Heavy Electrons at Metallic Fermi Surfaces, a Superlattice Property

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(Received 16 November 1995)

The near-E_F electronic structure and Fermi surface of Cu/Co superlattices are investigated by a tight-binding model and the Green function matching method. The more striking feature is the development of extremely dispersionless bands. Variation of the Cu and Co slab thicknesses changes the superlattice bands' energy. For periodic values of the Co thickness, Cu/Co superlattices exhibit a one-particle *flat band* at the Fermi level. As a consequence, a significant region of the superlattice Fermi surface has three-dimensional character. [S0031-9007(96)00490-5]

PACS numbers: 75.70.Cn, 71.18.+y, 71.20.Be

Metallic magnetic superlattices (SLs) exhibit new and interesting physical effects. The oscillatory exchange coupling and the negative giant magnetoresistance have been the principal subject of intense investigation in these systems [1,2]. Nevertheless, the range of peculiar effects extends to a great variety of physical phenomena, such as magneto-optics, transport properties, magnetostriction, or magnetothermoelectric power [3–5]. For example, it has been shown recently that the resistivity and anisotropic magnetoresistance of Co/Ni multilayers oscillate with the Co and Ni layer thicknesses and that the oscillation is a superlattice effect [6]. On the other hand, angle resolved photoemission and inverse-photoemission experiments on Cu thin films grown on Co(001) substrates show that Cu d-derived quantum-well states have flatter in-plane dispersion relations that those of the corresponding Cu bulk crystal [7]. In this Letter, we show that magnetic SLs present characteristic electronic properties due to the SL structure. We report on a mass-enhancement effect caused by the SL potential and demonstrate that, for specific values of the Co thickness, Cu/Co(001) SLs develop a *flat band* at the Fermi level almost dispersionless in an extended k-space region. As a consequence, a significant portion of the SL Fermi surface (FS) has three-dimensional (3D) character. The development of the 3D region in the SL Fermi surface is periodic with the Co thickness.

We consider ideal Cu_nCo_m SLs grown on the (001) direction with matched lattice parameters; n and m are the number of Cu and Co atomic layers, respectively. The SL Bravais lattice belongs to the tetragonal system, being simple tetragonal if $n + m$ is even and body-centered tetragonal if $n + m$ is odd. In ferromagnetically (FM) coupled SLs the unit vector in the growth direction is $(n + m)a$, where a is the (001) interlayer distance. For the antiferromagnetic (AF) configuration the unit vector is twice the ferromagnetic one, $2(n + m)a$. In addition, electrons with spin σ ($\sigma = \uparrow, \downarrow$) are the majority in the ferromagnetic slab whose magnetization is pointing in the same direction and the minority in the successive magnetic slabs. Therefore, due to the symmetry under the interchange of layers whose magnetization points in opposite directions, energy bands, density of states (DOS), and charge density are identical for spin-up and spin-down electrons in AF arrangements. Empirical tight-binding Hamiltonians with second-nearest-neighbor interactions and spd orbital basis are used to describe the bulk crystals. The Co Hamiltonian includes diagonal band-dependent exchange interactions [8]. The calculation of the SL band structure and FS is based on the Green function matching method. [9,10]. The FS contours were evaluated on a mesh of 5000 k points in the 1/8 irreducible of the SL Brilloiun zone (BZ).

As is well known, SL bands correspond to distorted bulk electronic states of different k points that, due to the supersymmetry, project into the same point of the SL BZ. Figure 1 shows near the Fermi energy dispersion relations along high symmetry directions of the SL BZ for a ferromagnetically coupled Cu_6Co_4 SL. In the SL growth direction ΓZ, two different types of states are clearly identified. Dispersed bands are separated by minigaps and localized bands with almost constant energy along the entire direction. The former have main sp character and arise from hybridization between sp-like Cu and Co states. In real space, their wave functions are extended to both Cu and Co slabs. However, the dispersionless states have a predominant d character, and their wave functions have preferential localization in one of the SL constituents, mainly in the Co film for bands close to E_F [10]. In the in-plane directions, Δ and Σ, the more striking feature for both spin dispersions is the occurrence of flat bands. In fact, most bands have mixed sp-d character, since interactions among allowed bands for a given k become important, and strong hybridization occurs. This results in an enhancement of the effective mass of SL states. Consequently, *flat bands*, almost dispersionless in an extended k-space region, develop. Near E_F the SL spin-up bands remain nearly free-electron-like, while those of spin-down electrons are greatly distorted by hybridization with Co d bands. Thus, most spin-down Fermi states have a predominant d character and, consequently, large effective mass. For AF coupling the general picture is similar to that of spin-down bands in the FM configuration,

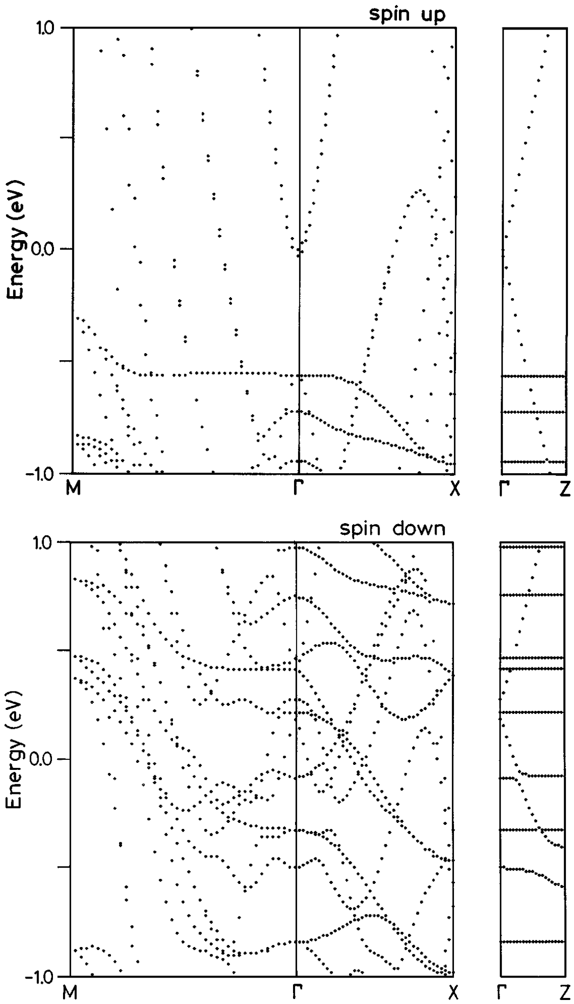

FIG. 1. Dispersion relations along high symmetry directions of a ferromagnetically coupled Cu_6Co_4 SL. Spin-up and spin-down states are represented at the top and bottom, respectively. The energies in eV are in reference to the Fermi level. Along the ΓZ direction the scale has been multiplied by 2.

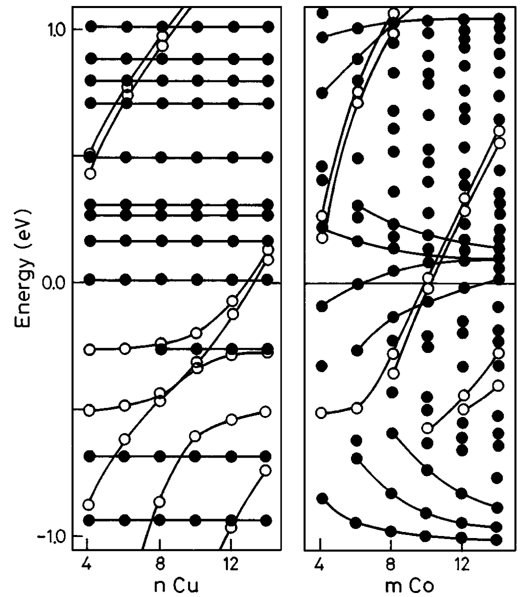

FIG. 2. Binding energy of spin-down SL states as a function of slab thickness. The evolution for Cu_nCo_6 SLs vs n and Cu_6Co_m vs m are shown in the left and right panels, respectively. Open and full circles correspond to SL states with main sp- and d-like character.

although hybridization is stronger due to the large increase in the number of allowed bands for a given k [10].

As has been extensively investigated in semiconductor SLs, the energy of SL states depends on n and m [9]. Thus, by changing the thickness of the SL constituents, the energy of a given band can be tuned. Figure 2 represents the energy of the spin-down SL states at Γ as a function of the slab thicknesses. Straight lines join SL states with the same symmetry and number of maxima in their wave function. With increasing Cu thickness, two types of behavior are obtained; either the energy remains constant or continuously moves up towards higher energy. The former corresponds to Co d-derived SL bands, well localized in the Co slab, and, consequently, its energy is independent of the Cu layer thickness. The second is followed by extended pure sp or strongly hybridized sp-d SL states. Conversely, all SL bands change their energy for increasing Co thickness. Nevertheless, the energy of states with main sp-like character changes quickly, while the dependence of energy bands with predominant d-like character is smooth. In this energy interval, due to the complexity of the d band, various series of d-derived Co states coexist. They originate from Co bulk extrema of different symmetry. A detailed analysis of the spatial and orbital symmetry together with their evolution with the number of Co layers allows us to identify their origin [10]. For the sake of clarity, only those associated to Γ_{12} and $\Gamma_{25'}$ have been marked in Fig. 2. In particular, the spin-down Γ_{12} state of bcc Co is just above E_F. However, for small Co thickness, the Δ_1 derived SL state is below E_F. Note the line crossing the Fermi level at $m = 6$ in the right panel of Fig. 2. Moreover, the next states of the series, $N = 2$, $N = 3, \ldots$, intersect E_F at periodic values of Co thickness, with an approximated period of 6 ml. Therefore, at Γ, spin-down electrons of Cu_nCo_{6p} $(p = 1, 2, \ldots)$ SLs have a band which lies within $\approx$20 meV of E_F.

Figure 3 shows the spin-down dispersion relations of the FM Cu_6Co_6 SL. The band at the Fermi level is completely flat through the SL growth direction ΓZ. Even more, due to the interaction with nearest bands, the in-plane dispersion around Γ is lower than that of the original bulk Δ_1 Co band [8]. The spatially averaged spectral strength at E_F along the ΓX direction is almost constant up to $k_{\parallel} \approx 0.07$. The constancy of the DOS shows the flattening of the Δ_1 band by the SL potential, which induces an enhancement of the effective mass of the SL state. An approximated estimation gives a value

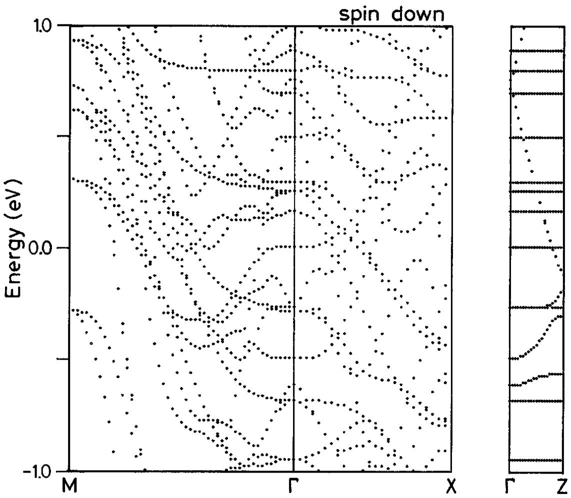

FIG. 3. Same as Fig. 1 for the spin-down electrons of a Cu_6Co_6 SL.

of ≈ 6 as the ratio between the SL and bulk effective masses. Furthermore, the SL state at Fermi is *flat* in all in-plane directions.

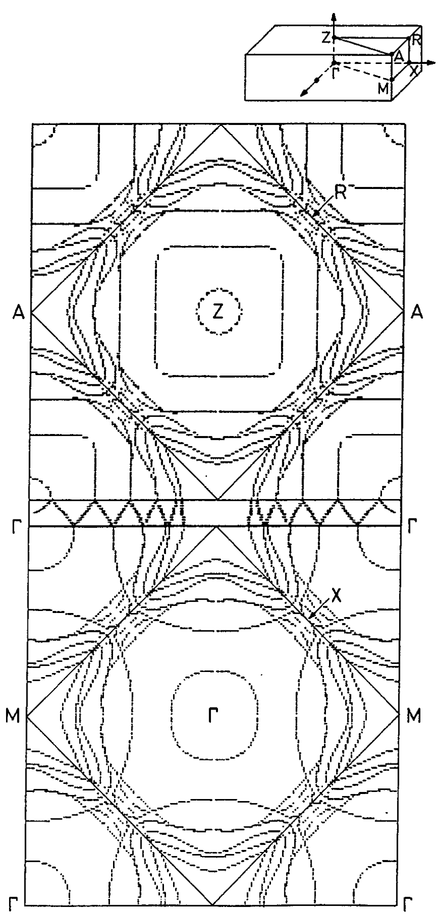

FIG. 4. Cross sections of the spin-up Fermi surface of a Cu_6Co_6 SL. The displayed cross sections correspond to the major-symmetry planes of the Brillouin zone of the simple tetragonal lattice.

Figures 4 and 5 show FS cross sections in the major symmetry planes of the SL Brillouin zone for both spin-up and spin-down electrons, respectively. The extension of the *flat band* in k space is indicated in Fig. 5 as cross-hatched areas. It is approximately a cylinder of diameter ≈ 0.14 in ΓX units. In this region, the Fermi surface has 3D character. That is, for all the values of k bounded by the cylinder there are allowed SL states with the Fermi energy and equal orbital character and symmetry. Besides, the location of a *flat band* at the SL Fermi level depends only on the Co thickness. Thus, it occurs in both FM and AF coupled SLs [10]. The 3D region in the SL FS induces an increase of the DOS at E_F.

Figure 6 presents the spatially averaged total DOS at the Fermi level as a function of the Co number of layers. It illustrates the periodic enhancement of the number of Fermi states. Therefore, physical properties which depend either on the DOS at E_F or on its gradient, such as electron specific heat, magnetic susceptibility, thermoelectric power, or electrical conductivity, should oscillate with the Co thickness. In addition, the occurrence of Fermi states in a 3D k-space zone may drastically affect SL scattering mechanisms, in which selection rules and momentum conservation play an important role, such as, for example, the electron-phonon interaction.

The unique requirement for the development of a *flat band* at the SL Fermi surface is the existence of a narrow band close to E_F in the SL constituents [8]. This band

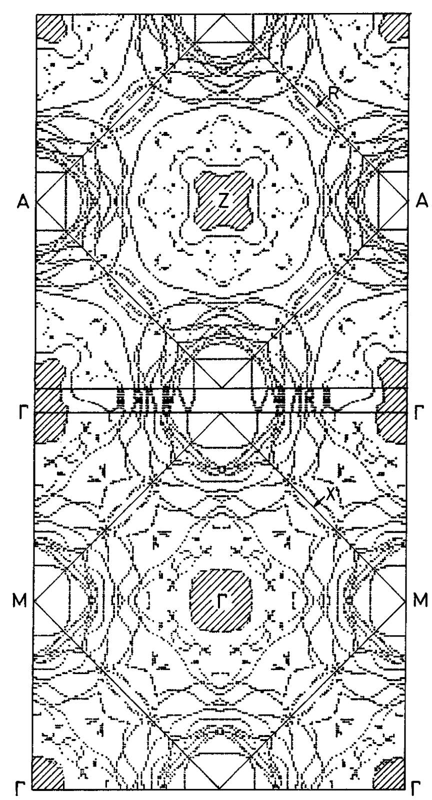

FIG. 5. Same as Fig. 4 for the spin-down Fermi surface.

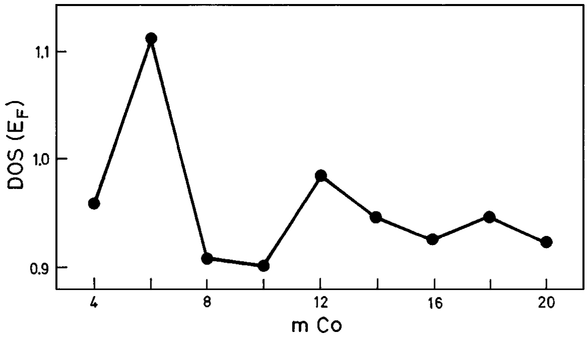

FIG. 6. Total density of states at the Fermi level for Cu_6Co_m SLs as a function of m.

has to be occupied in one of the SL component crystals and empty in the other. An appropriate election of the SL constituent thicknesses locates the SL *flat state* at E_F. The *flat-band* condition is also satisfied by minority-spin bands of Ni at L and majority-spin bands of Fe at H. Therefore, FS *flat bands* are expected in Ni and/or Fe SLs. Recently, oscillations of the GMR, saturation magnetoresistance, and magnetothermoelectric power have been reported in Fe/Cr, Co/Cu, and Co/Ni magnetic multilayers [6,11–13].

In addition to the 3D region discussed above, the SL Fermi surface presents a nested structure—see Figs. 4 and 5. It consists of concentric distorted conical sheets separated by minigaps. Analogously to the results obtained for the major symmetry directions (Fig. 2), nearly free sp sheets constitute the spin-up FS. They correspond to slightly distorted Cu and spin-up Co FS sheets [8] that, due to the SL supersymmetry, fold in the SL BZ. However, in the spin-down SL FS, strong hybridization between Cu sp-like and minority d-like Co bands occurs. Thus, the spin-down Fermi states have mixed sp-d character along the entire BZ. Furthermore, SL FSs present zones with a large density of sheets—see, for example, the Δ direction close to the X point on the spin-up FS, Fig. 4. In principle, these zones could be considered quasi-3D. However, there is a significant difference between these densely occupied zones and the *flat-band* 3D region discussed above. In the present case the sheets came from different bands, which cross the Fermi level at close values of k. Then, different sheets may have different orbital character, symmetry, and effective mass. Therefore, their effects on SL macroscopic properties are different.

In summary, we have demonstrated that for periodic values of the Co layer thickness Cu/Co SLs support *flat bands* at the Fermi level. They are caused by a SL mass-enhancement effect due to the interplay between sp-d hybridization and thickness dependence of SL energy bands. The location of a *flat band* at the Fermi level gives rise to an extended 3D region in the SL Fermi surface.

This work was supported by the Spanish Dirección General de Investigación Cientifica y Técnica under Grant PB93-1252.

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