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Magnetization of carbyne formed on $3d$ magnetics

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Within the scope of the adsorption approach to the description of epitaxial layer electronic structures, analytical expressions for magnetization of cumulene and polyyne formed on magnetic substrates have been obtained. To describe the densities of states of Fe, Co and Ni subbands, Friedels model were used. It has been shown that the spin moment of carbon adatom is proportional to the spin shift between σ-subbands.

Keywords: cumulene, polyyne, occupation number, magnetic moment.

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Once the graphene research area has emerged, there has increased interest in one-dimensional carbon structures (see [1–6]), or carbynes, which are carbon chains existing in two modifications: metallic cumulene with double bonds and semiconducting polyyne with alternating single and triple bonds. By now, researches managed to synthesize sufficiently long carbyne chains on various substrates [2,3] (see also [7,8]). Along with the known ability of atoms adsorbed on the grooved transition-metal faces to form one-dimensional structures [9], this fact prompted one of the authors to consider the possibility of forming carbynes on non-magnetic transition-metal substrates [10]. In this study, $3d$-magnetics Fe, Co and Ni were chosen as substrates; the main task was to determine the magnitudes of carbyne spin moments induced by the substrates (proximity effect). Here we propose a simple model for the proximity effect, which is not associated with a specific crystallographic structure of the interface and enables obtaining analytical solutions.

Using the Green functions for free cumulene (polyyne)

$$G^{-1}_{cum(pol)}(\omega, k) = \omega - \varepsilon_{cum(pol)}(k) + i0^{+}, \qquad (1)$$

where ω is the energy, $\varepsilon_{cum(pol)}(k)$ is the electron dispersion law for cumulene (polyyne), k is the wave vector [4], we have easily obtained their energy density of states

$$\rho_{cum}(\omega) = \begin{cases} 1/\pi\sqrt{4t^2 - \omega^2}, & \omega^2 \leqslant 4t^2, \\ 0, \ \omega^2 > 4t^2, & \end{cases}$$

$$\rho_{pol}(\omega) = \begin{cases} |\omega|/\pi\sqrt{(4t^2 - \omega^2)(\omega^2 - \Delta t^2)}, \ \Delta t^2 \leqslant \omega^2 \leqslant 4t^2, \\ 0, \ \omega^2 < \Delta t^2, \ \omega^2 > 4t^2. \end{cases} \qquad (2)$$

Here t is the energy of electron hopping between the nearest neighbors in cumulene and the arithmetic mean of hopping energies (for the single and triple bonds) in polyyne, $\Delta t = \Delta_{pol}/2$, where Δ_{pol} is the energy gap in the polyyne spectrum. As per estimates made in [4], $\Delta_{pol} \approx 0.32$ eV at $t \approx 3$ eV. Note that (2) presents an exact expression for the polyyne density of states derived in [11,12] according to the SSH-model (Su–Schrieffer–Heeger) that accounts for the difference in the matrix elements of the electron transition between neighbors with triple and single bonds but ignores the difference in the bond lengths; in [4], both of these factors are taken into account, but the density of states is represented by an approximate expression (anzats).

According to the adsorption approach to describing epitaxial monolayers [13], obtain from the Dyson equation Green functions of epitaxial carbynes (epicarbynes)

$$[\tilde{G}^{\sigma}_{cum(pol)}(\omega, k)]^{-1} = G^{-1}_{cum(pol)}(\omega, k) - \Sigma^{\sigma}(\omega),$$

where $\Sigma^{\sigma}(\omega)$ is the self-energy part describing the substrate influence on the carbyne electron states, σ is the spin index [4,10,13,14]. As a model for the magnetic $3d$-substrate density of states $\rho^{\sigma}_{d}(\omega)$ necessary for calculating $\Sigma^{\sigma}(\omega)$, the Friedel pedestal-type model [15] was used:

$$\rho^{\sigma}_{d}(\omega) = \begin{cases} 5/W_d, & |\Omega_\sigma| \leqslant W_d/2, \\ 0, & |\Omega_\sigma| > W_d/2. \end{cases} \qquad (3)$$

Here W_d is the d-band width, $\Omega_\sigma = \omega - \omega_{0\sigma}$, $\omega_{0\sigma}$ is the energy of the σ-subband center. Assuming that

$$\Sigma^{\sigma}(\omega) = \Lambda^{\sigma}(\omega) - i\Gamma^{\sigma}(\omega),$$

obtain the functions of the substrate states' broadening and shift which are defined, respectively, as

$$\Gamma^{\sigma}(\omega) \equiv \Gamma = 5\pi V^2/W_d \quad \text{at} \quad |\Omega_\sigma| \leqslant W_d/2,$$

$$\Gamma^{\sigma}(\omega) = 0 \quad \text{at} \quad |\Omega_\sigma| > W_d/2,$$

$$\Lambda^{\sigma}(\omega) = (\Gamma/\pi)\ln|(2\Omega_\sigma + W_d)/(2\Omega_\sigma - W_d)|,$$

where V is the effective matrix element of the carbyne–substrate bond. Functions $\rho^{\sigma}_{d}(\omega)$ and $\Lambda^{\sigma}(\omega)$ are schematically shown in Fig. 1.

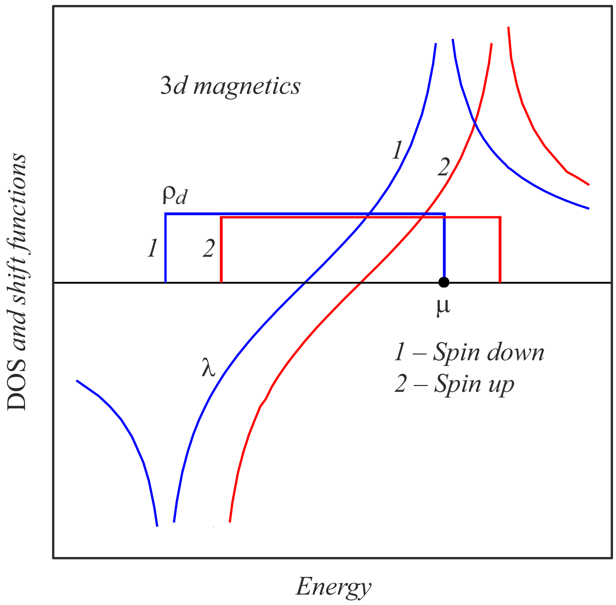

Figure 1. Dimensionless state densities of σ-subbands $\rho_d \equiv 2\pi t \rho_d^\sigma$ and corresponding dimensionless shift functions $\lambda \equiv \pi\Lambda^\sigma/\Gamma$ for cumulene. *1* — spin-down states, *2* — spin-up states, μ — chemical potential.

As the substrates, consider Fe, Co and Ni whose d-band widths W_d calculated in [16] with neglecting the spin are presented in the Table. Then, rounding off (for simplicity) the $d\sigma$-subband occupation numbers [17], assume that the $\downarrow$-subband is completely occupied for all the three metals, i. e. $N_{d\downarrow} = 5$, while $N_{d\uparrow} = 2$, 3 and 4 for Fe, Co and Ni, respectively. The d-band width per spin is $W_d^{(1)} = W_d/5$, while the resulting d-band width is $W_d^{(\sigma)} = W_d + W_d^{(1)}(10 - N_\downarrow - N_\uparrow)$ if the shift of the spin-down and spin-up subbands is taken into account; this relation gives the values given in the Table. The found $W_d^{(\sigma)}$ values agree with experimental bandwidths W_d^{exp} [8] significantly better than spinless W_d values. According to [18], iron work function φ_d is 4.67 and 4.81 eV for faces (100) and (111), respectively; that for the cobalt polycrystal is $\varphi_d = 4.41$ eV, that for the nickel polycrystal is $\varphi_d = 4.5$ eV. Since this study was aimed at obtaining high-quality results, let us set in further estimations the Fe, Co and Ni work functions to $\varphi_d = 4.5$ eV that is equal to expected carbyne work function φ_{car}. Then the conduction band bottom energy E_{bot} relative to the d-magnetics' chemical potential level is $E_{bot} = -W_d$ for all the substrates, while the conduction band top energy is $E_{top} = W_d^{(1)}(10 - N_\downarrow - N_\uparrow)$. Energy intervals of the $d\uparrow$-subbands are $(E_{bot}^\uparrow = -W_d^{(1)}N_\uparrow,\ E_{top}^\uparrow = W_d^{(1)}\ (5 - N_\uparrow))$; thus obtain (in eV): $(-1.92,\ 2.88)$ for Fe, $(-2.61,\ 1.74)$ for Co and $(-3.04,\ 0.76)$ for Ni. Then the energies of σ-subband centers are $\omega_{0\downarrow} = -2.5W_d^{(1)} = -W_d/2$ and $\omega_{0\uparrow} = W_d^{(1)}(2.5 - N_\uparrow)$; their numerical values are given in the Table. Note that the highest energy parameters in the problem under consideration are $2t \sim W_d^{(\sigma)} \sim 6$ eV, the lowest are $\Delta_{pol} \sim 0.3$ eV.

To continue, it is necessary to calculate the epicarbyne state densities

$$\tilde\rho^\sigma_{cum(pol)}(\omega) = -\pi^{-1}\mathrm{Im}\int\limits_{\mathrm{BZ}} \tilde G_{cum(pol)}(\omega, k)dk,$$

where integration is performed over the cumulene (polyyne) Brillouin zone. Occupation numbers of epicarbyne atoms at $T = 0$ are

$$\tilde n^\sigma_{cum(pol)} = \int\limits_{-\infty}^{\mu} \tilde\rho^\sigma_{cum(pol)}(\omega)d\omega,$$

$$\tilde n_{cum(pol)} = \sum_\sigma \tilde n^\sigma_{cum(pol)},$$

where μ is the chemical potential; now derive the substrate-induced spin moments of epicarbyne: $\tilde m_{cum(pol)} = \tilde n^\downarrow_{cum(pol)} - \tilde n^\uparrow_{cum(pol)}$.

Since the expressions for state density and occupation number cannot be obtained in the analytical form, we have to resort to simplifications. As the analysis [4] shows, in the limit of weak carbyne-to-substrate coupling when $\Gamma^2 \ll t^2$, the density of states and occupation number of epitaxial carbyne cumulene may be approximated by the following expressions:

$$\tilde\rho^\sigma_\pm(\omega) = \frac{1}{\pi}\frac{\Gamma}{(\omega - \omega^\sigma_\pm)^2 + \Gamma^2},\ \tilde n^\sigma_\pm = \frac{1}{\pi}\mathrm{arccot}\left(\frac{\omega^\sigma_\pm}{\Gamma}\right), \quad (4)$$

where energies $\omega^\sigma_\pm$ are the roots of equation $\omega - \Lambda^\sigma(\omega) = \pm 2t$ whose solution is graphically illustrated in Fig. 2 using the example of a single σ-subband: introduction of functions $F^\sigma_\pm(\omega) = \pi(\omega \mp 2t)/\Gamma$ allows reducing the problem to equations $F^\sigma_\pm(\omega) = \Lambda^\sigma(\omega)$ whose roots are determined by abscissas of points of intersection between inclined straight lines $F_\pm$ (Fig. 2) and curve λ (Figs. 1 and 2). Assuming that $\Gamma \ll \min\{|E^\sigma_{bot}|, |\omega_{0\sigma}|\}$As, obtain as a result $\omega^\sigma_\pm \approx \pm 2t$. Note that the case of $\Gamma^2 \gg t^2$ is not interesting, since in this limit carbyne disintegrates into a chain of weakly bound carbon adatoms.

In the case of polyyne, the arc cotangent argument in the expression for $\tilde n^\sigma_\pm$ is $(\omega^\sigma_\pm - \Delta_{pol}/2)/\Gamma$. Total occupation number of the carbyne adatom is $\tilde n = \sum_{\sigma, p=\mp} \tilde n^\sigma_p = 1$, since we have equated work functions of carbyne φ_{car} and substrates φ_d and, therewith, no charge transfer exists between them. The substrate-induced spin moment is $\tilde m = \sum_{p=\pm}(\tilde n^\downarrow_p - \tilde n^\uparrow_p)$, which gives for carbyne $|\tilde m| \sim \Gamma|\omega_{0\downarrow} - \omega_{0\uparrow}|/4t^2$.

Assuming that parameter Γ is approximately the same in all the cases, we can see that for the Fe–Co–Ni series the spin moment magnitude decreases as 1:0.9:0.3. Based on exact values of the σ-subband occupation numbers N_σ (see Table 2.2 in [18]), obtain 1:0.8:0.3. If $\Gamma = 1$ eV, obtain $|\tilde m| \approx 0.08$, 0.07 and 0.02 for Fe, Co and Ni, Band parameters of $3d$-magnetics (all the energy characteristics are given in eV)

Metal	W_d	$N_\downarrow, N_\uparrow$	$W_d^{(1)}$	$W_d^{(\sigma)}$	W_d^{exp}	$-E_{bot}, E_{top}$	$-E_{bot}^{\uparrow}, E_{top}^{\uparrow}$	$-\omega_{0\downarrow}, \omega_{0\uparrow}$
Fe	4.82	5, 2	0.96	7.71	8.5	4.82, 0	1.92, 2.88	2.41, 0.48
Co	4.35	5, 3	0.87	6.09	6.9	4.35, 0	2.61, 1.74	2.18, 0.43
Ni	3.78	5, 4	0.76	4.54	5.4	3.78, 0	3.04, 0.76	1.89, -1.12

Footnote. W_d is the theoretical d-band width without reference to spin, $N_\downarrow(N_\uparrow)$ is the number of electrons in the spin-down (up) subband, $W_d^{(1)}$ is the subband region width per spin, $W_d^{(\sigma)}$ is the theoretical d-band width with the reference to spin, W_d^{exp} is the experimental value of the d-band width, $E_{bot}(E_{top})$ is the bottom (top) boundary of the d-band with bandwith $W_d^{(\sigma)}$, $E_{bot}^{\uparrow}(E_{top}^{\uparrow})$ is the bottom (top) boundary of the spin-up subband, $\omega_{0\downarrow}(\omega_{0\uparrow})$ is the energy of the spin-down (up) subband center.

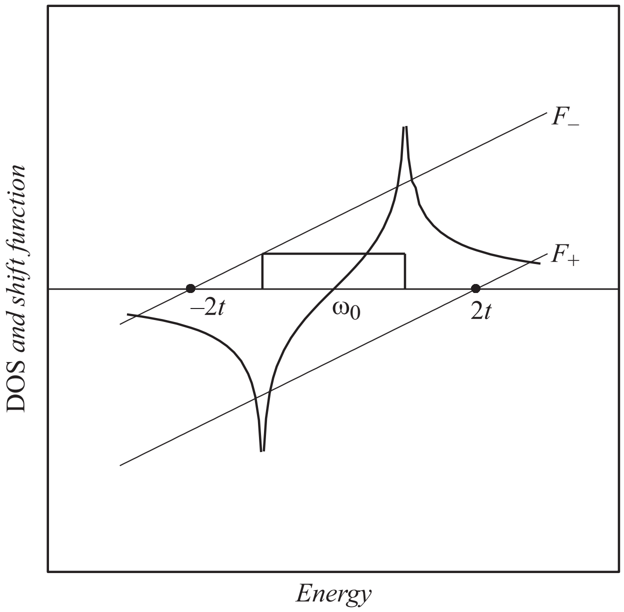

Figure 2. Illustration to the equation $F_\pm = \pi(\omega \mp 2t)/\Gamma$ solution.

respectively. Since $\Gamma = 5\pi V^2/W_d$ and, as shown in the Table, $5/W_d \sim 1\,\text{eV}^{-1}$, condition $\Gamma = 1\,\text{eV}$ reduces to $V \sim 1/\sqrt{\pi}\,\text{eV}$ or 0.5 eV. Note that theoretical evaluation of matrix element V is a rather complex task (see [19]).

The calculation scheme for epicarbyne induced magnetization used in this study (also valid for other epitaxial and encapsulated structures) is apparently the simplest one since it makes unnecessary the often-unavailable information on geometry of the contact between the magnetic and non-magnetic monolayer. The basic approximation technique used in this study is using ansatz for state density $\tilde{\rho}_\pm^\sigma(\omega)$. The model refinements that do not hinder obtaining analytical results are evident: this is accounting for parameter G dependence on spin, which may be performed using the data from Table 2.2 given in monograph [18]. However, such a procedure seems premature, since, as far as we know, the carbyne$-3d$-magnetic system has been studied rather poorly [20,21]. Paper [20] presents the results of DFT (Density Functional Theory) calculations of the structure and formation energy of carbynes formed on transition metals (e.g. Cu and Ni); however, there are considered short chains consisting of about ten atoms. Work [21] considered an ohmic contact between organic semiconductor (polyyne) and metal film (e.g. copper and nickel) used in device structures. Unfortunately, those papers do not contain data necessary for refining our models. In conclusion, emphasize that magnetized low-dimensional carbon structures are of interest for creating new thermoelectric devices [22–25] based on the Seebeck spin effect. Furthermore, the possibility of direct integration of one-dimensional magnetic nanostructures into electronic circuits is crucial to realizing their enormous potential as components of magnetic storage devices, logic devices, and other spintronic elements [26]. A unique feature of one-dimensional magnetism is its applicability in individual spin chains, which has become possible due to separation of the structures' magnetic chains by a distance sufficient for ensuring the minimal interaction between adjacent chains [27]; another opportunity is developing and manufacturing highly efficient materials able to absorb electromagnetic waves [28].

Conflict of interests

The authors declare that they have no conflict of interests.

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