Magnetic properties and electronic structure
of LaFeAsO$_{0.85}$F$_{0.1}$

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The magnetic properties of LaFeAsO$_{0.85}$F$_{0.1}$ compound were investigated by measurements of dc magnetization at different values of the magnetic field, $H = 0.02$, 1.0 and 2.0 T, in the temperature range 4.2–300 K. The superconducting behavior was found below 26 K, whereas a distinct peculiarity in the low-field dependence of the magnetic susceptibility $\chi(T)$ was clearly observed at $T_M \simeq 135$ K, which resembles a weak ferromagnetic (FM) response with saturation magnetic moment of about 10^{-4} μ_B per formula unit at 50 K. The transition at T_M is presumably not governed by magnetic impurities but rather correlated with the antiferromagnetic (AFM) transition in the undoped LaFeAsO compound at about the same temperature. We suggest, that observed magnetic properties of the LaFeAsO$_{0.85}$F$_{0.1}$ sample are due to an interplay of FM and AFM transitions, and presumably related to an intrinsic feature of a small portion of the undoped LaFeAsO phase inherent in our sample. In order to shed light on the problem of magnetic instability of the LaFeAsO, the *ab initio* DFT calculations of electronic structure and paramagnetic susceptibility were performed within the local spin density approximation. It is shown, that a V-shaped peculiarity in the density of electronic states in a close vicinity of the Fermi level can govern magnetic properties of LaFeAsO under fluorine doping and/or oxygen deficiency.

1. Introduction

The recent report on superconductivity with $T_c \simeq 26$ K in LaFeAsO$_{1-x}$F$_x$ [1] has opened a new class of the quarternary «1111» iron-based layered superconductors and stimulated intensive studies of their physical properties. A large increase of the superconducting transition temperature in LaFeAsO$_{1-x}$F$_x$ was later observed under high pressure (up to 43 K at $P \sim 4$ GPa [2]) and with substitution of rare earths for La (the highest $T_c \simeq 55$ K was reported for SmFeAsO$_{1-x}$F$_x$ [3]). The comprehensive reviews of experimental and theoretical reports on properties of the iron-pnictide superconductors were recently published (see, e.g., Refs. 4–7).

The parent undoped compound LaFeAsO is not superconducting, but shows a number of peculiarities of its physical properties (e.g., electrical resistivity, magnetic susceptibility, specific heat, etc. [1,8–10]), which are caused by a structural tetragonal–orthorhombic transition at $T_S \approx 160$ K and antiferromagnetic (AFM) spin ordering at $T_N \approx 140$ K [8,11–13]. Upon electron or hole doping with F substitution at the O site [1,9,10,12–14], or with oxygen vacancies [15–17] both transformations are suppressed and superconductivity emerges that suggests a relationship between magnetic (and structural) properties and superconductivity. The electron–phonon interaction is estimated to be small in the pure and F-doped LaFeAsO to provide the conventional superconductivity, and there is growing evidence that proximity to magnetic instability plays an essential role in the nature of superconductivity in these compounds [4–7]. It has been suggested that superconductivity

is driven by spin-fluctuations due to strong AFM [18,19] or FM [20] instability in LaFeAsO and related compounds.

However, a nature of the complex interplay between magnetism and superconductivity in RFeAsO is still not well characterized and understood. Also, the recent experimental data on behavior of magnetic susceptibility of «1111» systems in the normal state are still incomplete and contradicting [9,12,20,21]. Therefore, further studies of the magnetic and superconducting properties and their evolution with doping, pressure, temperature, etc. can help to elucidate a mechanism of the high-T_c superconductivity in the new class of the Fe-based superconductors.

In this contribution we report the experimental results on the magnetic susceptibility in the normal state for the superconductor LaFeAsO$_{0.85}$F$_{0.1}$, which is fluorine-doped but contains about 0.05 of vacancies in the oxygen sublattice. The present experimental study is supplemented by the *ab initio* DFT calculations of the electronic structure and magnetic susceptibility for a number of LaFeAsO based systems in the normal state within the local spin density approximation (LSDA). The aim of this investigation is to shed more light on the relation between the chemical composition, magnetic properties, and the interplay between superconductivity and magnetic instability in the «1111» systems.

2. Experimental details and results

Polycrystalline sample of LaFeAsO$_{0.85}$F$_{0.1}$ was prepared using a two-step solid state reaction technique, similar to that described in Ref. 22. The crystal structure and the composition were investigated by powder x-ray diffraction and wavelength-dispersive x-ray spectroscopy. The basic phase content was determined to be about 97%.

Magnetic properties of LaFeAsO$_{0.85}$F$_{0.1}$ were studied by an in-house SQUID magnetometer in the temperature range 4.2–300 K. The sample of mass ~ 0.3 g had the cylindrical form with diameter of 5 mm and height of 2.5 mm. The temperature dependence of the magnetic susceptibility $\chi(T)$ was measured under cooling to helium temperature in zero magnetic field (ZFC) followed by a slow heating with the rate of about 1.5 K/min at applied magnetic fields of $H = 0.02$, 1.0 and 2.0 T. The $\chi(T)$ dependence was also measured by cooling in the magnetic field $H = 0.02$ T (FC). As can be seen in Fig. 1, the studied sample shows the superconducting transition at temperature $T_c \simeq 26$ K, which is typical for the fluorine doped LaFeAsO systems.

For the normal state, the $\chi(T)$ dependence, measured in $H \geq 1$ T, appears to be relatively flat and roughly described by the mean value of $\chi_{av} \sim 5 \cdot 10^{-4}$ emu/mol. This value is comparable with the recently published data for magnetic susceptibility of the F-doped LaFeAsO at room temperature [9,20]. It should be noted, however, that the temperature dependencies of χ for the F-doped
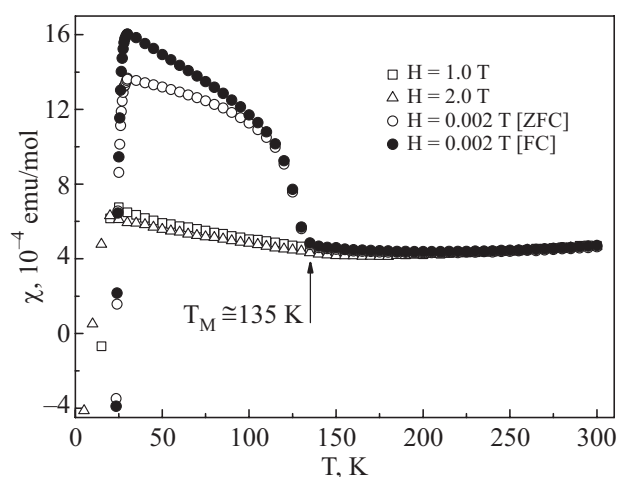

Fig. 1. Temperature dependencies of dc magnetic susceptibility of LaFeAsO$_{0.85}$F$_{0.1}$ at different magnetic fields: $H = 2$ T ($\triangle$); 1 T ($\square$); 0.02 T (ZFC — $\circ$, FC — $\bullet$).

LaFeAsO are essentially different between the above two reports. The data obtained in Ref. 20 provide an increasing χ with decreasing temperature, whereas that reported in Ref. 9 show a gradual decrease of χ with decreasing temperature, as in the undoped LaFeAsO compound. The latter $\chi(T)$ behavior is consistent with the temperature dependence of the ^{75}As-Knight shift in LaFeAsO:F [23], whereas the former dependence (increasing χ with decreasing temperature [20]) is considered to be due to impurity phases which amount to a few wt.% [12]. One can note an intermediate character of the relatively flat $\chi(T)$ dependence for our sample measured in high magnetic fields (see Fig. 1).

As is obvious from Fig. 1, the peculiar features of the low-field magnetic susceptibility of LaFeAsO$_{0.85}$F$_{0.1}$ is a clear cusp at $T \simeq 135$ K with a sharp rise of χ with cooling from $T_M \simeq 135$ K to $T_c \simeq 26$ K. Based on the mag-
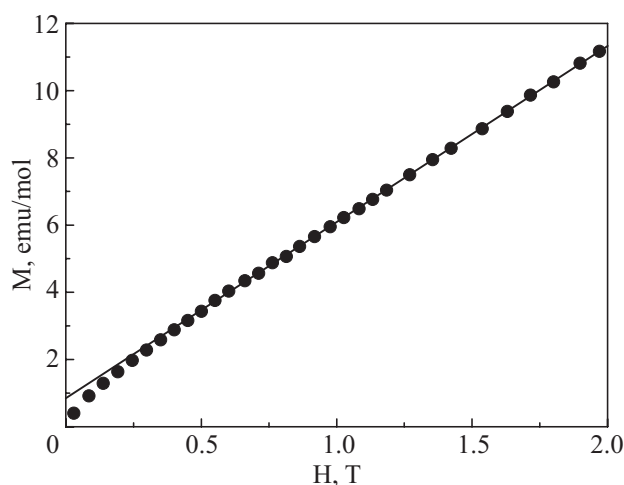

Fig. 2. Magnetization versus field for LaFeAsO$_{0.85}$F$_{0.1}$ at $T = 50$ K.

netization data in Fig. 2, we can assume the emergence of weak FM response at $T \leq T_M$. The corresponding saturation moment at $T = 50$ K amounts to approximately 1 emu/mol or $\sim 1.5 \cdot 10^{-4}$ μ_B/f.u., being about four orders of magnitude smaller than the magnetic moment at Fe site for the undoped LaFeAsO in the AFM state (~ 0.36 μ_B [11]). A similar nonlinear behavior of $M(H)$ in the low-field region, and the same order of the ferromagnetic moments were reported in Refs. 12, 21, that were considered to be caused by impurity phases. Typically, in the F-doped LaFeAsO samples one can expect the formation of such AFM iron-bearing secondary phases as FeAs, FeF$_2$ (both with $T_N \leq 78$ K) and Fe$_2$As ($T_N \sim 350$ K) [12,21, 24,25]. Consequently, the observed FM transition at $T_M \simeq 135$ K is presumably not affected by the above secondary magnetic phases. On the other hand, the FM transition evidently correlates with a point of the AFM transition in the undoped LaFeAsO compound [7,11].

3. Computational details and results

The undoped parent LaFeAsO compound, as well as the LaFeAsO$_{1-x}$F$_x$ and LaFeAsO$_{1-y}$ systems, possess the tetragonal ZrCuSiAs-type crystal structure (space group $P4/nmm$) [1,2]. With the c/a ratio close to 2.16, the tetragonal structure of LaFeAsO exhibits strong two-dimensional features. The crystal lattice is composed by alternating La–O and Fe–As triple-layer slabs, which are stacked along the c axis. Each iron (oxygen) layer is sandwiched between two nearest-neighbor As (La) atomic layers, which form edge-shared tetrahedrons around the iron (oxygen) sites. The positions of As or La sheets are fixed by internal parameters z_{As} and z_{La}, which define the inter-layer distances of Fe–As and La–O, respectively. It is suggested that there is partial ionic bonding between Fe–As and La–O layers, which is increased upon fluorine doping [4,6].

The previous *ab initio* calculations of the electronic structure of the «1111»-type iron-based oxypnictides were predominantly related to studies of the ground state AFM ordering in the undoped «1111» compounds (see [18,19,26–28] and references therein). In this paper the detailed calculations of the electronic structure are carried out for the paramagnetic phase of LaFeAsO based systems with the aim to study a paramagnetic response in an external magnetic field, and to shed more light on the nature of paramagnetism and interplay between superconductivity and magnetic instability in «1111» systems.

In the present *ab initio* calculations of the electronic structure we employed a full-potential all-electron relativistic linear muffin-tin orbital method (FP-LMTO, code RSPt [29,30]). No shape approximations were imposed on the charge density or potential, what is especially important for the anisotropic layered crystal structures. The exchange-correlation potential was treated in the LSDA [31] and generalized gradient (GGA, [32]) approximations of the density functional theory (DFT). The effect of the spin–orbit coupling, included in the Hamiltonian, appeared to be important for the precise calculations of atomic volume dependent density of states (DOS) at the Fermi level E_F. The FP-LMTO calculations were carried out for the LaFeAsO compound and also for LaFeAsO with oxygen replaced by virtual atoms with $Z = 7.9$ and $Z = = 8.1$ in order to simulate doping.

The calculations were performed for a number of lattice parameters a close to the experimental ones [1,5], with parameters c/a, z_{As} and z_{La} fixed to their experimental ambient pressure values. The total energies E were calculated as a function of volume V, and were fitted to the Murnaghan analytical parametrization for the equation of state [29]. Then the theoretical lattice spacings and the bulk moduli B were determined from calculated volume dependencies of the total energy $E(V)$ with both LSDA [31] and GGA [32] exchange-correlation potentials. The theoretical lattice parameter a appeared to be close to the experimental one [1,2,5] (about 1% smaller for the LSDA potential). The estimated bulk moduli of LaFeAsO, $B_{LSDA} \simeq 1.3$ Mbar and $B_{GGA} \simeq 1$ Mbar, are in agreement with the earlier reported theoretical value of $B_{theor} = = 0.98$ Mbar [33].

According to our calculations, in the vicinity of the Fermi level E_F the electronic structure of LaFeAsO is governed by a moderate hybridization of d (Fe) and p (As) states within the Fe–As layers. The Fe d states provide the dominant contribution to the density of states (DOS) $N(E)$ extending between –2 eV and 2 eV around $E_F = 0$, where the partial contributions of other states are substantially smaller. The p states of As are predominantly extended in the interstitial region, and there is no clear separation of the $3d$ states of Fe into the e_g and t_{2g} manifolds in the crystal field of As tetrahedron. In fact, a pseudogap at $\simeq 0.3$ eV above E_F corresponds to the occupation d^6 of Fe^{2+}. These calculated basic features of electronic structure and DOS(E) of LaFeAsO are in a qualitative agreement with results of earlier calculations [18,26,28].

As is seen in Fig. 3, in LaFeAsO the Fermi level E_F lies at the steep slope of $N(E)$, rapidly decreasing with energy. We found that E_F is located very close to the V-shaped local minimum of $N(E)$, which is also seen in Fig. 3. This V-shaped feature of DOS is related to a Fermi surface driven instability, reported in Refs. 18, 27, 28, which forces the undoped LaFeAsO into the stripe AFM state.

The calculated $N(E)$ for LaFeAsO with oxygen replaced by virtual atoms with $Z = 7.9$ and $Z = 8.1$ are also presented in Fig. 3. Within the virtual crystal approximation (VCA) the true atom in the phase is replaced by an «average» atom which is interpolated linearly in charge between the corresponding pure atoms. Hence, the VCA
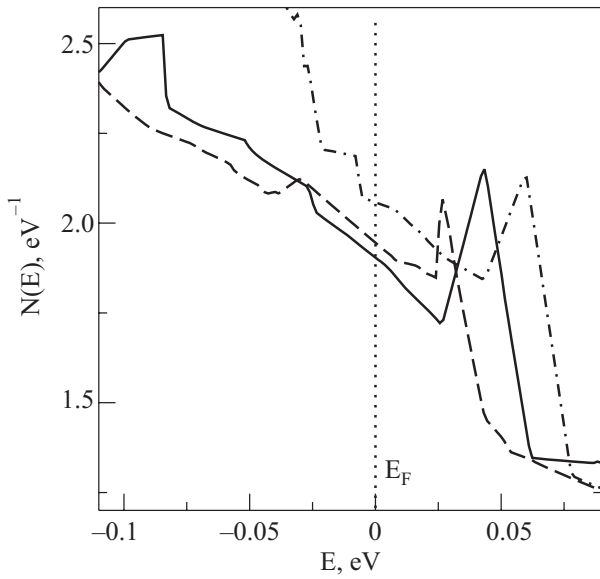
Fig. 3. LSDA density of states of the paramagnetic LaFeAsO around E_F for the undoped compound (solid line), and for LaFeAsO with oxygen replaced by virtual atoms with $Z = 7.9$ (dashed-doted line) and $Z = 8.1$ (dashed line). Calculations are performed with the fine energy mesh of 0.001 eV. The Fermi level position (at 0 eV) is marked by a vertical line.

calculations have taken into account the hybridization and band-filling effects, but neglected randomness and have not properly taken into account the charge transfer effect. The chosen approximation has an advantage due to its simplicity and hence we can be able to study small concentrations of F in the oxygen sublattice. The scattering effect of disorder is expected to be weak, since oxygen ions do not participate in the states at E_F. For all studied systems one can see a peculiar $N(E)$ behavior, with the V-shaped feature at the Fermi level. Also, the evaluated volume derivatives of $N(E_F)$ were found to be positive ($d\ln N(E_F)/d\ln V \simeq 0.9$ for the undoped LaFeAsO), and this suggests the reduction of $N(E_F)$ with pressure for the LaFeAsO$_{1-x}$F$_x$ systems.

Calculated magnetic properties

The FP-LMTO-LSDA calculations of the field-induced spin and orbital (Van Vleck) magnetic moments were carried out self-consistently within the procedure described in Ref. 30 by means of the Zeeman operator,

$$H_Z = \mu_B H (2\hat{s} + \hat{l}), \qquad (1)$$

which was incorporated in the original FP-LMTO Hamiltonian. Here H is the external magnetic field, $\hat{s}$ and $\hat{l}$ the spin and orbital angular momentum operators, respectively. The field induced spin and orbital magnetic moments were calculated in the external field of 10 T and

provided estimation of the related contributions to the magnetic susceptibility, χ_{spin} and χ_{orb}.

For the tetragonal crystal structure of LaFeAsO, the components of the paramagnetic contributions χ_{spin} and χ_{orb} were derived from the magnetic moments obtained in an external field, applied parallel and perpendicular to the c axis. The evaluated magnetic anisotropy, which is determined by the orbital contribution, $\Delta\chi_{orb} = \chi_{orb\|} - \chi_{orb\perp}$, was found to be negligible, in comparison with the dominant χ_{spin} contribution. The orbital Van Vleck contribution χ_{orb} itself is at least an order of magnitude smaller than the strongly enhanced spin susceptibility, and comes almost exclusively from the d states of Fe. For the theoretical LSDA equilibrium volume the contributions χ_{spin} and χ_{orb} are found to be equal to $5.45 \cdot 10^{-4}$ emu/mol and $0.46 \cdot 10^{-4}$ emu/mol, respectively. The Langevin diamagnetism of filled shells, $\chi_{dia} \simeq -0.54 \cdot 10^{-4}$ emu/mol, was estimated according to Ref. 35, and assumed to be close to a free-ionic diamagnetic susceptibility.

Due to the close proximity of the induced spin-polarized state to the spontaneous magnetic ordering for the experimental lattice parameters, the calculated total magnetic moment rises to $\simeq 0.2\mu_B$, which in fact is close to the experimentally observed magnetic moment of $0.36\mu_B$ at Fe site in the AFM state [11]. This is however not an induced magnetization, since it turns out that FM state with quite small moment is actually more stable than the paramagnetic solution. Actually, as it is seen in Fig. 4,
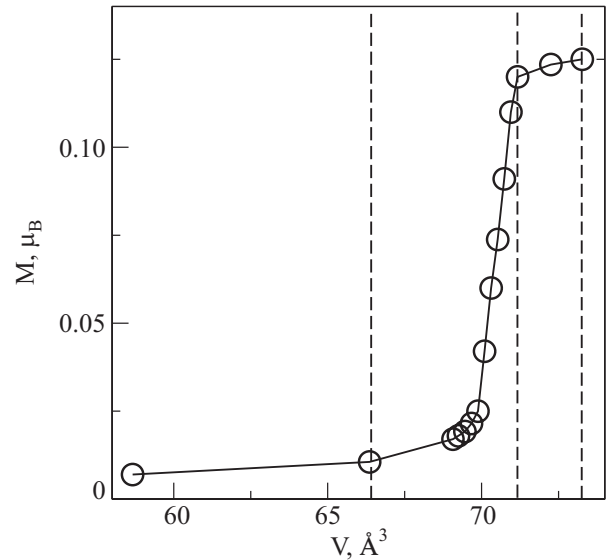

Fig. 4. Magnetic moment induced in the field $H = 10$ T as a function of volume with lattice parameters c/a, z_{As} and z_{La} fixed to their experimental ambient pressure values for undoped LaFeAsO. Dashed vertical lines denote the calculated LSDA equilibrium volume, the experimental volume and the calculated GGA equilibrium volume of LaFeAsO (from left to right).

the spontaneous spin polarization occurs in the field-induced calculations at lattice parameters above a_{LSDA}, whereas for $a \leq a_{LSDA}$ (approximately 2% lower than the experimental value), a paramagnetic response was obtained.

The enhanced Pauli spin contribution to the magnetic susceptibility was also calculated within the Stoner model:

$$\chi_{\text{ston}} = S\chi_P \equiv \mu_B^2 N(E_F)[1 - IN(E_F)]^{-1}, \qquad (2)$$

where $\chi_P = \mu_B^2 N(E_F)$, S is the Stoner enhancement factor, and μ_B the Bohr magneton. The multi-band Stoner integral I, representing the exchange-correlation interactions for conduction electrons and appropriate for compounds, can be expressed in terms of the calculated parameters of the electronic structure [34]:

$$I = 1 / N(E_F)^2 \sum_{qll'} N_{ql}(E_F) J_{qll'} N_{ql'}(E_F). \qquad (3)$$

Here $N(E_F)$ and $N_{ql}(E_F)$ are the total density of electronic states and site, q, and angular momentum, l, projected DOS at the Fermi level, respectively. The parameters of the exchange interaction $J_{qll'}$ are defined in terms of the intra-atomic exchange integrals:

$$J_{qll'} = \int g(\rho(r))\phi_{ql}(r)^2 \phi_{ql'}(r)^2 \, dr, \qquad (4)$$

and therefore depend upon the corresponding partial wave functions $\phi_l(r)$. Here $g(\rho(r))$ is a function of the electron density [31], l and l' are the corresponding angular-momentum quantum numbers.

The calculated value of the enhanced Pauli susceptibility ($\chi_{\text{ston}} \sim 5 \cdot 10^{-4}$ emu/mol for $a_{LSDA} \leq a \leq a_{\exp}$) is close to the field-induced evaluated χ_{spin} for the same range of lattice parameters. The Stoner criterion is nearly fulfilled for LaFeAsO, and the calculated susceptibility enhancement factor S appears to be about 8, which is comparable with the earlier estimation ($S \simeq 6$, [26]). This means nearness to a quantum critical point in the pure LaFeAsO compound and a possibility of competition between FM and AFM spin fluctuations.

4. Discussion

To our best knowledge, no clear anomalies were observed at $T \simeq 135$ K in $\chi(T)$ dependencies of the superconducting doped LaFeAsO$_{1-x}$F$_x$ systems, similar to that found in the present study (see Fig. 1). The disappearance of the static AFM order in the doped «1111» superconducting materials is widely reported [4–7], and it is believed to be favorable for the unconventional superconductivity [18,19].

One may speculate that the studied sample contains a fraction of the undoped (or weakly doped) parent phase, wherein a strong interplay of FM and different AFM spin

fluctuations can take place. Firstly, the Fe–As–Fe positions angle is larger than 90° and provides a possibility of AFM superexchange interaction (see, e.g., [36]) via the As p orbitals. Furthermore, a substantial direct Fe–Fe overlap in the Fe planes can yield an additional AFM exchange [26]. Finally, the calculated band structure indicates a possibility of the nesting-related AFM spin-density-wave type [18,19,28].

The calculated for $a \leq a_{LSDA}$ volume-dependent field-induced moments allow to describe the experimental susceptibility of LaFeAsO in the paramagnetic region at temperatures above 140 K. The LaFeAsO compound is found to be on the verge of magnetic instability. The proximity to a quantum critical point is clearly seen in Fig. 4, and this nearness results in strong FM spin fluctuations [26] and can provide a weak FM ordering in the doped phase of the LaFeAsO$_{0.85}$F$_{0.1}$ sample.

On the other hand, it seems probable that magnetization found at low temperatures is due to a weak ferromagnetism (or canted antiferromagnetism) of Dzyaloshinsky–Moriya (DM) type [37,38]. In this case the DM antisymmetric exchange interaction can provide incomplete cancellation of the magnetic moments at Fe sites for the AFM LaFeAsO phase. Also, a presence of defects in the iron sublattice, as well as crystal structure distortions, can not be ruled out. Then the environments of the Fe sites are different, and this can be assumed as another origin of the observed weak FM. It has been recently shown [39], that the combined effects of spin orbit coupling, lattice distortion, and p–d hybridization in tetrahedrally coordinated Fe in LaFeAsO can provide a highly anisotropic magnetic moment with an in-plane value of 0.25–0.35 μ_B per Fe with a small z projection $M_z \simeq 0.05\mu_B$. Curiously, the total moment of about $10^{-3} \mu_B$ was roughly estimated for the ground AFM state of LaFeAsO [12] from the calculated not fully equivalent densities of spin-up and spin-down electrons for 16-atom supercell. However, this result may be rather due to incomplete convergence of the DFT calculations of Ref. 12 for the AFM phase.

The present FP-LMTO calculations revealed a peculiar non-monotonous behavior of the density of states in the immediate vicinity of E_F. As seen in Fig. 3, for the undoped LaFeAsO the V-shaped minimum of $N(E)$ is followed by a local maximum of DOS, about 0.05 eV above E_F. Our calculations for LaFeAsO with oxygen replaced by virtual atoms with $Z = 7.9$ and $Z = 8.1$ also provided similar behavior of $N(E)$ (see Fig. 3). Obviously, the VCA calculations are unable to reproduce the relative positions of E_F and the fine $N(E)$ features with resolution better than 0.05 eV, which is basically the accuracy of LSDA calculations. However, one can expect that with the up-shifting of the Fermi level upon F doping in LaFeAsO$_{1-x}$F$_x$, the density of states $N(E_F)$ slightly bounces up due to the local DOS maximum, but then eventually descends down with increased fluorine con-

tent x. Note, that the local DOS peak in Fig. 3 can be «smeared» substantially due to the scattering effect of disorder.

We presume, that within the Stoner model (2) such $N(E_F, x)$ behavior can affect the spin paramagnetic susceptibility and can explain qualitatively the reported experimental $\chi(T)$ and $\chi(x)$ dependencies in LaFeAsO$_{1-x}$F$_x$ [9,12,20,21]. In particular, it has been shown in Ref. 12, that the paramagnetic susceptibility in the normal conducting state of LaFeAsO$_{1-x}$F$_x$ is enhanced with the F-doping, showing a maximum around F content of 5%. Also, within the Stoner model (2), the observed weak $\chi(T)$ behavior for LaFeAsO$_{0.85}$F$_{0.1}$ in the range 140–300 K (see Fig. 1) is qualitatively consistent with the calculated non-monotonous $N(E)$ dependence in Fig. 3, provided the E_F is varied slightly in the range about 0.05 eV, which is well within the accuracy of *ab initio* calculations.

A detailed theoretical study of $\chi(T)$ and $\chi(x)$ in LaFeAsO$_{1-x}$F$_x$ merits a separate examination beyond the scope of this study. It would obviously require a more rigorous calculation of $N(E)$ in the alloys, presumably employing CPA (coherent potential approximation) method. Also, the thermal expansion and spin fluctuation effects have to be taken into account. Finally, according to the present calculations, the density of states $N(E_F)$ in LaFeAsO$_{1-x}$F$_x$ is found to be decreasing with pressure, as well as the enhanced Pauli susceptibility.

5. Conclusions

Magnetic susceptibility of the LaFeAsO$_{0.85}$F$_{0.1}$ compound was investigated in the temperature range 4.2–300 K, and the superconducting transition is detected at 26 K. A clear cusp at $T_M \simeq 135$ K was observed in the low-field dependence of magnetic susceptibility $\chi(T)$ with a sharp rise of χ with further cooling to $T_c \simeq 26$ K. The obtained magnetization data $M(H)$ indicate the emergence of FM phase at $T \leq T_M$.

Ab initio calculations of the electronic structure and paramagnetic contributions to susceptibility of the parent LaFeAsO compound have revealed that this system is in close proximity to the quantum critical point. It is shown, that the paramagnetic susceptibility calculated in external magnetic field appears to be close to the experimental value. The Van Vleck contribution to χ comes mainly from d electrons of Fe and amounts up to 10% of total susceptibility.

The V-shaped minimum and local maximum are revealed in the density of electronic states in the immediate vicinity of the Fermi level, which can govern magnetic properties of LaFeAsO$_{0.85}$F$_{0.1}$ under fluorine doping and/or oxygen deficiency. Our calculations for LaFeAsO$_{1-x}$F$_x$ indicate, that the main role of pressure (and F-doping $x \gtrsim 0.1$) is to reduce the density of states at the Fermi level and to shift the «1111» system away from the FM instability. In general, the reported results point out that itinerant magnetism theory is relevant to describe magnetic properties of the LaFeAsO based systems.

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