Diamagnetism of two-dimensional graphite with quasilinear dispersion law

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The orbital susceptibility of two-dimensional graphite with a linear dispersion law is calculated. It is shown that this quantity is determined entirely by the band-band contribution of the filled-valence-band states excited by the magnetic field into the conduction band, and is inversely proportional to the state density on the Fermi level in the temperature-degenerate case. A quasilinear dispersion law with a forbidden gap $\sim 10^{-3}$ eV between the degenerate π bands is proposed for the description of the experimental temperature dependences of the diamagnetism. The obtained theoretical expressions describe satisfactorily the experimental data in the entire measurement-temperature range.

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1. INTRODUCTION

Graphites have the largest specific diamagnetism of all the presently known materials. Thus, the susceptibility of single-crystal graphite in the c-axis direction amounts to $\sim -30 \cdot 10^{-6}$ cgs emu/g at a temperature lower than 77 K.[1] There exist, however, "two-dimensional" graphite-like structures with a magnetic susceptibility greatly exceeding this value.[2,3] These "two-dimensional graphites" contain as their principal structural units graphite-like layers that hardly interact with one another; this makes it possible to describe the electronic structure of such materials by means of two-dimensional band models.[4]

An ideal graphite-like layer is, if spin-orbit interaction is disregarded, a gapless semiconductor with a linear dispersion law near the corners of the band[5,6]:

$$\varepsilon_{1,2}(\mathbf{k}) = \pm \hbar p_0 k/m, \tag{1}$$

where k is the distance in k-space from the corner of the band, p_0 is the constant of the band structure of the graphite,[6] and m is the mass of the free electron. The signs + and − pertain respectively to the conduction and valence bands.

In this paper we calculate the orbital susceptibility of a graphite-like layer, for the purpose of ascertaining the origin and the structure of the large diamagnetic contribution to the susceptibility of the two-dimensional graphites.

The present difficulties in the description the diamagnetism of two-dimensional graphite[7-9] in the entire range of measurement temperatures are due to one shortcoming: the orbital susceptibility is calculated there by using energy levels that were not corrected for the terms quadratic in the magnetic field H, whereas all the diamagnetic effects manifest themselves just in the second order in H.[10,11] In fact, a more correct use of the Euler-Maclaurin summation than in Refs. 8 and 9 leads only to a diamagnetism that oscillates about zero. At the same time, the oscillation mechanism proposed by McClure[7] for the description of the high-temperature contribution to the magnetic susceptibility does not operate below the degeneracy temperature.

2. ORBITAL SUSCEPTIBILITY OF TWO-DIMENSIONAL GRAPHITE WITH A LINEAR DISPERSION LAW

The orbital susceptibility χ_{orb} of two-dimensional graphite with a linear dispersion law (1) was calculated from the general expression proposed by Roth and Wannier[10,11] for the magnetic susceptibility of a system of noninteracting Bloch electrons in the limit of weak fields ($H \to 0$). Expanding the tensor products, we rewrite expression (103) of Ref. 10 for the case of a two-band structure (1) in the presence of an inversion center. In a magnetic field H directed along the z axis perpendicular to the plane of the layer we can write

$$\chi_{orb} = \chi_{LP} + \chi_{bb}, \tag{2}$$

where χ_{L-P} is the Landau-Peierls susceptibility:

$$\chi_{LP} = \frac{1}{12}\left(\frac{e}{\hbar c}\right)^2 \sum_{n,\mathbf{k}} \frac{\partial f_0(\varepsilon_n-\mu)}{\partial \varepsilon_n}\left[\frac{\partial^2\varepsilon_n}{\partial k_x^2}\frac{\partial^2\varepsilon_n}{\partial k_y^2} - \left(\frac{\partial^2\varepsilon_n}{\partial k_x \partial k_y}\right)^2\right], \tag{3}$$

and χ_{bb} is the band-band contribution made to the diamagnetism by the carriers belonging to the entire Fermi distribution:

$$\chi_{bb} = -\frac{1}{4}\left(\frac{e}{c}\right)^2 \sum_{n,\mathbf{k}} f_0(\varepsilon_n-\mu)\left\{\frac{(x_{nn'})^2+(y_{nn'})^2}{m} - \frac{1}{\hbar^2}\left[(x_{nn'})^2\frac{\partial^2\varepsilon_n}{\partial k_y^2} + (y_{nn'})^2\frac{\partial^2\varepsilon_n}{\partial k_x^2} - 2y_{nn'}x_{nn'}\frac{\partial^2\varepsilon_n}{\partial k_x \partial k_y}\right]\right\}. \tag{4}$$

Here $\varepsilon_n(k)$ is the dispersion law in the first band ($n=1$, 2):

$$f_0(\varepsilon-\mu) = \left[1+\exp\left(\frac{\varepsilon-\mu}{\Theta}\right)\right]^{-1}$$

is the Fermi-Dirac distribution function, μ is the chemical potential of the system of impurity carriers, and Θ is the temperature in energy units. The summation sign stands for summation over the band numbers n and integration over the coordinates of the continuous variable k in the first Brillouin zone. The matrix elements in (4) are written in the representation of the Bloch function of the single-electron problem.

To obtain (4) we have used the following properties of the Adams coordinate operators[11,10]:

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$$x^{\nu}_{nn'}=\frac{\hbar}{mi}\frac{p^{\nu}_{nn'}}{\varepsilon_n(\mathbf{k})-\varepsilon_{n'}(\mathbf{k})} \quad \text{at} \quad n\neq n',$$
$$x^{\nu}_{nn'}=0 \quad \text{at} \quad n=n', \tag{5}$$

where ν are the Cartesian indices ($\nu=x,y$), $p_{nn'}=\langle n,\mathbf{k}|p^{\nu}|n',\mathbf{k}\rangle$ is the band-band matrix element of the momentum operator p^{ν}, and $|n,\mathbf{k}\rangle=u_{n\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$ is the Bloch function of the nth band.

To determine the matrices $p^{\nu}_{nn'}$, we express the periodic parts of the Bloch waves $u_{n,k}$ in terms of the wave functions $u_{1,0}$ and $u_{2,0}$, which are degenerate at the corners of the band. From the secular equation for the energy levels (1) we obtain in the $\mathbf{k}\cdot\mathbf{p}$ approximation[6]

$$u_{n,\mathbf{k}}=2^{-1/2}(u_{1,0}\mp e^{-i\alpha}u_{2,0}). \tag{6}$$

The signs – and + pertain respectively to the electron and hole states, and α is the angular coordinate of the vector $\mathbf{k}$. The wave functions (6) lead in first order in $\mathbf{k}$ to the linear spectrum (1).

Inasmuch as symmetry yields[6]

$$\langle 1.0|p^{x}|2.0\rangle=ip_0, \quad \langle 1.0|p^{y}|2.0\rangle=-p_0,$$

we obtain the sought relations:

$$p_{12}{}^{x}=ip_0\cos\alpha, \quad p_{12}{}^{y}=-ip_0\sin\alpha. \tag{7}$$

Taking into account the spin degeneracy and the fact that a unit cell contains two carbon atoms, we obtain with the aid of (5) and (7), normalizing to unit mass,

$$\chi_{orb}\equiv\chi_{bb}=\chi_1+\chi_2, \tag{8}$$

$$\chi_1=A\int_0^{\varepsilon_0}\frac{d\varepsilon}{\varepsilon}\left[\frac{\partial f_0(\varepsilon-\mu)}{\partial\varepsilon}+\frac{\partial f_0(\varepsilon+\mu)}{\partial\varepsilon}\right], \tag{9}$$

$$\chi_2=-B\int_{-\varepsilon_0}^{\varepsilon_0}f_0(\varepsilon-\mu)\frac{\partial\varepsilon}{|\varepsilon|}, \tag{10}$$

where ε_0 corresponds to the point of cutoff of the linear spectrum in the first Brillouin zone,

$$A=\frac{3}{32\pi\rho}\frac{a^2}{c_L}\left(\frac{e}{\hbar c}\right)^2\gamma_0{}^2=0.35\cdot10^{-6}\frac{\text{cgs emu}}{g}\cdot\text{eV}, \tag{11}$$

$$B=\frac{1}{4\pi\rho c_L}\frac{e^2}{mc^2}=0.15\cdot10^{-6}\frac{\text{cgs emu}}{g}. \tag{12}$$

We have used here the structure parameters of two-dimensional graphite: $a=1.456$ Å; $\rho=2.22$ g/cm^3 is the graphite density; $c_L=6.80$ Å is double the $\gamma_0=2\hbar p_0/3^{1/2}ma\approx2.8$ eV (Ref. 4) is the parameter of the intralayer interaction.[5,6] In the case degenerate in the temperature ($\Theta=0$) we have

$$\chi_1=-A/|\mu_0|, \tag{13}$$

$$\chi_2=-B\int_{-\varepsilon_0}^{\mu_0}\frac{d\varepsilon}{\varepsilon}, \tag{14}$$

where μ_0 is the Fermi level of the system.

Writing down the single-particle Hamiltonian in the presence of a magnetic field in a symmetrical gauge:

$$\mathcal{H}=\mathcal{H}_0-\frac{eH}{2mc}L_z+\frac{e^2H^2}{8mc^2}(x^2+y^2), \tag{15}$$

where $\mathcal{H}_0$ is the Hamiltonian in the absence of a field and L_z is the electron orbital-momentum operator, we can determine the origin of the two terms in (8).

An analysis of the structure of the diamagnetic contribution shows that the component

$$\mathcal{H}_1=-\frac{eH}{2mc}L_z,$$

that describes the interaction of the magnetic field with the orbital momentum of the electron is responsible for the quantity χ_1, whereas the component χ_2 is determined by the term

$$\mathcal{H}_2=\frac{e^2H^2}{8mc^2}(x^2+y^2)$$

in (15). The physical cause of both diamagnetic contributions lies in the interband transitions induced by the magnetic field.[10-12]

A remarkable consequence of the linear character of the dispersion law is the vanishing of the Landau-Peierls susceptibility (3), meaning the diamagnetism in two-dimensional graphite is entirely of band-band origin.

Relations (9) and (10) do not make it possible to calculate the value of the magnetic susceptibility at finite temperature, owing to the non-integrable singularity at zero in the integrands. This is a formal consequence of the fact that the matrix elements (5) become infinite at the band degeneracy point $\varepsilon=0$. The physical reason is that the magnetic field is a strong enough perturbation to upset the band structure near the degeneracy point, so that relation (5) becomes invalid in the region $\varepsilon\approx0$. Almost degenerate states lead then to a strong field dependence of the magnetic susceptibility (of the form $H^{-1/2}$).

We shall get rid of this divergence by changing over from the energy spectrum (1) to a more realistic one.

3. ENERGY SPECTRUM AND DIAMAGNETISM OF TWO-DIMENSIONAL GRAPHITE WITH A QUASILINEAR DISPERSION LAW

The gapless state produced in two-dimensional graphite by the symmetry of the crystal lattice should be made to vanish by perturbations that lower the symmetry. In the absence of band-band interaction, the role of such a perturbation can be played by the spin-orbit coupling.[6,14] The perturbed spectrum of the two-dimensional layer can be written in sufficiently general form[15,16]

$$\varepsilon_{1,2}(\mathbf{k})=\delta\pm[\gamma^2+(\hbar p_0/m)^2k^2]^{1/2}, \tag{16}$$

where γ and δ are certain small (compared with $|\mu_0|$) energy constants.

Thus, perturbation of the linear energy spectrum (1) leads to a quasilinear dispersion law with a small forbidden gap $\Delta\varepsilon=2\gamma$ between the valence and conduction bands.

We shall not specify the parameter γ more concretely, and retain it as a phenomenological constant whose value, as will be shown below, can be obtained by compar-

ing the theoretical and experimental temperature dependences of the diamagnetic susceptibility of two-dimensional graphites.

Neglecting the influence of the small perturbation γ on the matrix elements (7), we rewrite (9) and (10) with allowance for (16) (the energy origin is shifted by an amount δ from the corner of the band):

$$\chi_1 = A\int_\tau^{\varepsilon_0} \frac{d\varepsilon}{\varepsilon}\left[\frac{\partial f_0(\varepsilon-\mu)}{\partial\varepsilon}+\frac{\partial f_0(\varepsilon+\mu)}{\partial\varepsilon}\right], \tag{17}$$

$$\chi_2 = -B\left[\ln\frac{\varepsilon_0}{\gamma}+\int_\tau^{\varepsilon_0}\frac{d\varepsilon}{\varepsilon}\left[f_0(\varepsilon-\mu)-f_0(\varepsilon+\mu)\right]\right]. \tag{18}$$

In the temperature-degeneracy region

$$\chi_2 = -B\cdot\begin{cases}\ln\dfrac{\varepsilon_0}{|\mu_0|} & \text{at } \mu_0\leqslant-\gamma\\ \ln\dfrac{\varepsilon_0}{\gamma}+\ln\dfrac{\mu_0}{\gamma} & \text{at } \mu_0\geqslant\gamma\end{cases}. \tag{19}$$

Inasmuch as at $|\mu_0|\ll\varepsilon_0$ the value of χ_2 depends little on the cutoff energy, and $\varepsilon_0\approx 1$ eV, we can estimate χ_2 as a function of the position of the Fermi level at $\gamma = 5\cdot 10^{-4}$ (see Sec. 4):

μ_0, eV:	−0.3	−0.1	−0.01	0	+0.01	+0.1	+0.3
$-\chi_2\cdot 10^6$, cgs emu/g	0.18	0.34	0.70	1.14	1.58	1.97	2.10

Whereas for sufficiently deep states in the valence band $[\mu_0 = -(0.1-0.3)$ eV$]$ χ_2 is located at the level χ_{at} of the atomic diamagnetism, χ_2 can noticeably exceed χ_{at} in the case when the Fermi level is close to the degeneracy point or in the conduction band. However, the weak dependence of χ_2 on the position of the Fermi level and on the temperature make this quantity pseudoatomic in character.

Thus the large absolute value of the diamagnetism of two-dimensional graphite in a direction perpendicular to the layer plane is determined almost completely by the value of χ_1.

4. TEMPERATURE DEPENDENCE OF THE DIAMAGNETIC SUSCEPTIBILITY OF TWO-DIMENSIONAL GRAPHITE. COMPARISON WITH EXPERIMENT

Taking into account the rapid decrease of the integrand of (17) at large ε, we write down for $|\mu_0|\ll\varepsilon_0$:

$$\chi(\Theta)\approx A\int_\tau^\infty\frac{d\varepsilon}{\varepsilon}\left[\frac{\partial f_0(\varepsilon-\mu)}{\partial\varepsilon}+\frac{\partial f_0(\varepsilon+\mu)}{\partial\varepsilon}\right]. \tag{20}$$

We shall need now the temperature dependence of the chemical potential μ. At $|\mu_0|\gg\gamma$ we obtain after elementary transformations, from the electroneutrality condition,

$$\beta^2+4\int_0^\beta\ln(1+e^{-x})\,dx=\beta_0^2, \tag{21}$$

where

$$\beta=|\mu|/\Theta,\quad \beta_0=|\mu_0|/\Theta.$$

This yields an equation for the determination of β:

$$\beta^2+\frac{\pi^2}{3}-4\sum_{n=1}^\infty(-1)^{n+1}\frac{e^{-n\beta}}{n^2}=\beta_0^2. \tag{22}$$

The series (22) converges rapidly, but at $\beta\leqslant 1$ it is convenient to use the following expansion in powers of β:

$$\beta\ln 16+\frac{1}{6}\beta^3-\frac{1}{240}\beta^5+\ldots=\beta_0^2. \tag{23}$$

The values of β at a given temperature Θ and at a given Fermi level μ_0 are determined by iteration from (22) or (23). Figure 1 shows the dependence of μ on Θ in dimensionless coordinates.

We consider now (20) at $|\mu_0|\gg\gamma$. The use of $\Theta/|\mu_0|$ at low temperatures and of γ/Θ at high ones as the small parameters of the problem enables to distinguish between the contributions made to the magnetic susceptibility by the different energy states in the band. In the dimensionless coordinates $x=\varepsilon/\Theta$ and β we have an asymptotic estimate as $\gamma/\Theta\to 0$:

$$\chi(\Theta)\approx-\frac{A}{\Theta}\left[-\frac{\ln(\gamma/\Theta)}{2\mathrm{ch}^2(\beta/2)}+\Phi(\beta)\right]+o\left(\frac{\gamma}{\Theta}\right), \tag{24}$$

where

$$\Phi(\beta)=\int_1^\infty\frac{dx}{4x}\left[\mathrm{ch}^{-2}\frac{x-\beta}{2}+\mathrm{ch}^{-2}\frac{x+\beta}{2}\right]. \tag{25}$$

The first term in (24) corresponds to the contribution from the states located in the immediate vicinity of the band-degeneracy point $\varepsilon\approx 0$ and having the highest susceptibility.

It should be noted that the asymptotic form (24) describes satisfactorily the temperature dependence of $\chi(\Theta)$ in the entire temperature interval: at $\gamma/\Theta\sim 1$, when the asymptotic estimate of the first term in (24) is incorrect, this term vanishes, corresponding to the absence of carriers near the point $\varepsilon=0$.

The function $\Phi(\beta)$ (Fig. 2) and the susceptibility of two-dimensional graphite take in different temperature intervals the following forms:

1) $\Theta\ll|\mu_0|$—degeneracy. We have

$$\Phi(\beta)\approx\frac{1}{\beta}\left(1+\frac{\pi^2}{3}\beta^{-2}+\ldots\right), \tag{26}$$

$$\chi_0=\chi(0)=-\frac{A}{|\mu_0|+\gamma}\approx-\frac{A}{|\mu_0|}. \tag{27}$$

2) $\Theta\geqslant|\mu_0|$. Here

$$\Phi(\beta)=\sum_{k=0}^\infty(-1)^k a_{2k+1}\frac{2}{(2k)!}\beta^k\approx 0.296+0.0307\beta^2-0.0052\beta^4+\ldots, \tag{28}$$

where

$$a_{2k+1}=\sum_{n=1}^\infty(-1)^{n+1}n^{2k+1}[-\mathrm{Ei}(-n)];$$

$-Ei(-n)$ is the integral exponential function,[17] and

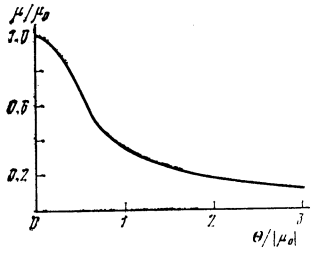

FIG. 1.

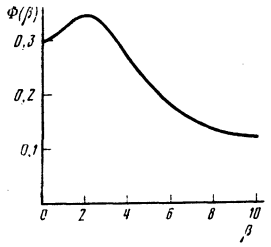

FIG. 2.

$$\chi(\Theta) \approx -\frac{A}{2\Theta}\left[-\ln\left(\frac{\gamma}{\Theta}\right)+0.59\right]. \quad (29)$$

The function (29) differs little from $1/\Theta$ and is not connected with the initial position of the Fermi level.

3) $\Theta \approx 0.5|\mu_0|$. A characteristic maximum of the diamagnetism is observed in this level. Its position practically coincides with the temperature Θ_m at which the relative fraction of the states with the maximum value of the susceptibility is maximal:

$$\Theta_m \approx 0.526|\mu_0|. \quad (30)$$

The amplitude of the maximum χ_m/χ_0 is determined only by the ratio $|\mu_0|/\gamma$ and depends little on μ_0:

$$\frac{\chi_m}{\chi_0} = \beta_{0m}\left[\frac{-\ln(\gamma/\Theta_m)}{2\,\mathrm{ch}^2(\beta_m/2)} + \Phi(\beta_m)\right] \approx 0.675 \ln\frac{\Theta_m}{\gamma} + 0.623. \quad (31)$$

Comparison of (31) with the experimental ratios χ_m/χ_0 makes it possible to estimate the parameter γ.

The theoretical relations (24) were compared with the experimental data of Marchand and Dupart,[18] who investigated the temperature dependence of the diamagnetism of boronized pyrocarbons in the temperature interval 77–1400 K. Pyrocarbons are homogeneous products obtained by precipitation of carbon from the gas phase when methane is thermally decomposed in vacuum. Alloying with boron makes it possible to vary the hole carriers. Experimental proof of the linear character of the state density of the impurity carriers in pyrocarbons with boron in a wide range of Fermi-level positions in the valence band (– 0.076 to 0.52 eV) is contained in a paper by one of us.[4] Thus, a pyrocarbon alloyed with boron can serve as a real approximation of two-dimensional graphite.

Figure 3 shows typical temperature dependences of the diamagnetic susceptibility for samples with different boron contents in the lattice.[16] The ordinates represent the differences of the principal values of the susceptibility, corresponding to the magnetic field directions perpendicular to the layer (χ_{33}) and along the layer (χ_{11}). The susceptibility χ_{11} along the layer amounts to $-(0.3-0.5)\cdot 10^{-6}$ cgs emu/g for all the materials investigated in Ref. 18, and is practically independent of temperature. This makes it possible to attribute χ_{11} to the atomic diamagnetism and the difference $\chi_{33}-\chi_{11}$ to the susceptibility of the π electrons.

The table lists the reduced results of the graphic material of Ref. 18. The experimental values of the constant A in Eq. (9) were estimated from (27) and (30):

$$A_{\exp} = 1.90|\chi_0|\Theta_m. \quad (32)$$

For comparison with experiment, the theoretical plots

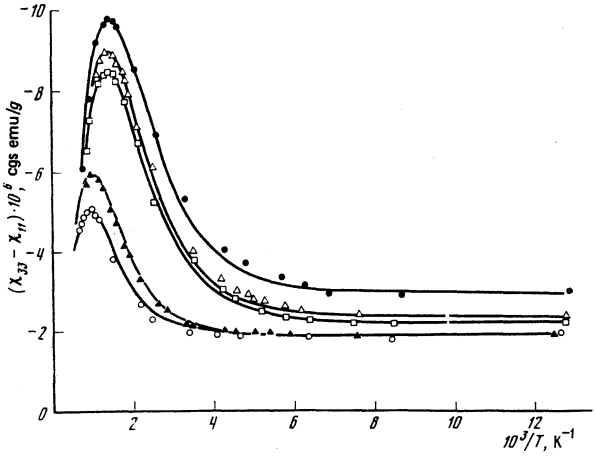

FIG. 3. Temperature dependence of the diamagnetic susceptibility of pyrocarbons with boron. The experimental data of Ref. 18 are represented by different symbols: ●—sample 40AS, △=40AP, □—56P, ▲—100P, and ○—150S. Solid lines—calculated curves for the parameters A and γ listed in the table.

of $\chi(\Theta)$ with the parameters A and γ from the table are shown in Fig. 3. The functional relation (24) describes satisfactorily the experimental curves in the entire temperature-measurement interval. It must be recognized in the analysis of the empirical constants A_{exp} and γ that the existing inhomogeneity of the distribution of the boron or of the intrinsic defect content in the lattices of the two-dimensional graphites should change the functional connections that follow from (27), (30), and (31). An elementary analysis shows that the inhomogeneity leads to a decrease of the empirical coefficient A_{exp} from (32) and of the ratio χ_m/χ_0 compared with the theoretical values (11) and (31).

Taking the last remark into account, we have estimated the mean value of γ to be $\sim 5\cdot 10^{-4}$ eV, which is close in order of magnitude to the splitting of the band degeneracy point $\varepsilon = 0$ on account of the spin-orbit interaction.[14] The estimate obtained by us for γ allows us to estimate roughly the theoretically attainable diamagnetism of two-dimensional graphite. It must be recognized here that in the case of the dispersion law (16) the Landau-Peierls diamagnetism differs from zero and reaches at $|\mu_0|/\gamma \sim 1$ values typical of the interband contribution χ_1. Taking this remark into account, χ_{max} is estimated at $\sim -400\cdot 10^{-6}$ cgs emu/g in the liquid-helium temperature region. We note that the maximum value of the diamagnetism corresponds to complete absence of carriers in the two-dimensional graphite.

TABLE I. Reduction of the experimental data of Ref. 18.

Sample no.	$A_{\exp}\cdot 10^6$, eV·cgs emu/g	χ_m/χ_0	$\gamma\cdot 10^4$, eV	Sample no.	$A_{\exp}\cdot 10^6$, eV·cgs emu/g	χ_m/χ_0	$\gamma\cdot 10^4$, eV
40bP	0.31	3.7	5.7	66S	0.24	4.2	2.8
40BS	0.29	3.7	6.5	100P	0.30	3.3	16.7
40AP	0.31	3.6	7.6	100S	0.28	3.6	12.4
40AS	0.26	4.0	4.0	150S	0.32	2.8	38.8
56P	0.24	4.0	3.6	160	0.46	3.3	21.5

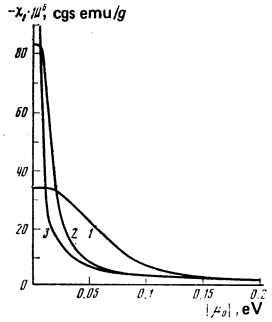

FIG. 4. Diamagnetic susceptibility of two-dimensional graphites as function of the position of the Fermi level ($\gamma = 5 \cdot 10^{-4}$ eV) at the temperatures 300 (1), 77 (2), and 4.2 K (3).

To attain such susceptibilities it is necessary to have defect-free graphite-like layers that do not interact with one another. Figure 4 shows plots of $\chi_1(\mu_0)$ calculated at $\gamma = 5 \cdot 10^{-4}$ eV at temperatures 300, 77, and 4.2 K. These make it possible to estimate the degree of perfection of the investigated graphites. The maximum attainable values of χ_1 are respectively $-31 \cdot 10^{-6}$ and $-84 \cdot 10^{-6}$ cgs emu/g at 300 and K, respectively.

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