (parallel coupling is favored) for an odd N_{Cr} and negative (antiparallel coupling is favored) for an even N_{Cr}. The result is consistent with the fact that the interlayer magnetic coupling oscillates with a two-monolayer period, and it means that in the Cr layer the AF order is more favourable than the half SDW one, in so far as $N_{Cr} \leqslant 21$. The calculation for the case of

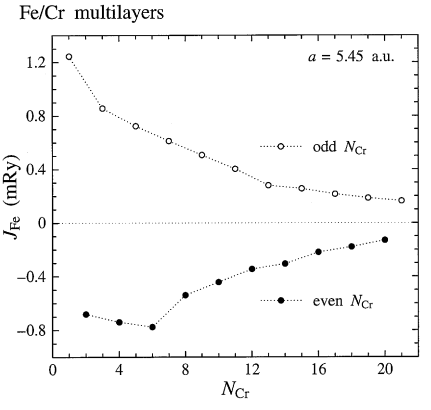

Fig. 1. The variation of the interlayer magnetic coupling between Fe layers J_{Fe} with respect to the spacer thickness of the Cr layer.

$a = 5.45$ a.u. illustrates the oscillation of J_{Fe} with a two-monolayer period but does not indicate the appearance of the SDW order in the Cr layer.

The calculation is furthermore carried out for two cases of $N_{Cr} = 9$ and $N_{Cr} = 19$ with varying the lattice constant a to determine an equilibrium lattice constant a_0 at which the total energy becomes minimum. In Fig. 2, we show E_p, E_{ap}, and their difference J_{Fe} as a function of the lattice constant a. It is found that E_p and E_{ap} become minimum at around 5.32 a.u., that is, $a_0 \simeq 5.32$ a.u. for both cases of N_{Cr}; this value is about 98% of the experimental value, which is common with the use of the LSD formalism. The curves of E_p and E_{ap} do not cross for $N_{Cr} = 9$, but they cross each other for $N_{Cr} = 19$, with a reversal of the sign of J_{Fe}, as can be seen in Fig. 2b. For the case of $a = a_0$, J_{Fe} is positive for $N_{Cr} = 9$ and negative for $N_{Cr} = 19$, which means that in the Cr layer the AF order is favourable for $N_{Cr} = 9$ whereas the half SDW order is favourable for $N_{Cr} = 19$. This is different from the case of $a = 5.45$ a.u., where the AF order is favourable even for $N_{Cr} = 19$. The difference between these two cases of a can be ascribed to the magnitude of the local magnetic moment of the Cr atom. For the case of $a = 5.45$ a.u., we have the larger magnitude of the local magnetic moment, which usually makes the AF order favourable. When the magnitude of the local magnetic moment is not so large and N_{Cr} is around 20, where the half SDW order approaches the SDW order of bulk Cr, an energy gain due to the nesting mechanism may become dominant to make the half SDW order favourable. Thus the calculation for the case of the equilibrium lattice constant surely indicates the appearance of the SDW order in the Cr layer.

Here we briefly discuss the interlayer magnetic coupling J_{Fe} for the case of $a = a_0$. We expect that the oscillation of J_{Fe} with a two-monolayer period basically does

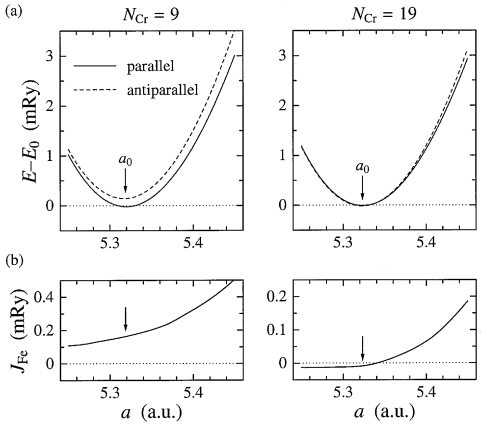

Fig. 2. Dependence of (a) the total energy per atom E_p, E_{ap} and (b) their difference J_{Fe} upon the lattice constant a for the cases of $N_{Cr} = 9$ and $N_{Cr} = 19$. The reference energy E_0 is E_p for the case of $a = 5.33$ a.u.

not change, since the oscillation may be in consequence of the commensurability within the Cr layer of the AF or half SDW order. We furthermore expect that there exists a critical N_{Cr} across which the relative stability between AF and half SDW orders is reversed between 9 and 19. At this critical N_{Cr}, correspondence between the sign of J_{Fe} and the parity of N_{Cr} is also reversed, and this reversal of the correspondence gives rise to a phase change by π in the oscillation of J_{Fe}, which is nothing but a phase slip of the oscillation.

In conclusion, we investigate the interlayer magnetic coupling between ferromagnetic Fe layers with respect to the spacer thickness of the Cr layer on the basis of the first-principles KKR-LSD calculation. It is shown that the interlayer magnetic coupling oscillates with a two-monolayer period of the Cr layer thickness. It is also demonstrated that an SDW order in the Cr layer can appear when N_{Cr} becomes large, and the relation between the appearance of the SDW order and the phase slip in the oscillation of the interlayer magnetic coupling is discussed.

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