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Proximity two bands Eliashberg theory of electrostatic field-effect-doping in a superconducting film of MgB_2.

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Abstract. A key aspect of field effect experiments is the possibility to induce charges on the first layers of a sample as a function of an applied gate voltage. It is therefore possible to study correlated phases of matter as a function of the induced charge density and the applied electric field. Moreover, resulting charge modulation along the direction of the applied electric field gives rise to junctions between perturbed and uneffected regions of the sample. In the framework of proximity effect Eliashberg theory, we investigate the consequence of an applied static electric field on the transition temperature of a two-band s-wave superconductor magnesium diboride. In most cases the only free parameter in the theory is the penetration depth of the applied electric field, whereas there is no freedom when the static perturbation is sufficiently weak. We come to the conclusion that the optimal way to enhance the critical temperature is to have a very thin film of magnesium diboride, otherwise the external electric field would not have substantial effect on superconductivity in this material.

PACS numbers: 74.45.+c, 74.62.-c,74.20.Fg

keywords: Field effect, Proximity effect, Eliashberg equations, Multiband superconductivity

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1. INTRODUCTION

The superconducting properties of magnesium diboride were discovered in 2001 [1] and early it was clear that this material is a standard phononic superconductor but with two conduction bands [2](σ and π) and a high critical temperature ($T_c = 39.4$ K). In a relatively short time all the physical properties of this material have been measured and well explained in the framework of two-band Eliashberg theory where the phonons are the superconductive glue [3]. It would be interesting to study how the modulation of the charge density would affect the properties of a multiband superconductor. This can be done with the aid of a field effect geometry characterized by a metallic gate, a dielectric (solid or liquid) and the material under examination. Through the application of a gate voltage it is possible to induce a pure charge doping on the first layers of the sample, without the inclusion of external dopants. To date there are several superconductors that show this feature such as iron compounds [4, 5] but only for the magnesium diboride we have the certainty of the mechanism that causes superconductivity [2, 6] and we know well the parameters that characterize the material in the way that we have no free parameters in the theory. The possibility to modulate the normal and superconductive properties of various materials by application of an electrostatic field has attracted much interest since many years. The first experiment was in the 1960 [7]. This technique has allowed enhancing the critical temperature of some superconductors [7, 8, 9], inducing metallic behavior in insulators [10] or even a superconducting phase transition in materials like $SrTiO_3$ [11]. Variations of the transport properties were observed also in the noble metals [12].

2. MODEL: PROXIMITY ELIASHBERG EQUATIONS

The objective of this study was to investigate the effect of an electrostatic field on sufficiently thick samples of magnesium diboride. Indeed, we consider a thickness larger than the electrostatic screening length in order to highlight the strong dependence of electronic properties along the z direction (i.e. the direction perpendicular to the sample surface). A similar situation was examined in the past [13] where a one-band s-wave superconductor, lead, was chosen as a case study. In that work, the spatial dependence of electronic properties along the direction of the applied electric field was modeled as the parallel of a surface layer and an unperturbed bulk. The first one is the part of material which is affected by the applied electric field, while the latter is considered uninfluenced. The two electronic systems were allowed to couple via superconducting proximity effect, resulting in a non-trivial response to the applied electric field that doesn't simply involve an adjustment of the superconducting properties of the surface layer alone [14] and strongly depends on both electrostatic screening length and total thickness of the film. Indeed, if we closely look at the superconductor/normal-metal interface, superconducting proximity effect involves both the opening of a finite energy gap in the normal metal and a reduction of the gap in the superconductor in a narrow

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region near the interface. The junction, composed by the surface layer (labelled by s) and the bulk (labelled by b), is depicted in figure 1. Due to field effect, charge is induced in the first atomic layers of the slab ($T_c = T_{c,s}$) while the underlying bulk remains unaffected ($T_c = T_{c,b}$). In a temperature range delimited by $T_{c,s}$ and $T_{c,b}$, the sample subjected to the electric field will behave as a superconductor/normal-material junction. By incrementing (decrementing) the magnitude of the applied electric field, the surface layer will be the superconductor (normal metal) and the bulk will be the normal metal (superconductor). In the present study we extend previous work on one-band s-wave superconductor, lead, to a two-band s-wave superconductor, magnesium diboride, in presence of an electric field. In order to do so we compute the superconductive critical temperature of the system exploiting the two-bands (1,2) s-wave Eliashberg equations with proximity effect [15, 16]. It is necessary here to clarify that this approach is used in the present case for magnesium diboride, nevertheless the theory is general. The theory consists in eight coupled equations for the gaps $\Delta_{j,\alpha}(i\omega_n)$ and the renormalization functions $Z_{j,\alpha}(i\omega_n)$ (with $j,k = 1,2$ and $\alpha = b,s$), where ω_n are the Matsubara frequencies. The imaginary-axis Eliashberg equations with proximity effect [17, 18, 19, 20, 21] are:

$$\omega_n Z_{j,\alpha}(i\omega_n) = \omega_n + \pi T \sum_{k,m} \Lambda^Z_{jk,\alpha}(i\omega_n, i\omega_m) N^Z_{j,\alpha}(i\omega_m) + \\ + \Gamma_{\mathrm{k},\alpha} N^Z_{k,\alpha}(i\omega_n) \tag{1}$$

$$Z_{j,\alpha}(i\omega_n)\Delta_{j,\alpha}(i\omega_n) = \pi T \sum_{k,m} [\Lambda^\Delta_{jk,\alpha}(i\omega_n, i\omega_m) - \mu^*_{jk,\alpha}(\omega_c) \times \\ \times \Theta(\omega_c - |\omega_m|)] N^\Delta_{k,\alpha}(i\omega_m) + \Gamma_{\mathrm{k},\alpha} N^\Delta_{k,\alpha}(i\omega_n) \tag{2}$$

where $\alpha^2_{jk,\alpha}F(\Omega)$ are the eight electron-phonon spectral functions, $\mu^*_{jk,\alpha}$ are the Coulomb pseudopotentials in the surface and in the bulk respectively, Θ is the Heaviside function and ω_c is a cutoff energy. In particular:

$$\Lambda_{jk,\alpha}(i\omega_n, i\omega_m) = 2\int_0^{+\infty} d\Omega \Omega \alpha^2_{jk,\alpha} F(\Omega)/[(\omega_n - \omega_m)^2 + \Omega^2] \tag{3}$$

$$\Gamma_{k,s(b)} = \pi |t|^2 A d_{b(s)} N_{k,b(s)}(0) \tag{4}$$

and, consequently, $\frac{\Gamma_{j,s(b)}}{\Gamma_{k,s(b)}} = \frac{N_{j,b(s)}(0)}{N_{k,b(s)}(0)}$,

$$N^\Delta_{j,\alpha}(i\omega_m) = \Delta_{j,\alpha}(i\omega_m)/\sqrt{\omega_m^2 + \Delta^2_{j,\alpha}(i\omega_m)} \tag{5}$$

and

$$N^Z_{j,\alpha}(i\omega_m) = \omega_m/\sqrt{\omega_m^2 + \Delta^2_{j,\alpha}(i\omega_m)} \tag{6}$$

$|t|^2$ is the transmission matrix equal to one in our case because the material is the same, d_s and d_b are the surface and bulk layer thicknesses respectively, such that ($d_s + d_b = d$ where d is the total film thickness), A is the junction cross-sectional area and $N_{j,s(b)}(0)$ are the densities of states for the j-th band at the Fermi level for the surface and bulk

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material. The value of $\Gamma_{k,s(b)}$ is independent from the junction area A: indeed it is possible to write $\Gamma_{k,s(b)}$ also in another way where A does not appear [17] but would introduce quantities that cannot be known a priori and which would require further approximations. Therefore we stick to the first way of writing $\Gamma_{k,s(b)}$. In order to show this property, we have verified that the variation of T_c is independent from the junction area A for a wide range of values ($10^{-10}m^2 \leq A \leq 10^{-5}m^2$).

The Coulomb pseudopotential, calculated for the magnesium diboride, for the first time in Ref. [3] is, in the bulk,

$$\mu^*_{jk,\alpha} = \mu_0[N_{1,\alpha}(0) + N_{2,\alpha}(0)] \begin{pmatrix} 2.23/N_{1,\alpha}(0) & 1/N_{1,\alpha}(0) \\ 1/N_{2,\alpha}(0) & 2.48/N_{2,\alpha}(0) \end{pmatrix} \tag{7}$$

where α is b or s. The value of the Coulomb pseudopotential in the surface layer is connected, in principle, also with the shift of chemical potential but it was demonstrated that this effect can be neglected [13] so it depends just from the variation of the densities of states at the Fermi level. Assuming a cutoff energy $\omega_c = 290$ meV and a maximum energy $\omega_{max} = 300$ meV in the Eliashberg equations, we are thus able to determine the value of the prefactor μ_0 of Coulomb pseudopotential in order to obtain the exact critical temperature in the absence of an electric field ($T_c = 39.4$ K and $\mu_0 = 0.033281$) by solving the unpertutbed s-wave standard two-band Eliashberg equations. Finally the electron-phonon coupling constants are defined as

$$\lambda_{jk,\alpha} = 2\int_0^{+\infty} d\Omega \frac{\alpha^2_{jk,\alpha}F(\Omega)}{\Omega} \tag{8}$$

Typically, the bulk values of $\alpha^2_{jk,b}F(\Omega)$ are known and can be found in the literature [3]. We determine the surface electron phonon spectral functions by assuming, in first approximation [22], that $\alpha^2_{jk,s}F(\Omega) = \frac{N_{j,s}(0)}{N_{j,b}(0)}\alpha^2_{jk,b}F(\Omega)$. This approximation is not so rough because we want calculate the order of magnitude of critical temperature variation and we think that, for this goal, it is enough. This means that we neglect the effect on critical temperature of small changes in the shape of spectral function but we consider just a global property as the electron-phonon coupling constant: this is the same approximation for the calculation of critical temperature by analytical equations as McMillan formula [23]. Values of A and d are taken from experiments and in the present work calculations were performed with an area of $10^{-7}m^2$ while we considered two possible values of the total thickness, $d = 10$ and $d = 40$ nm. One of the limitations of this method is the exact value of the penetration depth d_s: indeed, in the case of very strong electric fields at the surface of a thin film, this parameter is in general difficult to estimate *a priori* [14]. Thus, we leave it as a free parameter of the model, and we perform our calculations for different reasonable values. At this point we have to calculate just the values of $N_{j,s}(0)$ with density functional theory.

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3. METHODS: CALCULUS OF DENSITIES OF STATES

Density of states of bulk MgB_2 were computed ab-initio by means of density functional theory. In order to do so we exploited the Quantum Espresso package [24], which relies on pseudopotentials and on the expansion of valence-electrons wave functions in terms of plane waves. We made use of a Perdew-Burke-Ernzerhof generalized gradient approximation [25] in order to model the exchange-correlation functional for both Mg and B, while the core-electrons contribution was approximated with norm-conserving pseudopotentials built according to Troullier-Martins scheme [26] for both atomic species. Valence-electron wave functions were expanded in a plane-wave basis up to an energy cutoff of 35 Ry. Brillouin zone integration was performed on a Monkhorst-Pack grid of $16x16x12$ k-points both for the neutral and doped systems, with a Methfessel-Paxton first-order smearing [27] of 0.025 Ry. In order to reach convergence of the self-consistent solution of Kohn-Sham equations, we fixed to 10^{-9} Ry the threshold for the total energy. Assuming that the induced charge density spreads uniformly inside the superconductive part of the sample, we doped the system using a jellium model, i.e. with a uniform distribution of charges compensated by a background of opposite sign. This assumption is justified for not too high values of the electric field to which the sample is subjected. The densities of states of π and σ bands ($N_\pi(0)$ and $N_\sigma(0)$) were then computed by projecting the total density of states over the interested orbitals. In figure 2 the dependence of the two DOS (bands σ and π) from the charge doping is shown.

4. RESULTS

In a single band superconductor the physical situation is very clear: the application of an electrostatic field can increase or decrease the normal density of states at the Fermi level $N(0)$. The T_c is a monotonic increasing function of the electron-phonon coupling constant λ which is proportional to $N(0)$ in the way that if $N(0)$ increases T_c increases [13]. In a multiband superconductor the situation is more complex because the effect of an electrostatic field can be different on different bands and T_c may depend more strongly on the density of states of a particular band rather than another one. In particular in magnesium diboride the effect of an electrostatic field is similar on the two densities of states as it is shown in figure 2 but the critical temperature depends very weakly from $\lambda_{\pi\pi}$ (i.e. $N_\pi(0)$) while it is very sensible to variations of $\lambda_{\sigma\sigma}$ (i.e. $N_\sigma(0)$). There are also the interband contributions $\lambda_{\sigma\pi}$ and $\lambda_{\pi\sigma}$ but in MgB_2 they are weak [28]. We can see in figure 3 that the variation of critical temperature increases when the film thickness decreases and the surface layer increases. The first is a property of the system that we can control while the second is connected with our physical system. In particular materials the Thomas-Fermi model could fail for strong electric field and the penetration length of the electric field could be larger than that computed according to the Thomas-Fermi limit [14, 29], so we do calculations also for this possibility. From figure 3 we can

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understand that the effect on T_c strongly depends on the thickness of the surface layer and increases with it but, this is a property of the material that we can not modify for standard electrostatic fields. Unfortunately, because in the normal state MgB_2 behaves like a good metal it is probable that the Thomas-Fermi approximation works, at least for applied fields that are not too intense, so the critical temperature's variations should be small. In figure 4 we can see in which way the variation of critical temperature depends from charge doping for five different film thicknesses with the value of the surface layer fixed at $d_s = 0.05$ nm $\approx d_{TF}$ where d_{TF} is the Thomas-Fermi penetration length. As expected, the variation decreases when we increase the film thickness. These theoretical predictions can be compared with future experimental data. We have seen that the effect of the induced charge density due to the applied electric field on the critical temperature is very small because the Thomas-Fermi penetration length is of the order of 0.5 $\AA$ but, in principle, could be possible that, for very intense applied electrostatic fields, the Thomas-Fermi approximation is no more valid and the thickness of the surface layer increases so that the variations of critical temparture could be larger.

5. CONCLUSIONS

The aim of the present research was to examine the effect of charge doping on magnesium diboride by means of field effect. Analysis was based on the framework of proximity s-wave Eliashberg theory extended to the case of a two-band superconductor, thus generalizing the method previously used in the case of a one-band s-wave superconductor. One of the more significant findings to emerge from this study is that it is possible to realize T_c enhancements by means of Electric Doble-Layer gating (EDL) [12, 14]. Indeed, with usual values of the charge doping induced by field effect, we observed a shift in the critical temperature of the order of ~ 0.1 K in thin films of a standard phonon superconductor with a thickness ~ 10 nm.

6. ACKNOWLEDGMENTS

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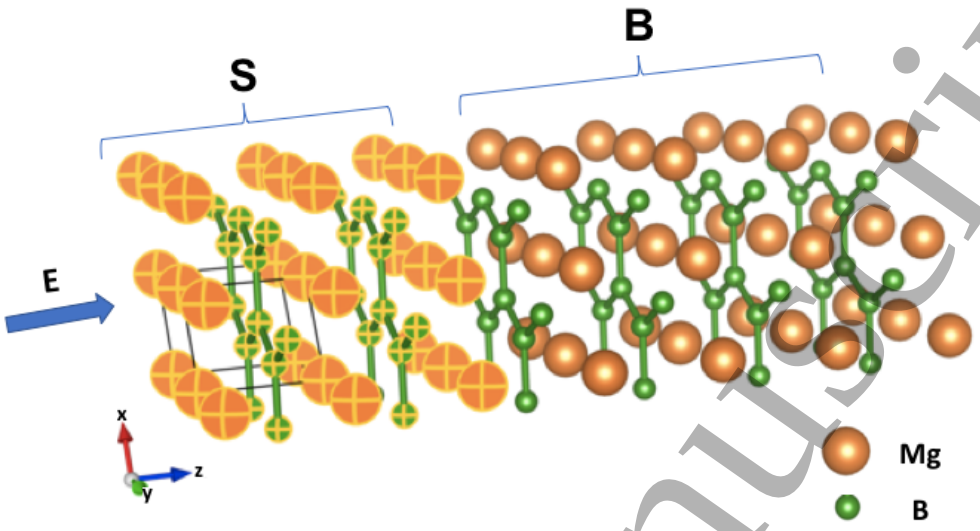

Figure 1. (Color online) Schematic view of magnesium diboride junction. S (B) is the label for the surface (bulk). E indicates the electric field directed perpendicularly to the sample surface.

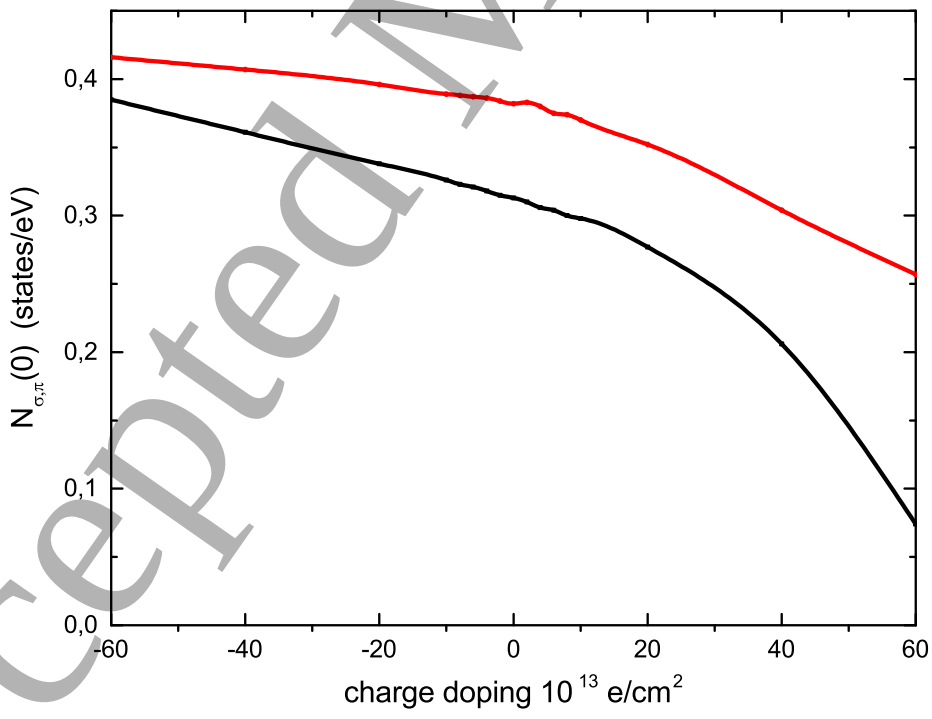

Figure 2. (Color online) Calculated densities of states $N_\sigma(0)$ (black solid line $states/eV$) and $N_\pi(0)$ (red solid line $states/eV$) at the Fermi level for different charge doping (e/cm^2).

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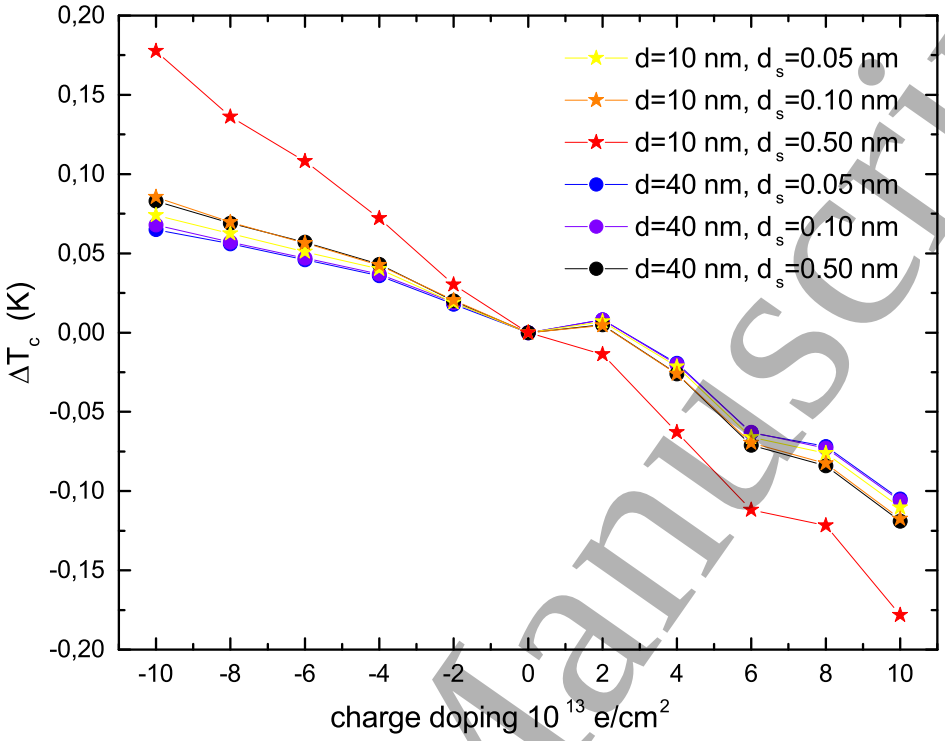

Figure 3. (Color online) Calculated variation of critical temperature (K) versus charge doping (e/cm^2) for two different values of film thickness $d = 10$ nm (pink with solid line, orange with dash line, red with point line stars) and $d = 40$ nm (dark blue with solid line, violet with dash line and black with point line circles) with surface layer thickness $d_s = 0.05$ nm $\approx d_{TF}$, $d_s = 0.1$ nm and $d_s = 0.5$ nm.

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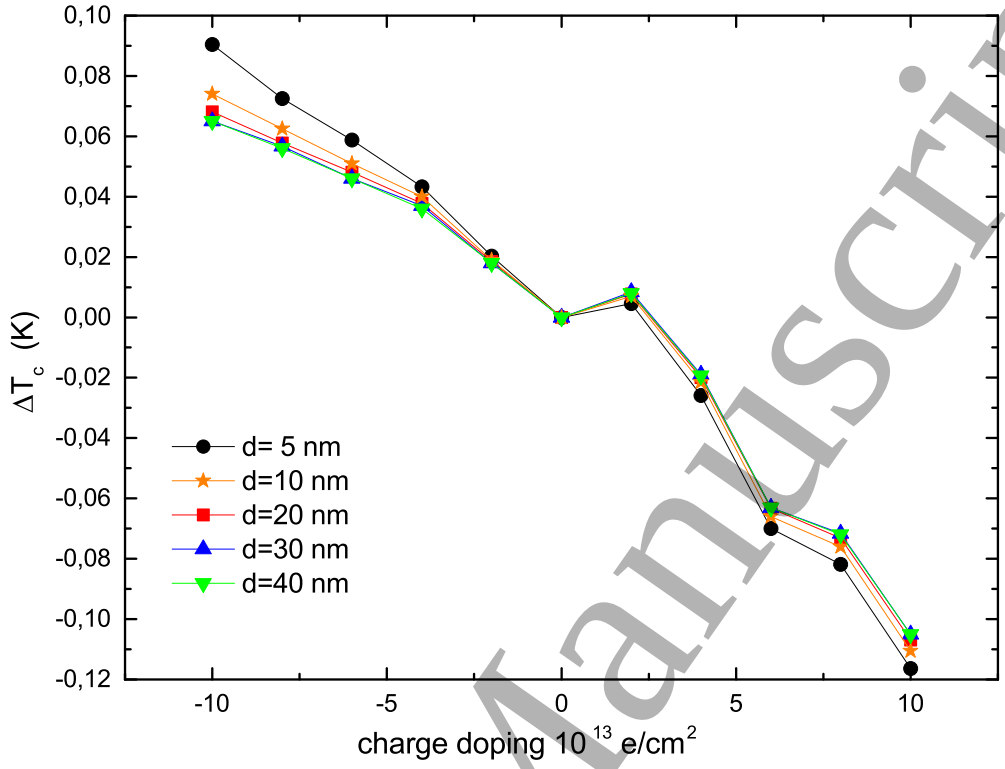

Figure 4. (Color online) Calculated variation of critical temperature (K) versus charge doping (e/cm^2) for six different values of film thickness $d = 5, 10, 20, 30, 40$ nm (black circles, orange stars, red squares, blue up triangles and green down triangle with surface layer thickness $d_s = 0.05$ nm $\approx d_{TF}$.

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