1. Introduction

CrO$_2$ is a rare example of stoichiometric oxide, which demonstrates metallic and ferromagnetic (FM) properties. It is widely used in magnetic recording and considered as one of the best particulate ever invented for these purposes [1, 2]. Besides magnetorecording, chromium dioxide has attracted a considerable scientific interest due to its half-metallic electronic structure [3–6], which is intensively investigated today because of its implication in various spin-dependent transport phenomena [7].

In our previous work [8], we have studied the microscopic origin of the half-metallic ferromagnetism in CrO$_2$ by combining first-principles electronic structure calculations with the model Hamiltonian approach and modern many-body methods for treating the electron correlations. We have demonstrated that the problem is indeed highly nontrivial: at the first glance, the ferromagnetism in CrO$_2$ can be easily explained by the Hund’s rule related exchange processes in the narrow $t_{2g}$ band, located near the Fermi level. However, the electron correlations, rigorously treated in the frameworks of dynamical mean-field theory (DMFT) [9], tend to destabilize the FM state. The ferromagnetism in the stoichiometric CrO$_2$ reemerges only if, besides conventional kinetic energy changes in the $t_{2g}$ band, to consider other mechanism, involving direct exchange and magnetic polarization of the...
The Fermi level is shown by the dot-dashed line. 

- In this case, the system is close to the insulating state, and one can expect antiferromagnetic (AFM) character of exchange interactions, caused by the superexchange mechanism [13]. Nevertheless, even in this case, the FM ground state can be ‘restored’ by the hole doping, which partially depopulates the occupied bands and, thus, activates the DE mechanism. Such scenario is also frequently realized in the colossal magnetoresistive manganites [11]. Then, even in the ideal electronic structure, depicted in figure 1(a), one unexplored possibility is the partial depopulation of the ‘narrow’ band, formed by more localized $t_{2g}$ orbitals: since it has finite bandwidth, it can also give rise to the DE interactions, which will compensate the decrease of the FM interactions, cause by the depopulation of the ‘wide’ bands. Thus, the situation is indeed very subtle and depends on the actual ratio of the widths of the ‘narrow’ and ‘wide’ bands, as well as other interactions, existing in the system beyond the conventional DE limit [10].

In the present work we systematically study the doping-dependence of interatomic exchange interactions in CrO$_2$, by using the effective low-energy electron model for the $t_{2g}$ bands, derived from the first-principles electronic structure calculations, and solving it by means of DMFT. The role of electron correlations beyond the local-spin-density approximation (LSDA) is one of disputable problems in the analysis of CrO$_2$. On the one hand, LSDA and generalized gradient approximation (GGA) provide a reasonable description for the structural, transport, and optical properties of CrO$_2$ [4, 14, 15]. On the other hand, it was also suggested that electron correlations are essential for understanding results of photoemission, x-ray absorption, optical, and resistivity measurements [16]. This is the main reason why in our work we use DMFT, being one of the rigorous methods for treating the electron correlations in solids, which becomes exact in the limit of large coordination numbers [9]. Particularly, DMFT allows us to consider the effect of dynamic correlations on the behavior of interatomic exchange interactions, which was also thoroughly investigated in our previous publication [8].

The rest of the article is organized as follows. In section 2, we will briefly discuss our method of construction of the effective low-energy electron model, the solution of this model by using DMFT, and the theory of infinitesimal spin rotations for interatomic exchange interactions [17, 18]. Then, in section 3, we will present our results. Particularly, we will discuss the
doping-dependence of interatomic exchange interactions and explain how it is related to the electronic structure of CrO$_2$ in DMFT. After that, we will use parameters of exchange interactions in order to evaluate $T_C$ and find the optimal concentration of $t_{2g}$ electrons ($n$), which maximizes $T_C$. We will also discuss the effect of the crystal structure on the doping dependence by considering the experimental rutile structure of CrO$_2$ and VO$_2$ and argue that in both cases the optimal $n$ is close to 1, which corresponds to the pristine VO$_2$. Finally, in section 4, we will present a brief summary of our work.

2. Method

In this section, we briefly remind the reader the main steps of our approach. More details can be found in [8]. All calculations have been performed using parameters of the experimental rutile structure (the space group $P4_2/mmm = D_{4h}^3$) for CrO$_2$ [19] and VO$_2$ [20].

The first step is the construction of the effective Hubbard-type model for the magnetically active $t_{2g}$ bands:

$$\hat{H} = \sum_{ij} \sum_{\sigma} t^{ab}_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_i \sum_{\sigma} \sum_{\sigma'} U^{ij}_{ab\sigma\sigma'} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma'} \hat{c}_{i\sigma'} \hat{c}_{j\sigma},$$

starting from the electronic band structure in LDA. The model itself is formulated in the basis of Wannier functions, which were obtained using the projector-operator technique [21, 22] and the orthonormal linear muffin-tin orbitals (LMTO’s) [23] as the trial wave functions. $\sigma(\sigma') = [1]$ in (1) is the spin indices, while $a$, $b$, $c$, and $d$ label three $t_{2g}$ orbitals, which have the following form in the global coordinate frame: $|1 \rangle = \pm \frac{1}{\sqrt{2}} |xy\rangle + \frac{\sqrt{3}}{2} |z^2 - r^2\rangle$, $|2 \rangle = \frac{1}{\sqrt{2}} |xz\rangle \pm \frac{i}{\sqrt{2}} |zx\rangle$, and $|3 \rangle = |x^2 - y^2\rangle$, where two signs correspond to two Cr (V) sites in the primitive cell. Since these $t_{2g}$ orbitals belong to different irreducible representations of the point group $mmm = D_{4h}$, all local quantities, including the DMFT self-energy and local Green’s function, will be diagonal with respect to the orbital indices. The indices $i$ and $j$ specify the positions of the Cr (V) atoms in the lattice. The parameters of the one-electron part, $\hat{t} = [t^{ab}_{ij}]$, are defined as the matrix elements of the LDA Hamiltonian in the Wannier basis [21].

The model Hamiltonian, obtained for CrO$_2$ and VO$_2$, are summarized in table 1.

After the construction of the model (1) was solved by means of DMFT [9], where the properties of the many-electron system are formally related to the frequency-dependent self-energy $\Sigma^{\uparrow\downarrow}(\omega)$, which describes all kind of correlation effects in the one-electron Green’s function $\hat{G}^{\uparrow\downarrow}(\omega, \mathbf{k})$ (in the reciprocal $\mathbf{k}$-space):

$$\hat{G}^{\uparrow\downarrow}(\omega, \mathbf{k}) = [\omega - \hat{\mathbf{t}}(\mathbf{k}) - \Sigma^{\uparrow\downarrow}(\omega)]^{-1}. \quad (2)$$

The basic approximation here is that $\Sigma^{\uparrow\downarrow}(\omega)$ does not depend on $\mathbf{k}$, which becomes exact in the limit of infinite dimensions (or coordination numbers). The main idea of DMFT is to map the initial many-body problem for the crystalline lattice onto the quantum impurity one, surrounded by an effective electronic bath, and find parameters of Green’s function of this bath, $G^{\uparrow\downarrow}(\omega)$, by solving the Anderson impurity model. For these purposes we employ the newly developed exact diagonalization scheme. The details can be found in [8, 25]. Then, $\Sigma^{\uparrow\downarrow}(\omega)$ is obtained from the Dyson equation:

$$\hat{G}^{\uparrow\downarrow}(\omega) = \hat{G}^{\uparrow\downarrow}(\omega) + \hat{G}^{\uparrow\downarrow}(\omega) \Sigma^{\uparrow\downarrow}(\omega) \hat{G}^{\uparrow\downarrow}(\omega), \quad (3)$$

where $\hat{G}^{\uparrow\downarrow}(\omega) = \sum_{\mathbf{k}} \hat{G}^{\uparrow\downarrow}(\omega, \mathbf{k})$, and the problem is solved self-consistently.

After the solution of the DMFT problem, we consider the mapping of the electron model (1) onto the spin Heisenberg model:

$$\hat{H}_S = -\frac{1}{2} \sum_{\mathbf{g}} \mathbf{J}_\mathbf{g} \cdot \hat{\mathbf{S}}_{\mathbf{g} \mathbf{g} + 1}. \quad (4)$$

In these notations, $\mathbf{J}_\mathbf{g}$ is the exchange coupling between two Cr (V) sites, located in the origin (0) and in the point $\mathbf{g}$ of the lattice, relative to the origin, and $\hat{\mathbf{S}}_\mathbf{g}$ is the direction of the spin moment at the site $\mathbf{g}$ (while the value of the spin itself is included in the definition of $\mathbf{J}_\mathbf{g}$). The mapping onto the spin model implies the adiabatic motion of spins when all instantaneous changes of the electronic structure adjust slow rotations of the spin magnetic moments. Then, the parameters of this model can be obtained by using the theory of infinitesimal spin rotations near the FM state [17, 18]:

$$\mathbf{J}_\mathbf{g} = \frac{1}{2\pi} \text{Im} \int_{-\infty}^{+\infty} d\omega \, T_R \left\{ \Delta \tilde{\Sigma}_\mathbf{g}(\omega) \hat{G}_\mathbf{g}(\omega) \hat{G}_\mathbf{g}(\omega) \right\}, \quad (5)$$

where $\hat{G}_\mathbf{g}(\omega) = [\omega - \hat{\mathbf{t}} - \tilde{\Sigma}_\mathbf{g}(\omega) \mathbf{1}]$ is the one-electron Green function between sites 0 and $\mathbf{g}$, $\Delta \tilde{\Sigma} = \tilde{\Sigma}^\uparrow - \tilde{\Sigma}^\downarrow$ is the intraatomic spin splitting, and $T_R$ denotes the trace over the

### Table 1. Parameters of electron model (in eV) for CrO$_2$ and VO$_2$: the crystal-field splitting of the $t_{2g}$ levels ($\delta_{00}$), the transfer integrals between nearest- and next-nearest neighbors ($\delta_{00}$ and $\delta_{02}$, respectively), and Kanamori parameters of the intra-orbital Coulomb ($U$) and exchange ($J$) interactions.

|        | CrO$_2$ | VO$_2$ |
|--------|---------|--------|
| $\delta_{00}$ | $-0.246$ | $-0.225$ |
| $\delta_{00}$ | $0.060$  | $0.081$  |
| $\delta_{02}$ | $0.212$  | $0.123$  |
| $\delta_{02}$ | $0.194$  | $0.178$  |
| $U$     | $0.212$  | $0.225$  |
| $J$     | $0.70$   | $0.71$   |

Note: The positions of the atomic sites 1 and 2, relative to the origin 0, are explained in figure 2.
Figure 2. (Left) Dependence of interatomic exchange interactions on the number of electrons \( n \) in the \( t_{2g} \) band of CrO\(_2\). Note that \( n = 2 \) corresponds to the pristine CrO\(_2\). (Right) Lattice of Cr sites with the notation of atomic positions and interatomic exchange interactions.

Figure 3. Partial densities of states as obtained in the DMFT calculations for CrO\(_2\) (left) and VO\(_2\) (right) for \( n = 1.0, 1.5, \) and 2.0 electrons in the \( t_{2g} \) band. The Fermi level is at zero energy (shown by dot-dashed line). Note that \( n = 2.0 \) and \( 1.0 \) corresponds to the pristine CrO\(_2\) and VO\(_2\), respectively.


3. Results and discussions

The band filling dependence of interatomic exchange interactions in CrO\(_2\) is explained in figure 2. We note that there are four relatively strong interactions, which mainly determine the magnetic behavior of this material: the nearest-neighbor (NN) interaction \(J_1\), the next-NN interaction \(J_2\), and two longer-range interactions \(J_6\) and \(J_7\). In the following, we discuss the behavior of these interactions in detail. Other interactions are considerably weaker.

First, let us explain the behavior of \(J_1\), which for CrO\(_2\) exhibits a nonmonotonous behavior with a peak at around \(n = 1\) (see figure 2). Due to the mmm symmetry of the NN bond (01), the matrices of transfer integrals, \(t_{01}\), and Green’s function, \(\hat{G}_{01}\), are diagonal with respect to the orbital indices. Therefore, \(J_1\) is the superposition of three individual contributions originating from the three \(t_{2g}\) orbitals. Due to the DE mechanism, which largely controls the behavior of \(J_1\), each contribution is expected to have a maximum near the half-filling of the \(\uparrow\)-spin band and then decrease with the decrease of \(n\) [10]. Therefore, near \(n = 2\), corresponding to the pristine CrO\(_2\), where the \(\uparrow\)-spin band formed by the orbital 1 is nearly fully populated while the bands 2 and 3 are approximately half-filled (see figure 3), \(J_1\) decreases with the decrease of \(n\). However, then the orbital 1 is gradually depopulated and becomes half-filled at around \(n = 1\), which formally corresponds to the pristine VO\(_2\). This explains the appearance of the additional peak around \(n = 1\) (figure 4). Indeed, the transfer integral between orbitals of the type 1 in the bond (01) is moderately strong (see table 1) [8]. Therefore, one can expect relatively large FM DE contribution and weak (in comparison with other orbitals) AFM contribution to the exchange coupling, which appears in the next order of the \((\Delta \hat{\Sigma})^{-1}\) expansion [8, 10]. The \(t_{2g}\) electrons, occupying the orbital 1 in CrO\(_2\), are sometimes considered as the localized ones, which participate only in the formation of the weakly AFM background (similar to \(t_{2g}\) electrons in manganites [11]), while the ferromagnetism is entirely related to the itinerant electrons in the bands, formed by the orbitals 2 and 3 [12]. As we have seen above, such interpretation is not quiet correct and the orbital 1 can also contribute to the ferromagnetism, at least in the case of the hole doping.

For the next-NN bond (02), the transfer integrals are strongly off-diagonal with respect to the orbital indices (see table 1). Moreover, the matrix element \(t_{11}^{02}\) is small. Therefore, the contribution of the orbital 1 to \(J_2\) will be also small and entangled with other orbitals. In such situation, the behavior of \(J_2\) is basically controlled by the population of the orbitals 2 and 3. This is the main reason why \(J_2\) monotonously decreases with the decrease of \(n\).

![Figure 4. Partial contributions of three \(t_{2g}\) orbitals to the nearest-neighbor exchange coupling \(J_1\) and long-range interactions \(J_6\) and \(J_7\) in CrO\(_2\). Note that \(n = 2\) corresponds to the pristine CrO\(_2\).](image-url)
Note that in the DMFT calculations, we have obtained the half-metallic FM solutions for all values of $n$. Therefore the spin magnetic moment is equal to $n$ and the effective spin ($S$), that we use in Tyablikov’s model is $n/2$. The results are explained in figure 5. As any mean-field approach, the DMFT is expected to overestimate the magnetic transition temperature because of neglect of the spacial correlations [9]. However, these spacial correlations are taken into account in Tyablikov’s RPA (though in some approximate form), which typically provides a realistic estimate for $T_C$ [29]. In this sense, it is a step beyond the mean-field approximation. Nevertheless, the price to pay for this is the additional mapping of the DMFT energies onto the spin Heisenberg model (4). The definition of $T_C$ is only meaningful when the FM state is stable. In Tyablikov’s approach, this is defined by the magnon frequencies $\omega_\ell(q)$ for two branches $\ell$: if some of $\omega_\ell(q)$ are negative, the FM state is considered to be unstable. These regions of stability (and instability) of the FM state are also shown in figure 5. One can see that, for $n = 2$ the FM state in our model is unstable. This is of course a limitation of our model analysis, which was thoroughly investigated in our previous work [8]. Note that in our model we do not consider the contributions caused by direct exchange interactions and the polarization of the oxygen band, which are indeed crucial for stabilizing the FM ground state in CrO$_2$ [8]. However, it is reasonable to expect that the doping-dependence of these interactions is relatively weak, because the doping affects mainly the magnetic interactions in the $t_{2g}$ band. Therefore, we do not consider here the direct exchange interactions as well as the magnetic polarization of the oxygen band, assuming that, if necessary, these (weakly dependent on $n$) FM contributions can be simply added to the ones in the $t_{2g}$ band, which we explore in the present work. Then, judging from figure 5, $J_0$ and $T_C$ reach the maximums at around $n = 1.3$ and 0.9, respectively, mainly as the joint effect of $J_1$, $J_6$, and $J_7$. The maximal value of $T_C$ is about 1400 K, which is indeed very high.

Figure 5. Total exchange coupling around each transition-metal site ($J_0$) and the Curie temperature ($T_C$), evaluated in the framework of Tyablikov’s random-phase approximation, as the function of the number of $t_{2g}$ electrons in CrO$_2$ (left) and VO$_2$ (right). Note that $n = 2$ and 1 corresponds to the pristine CrO$_2$ and VO$_2$, respectively.

$$T_C = \frac{nS(S + 1)}{3k_BT}\left(\sum_{q}^{2} \sum_{\ell=1}^{2} \frac{1}{\omega_\ell(q)}\right)^{-1}.$$

Figure 6. Dependence of interatomic exchange interactions on the number of electrons in the $t_{2g}$ band of VO$_2$. Note that $n = 1$ corresponds to the pristine VO$_2$.
Finally, we discuss the effect of the crystal structure on the considered properties. For these purposes, instead of CrO$_2$, we take the experimental crystal structure of VO$_2$ and perform the same calculations. Indeed, if the optimal band-filling in CrO$_2$ is around $n = 1$, that corresponds to the pristine VO$_2$, one can also try to consider the possibility of the electron or hole doping of the latter compound. The obtained band-filling dependence of interatomic exchange interactions in VO$_2$ is explained in figure 6 and corresponding densities of states are shown in figure 3. We observe that in this case, as well as in the case of CrO$_2$, the strongest exchange interactions are $J_1$, $J_2$, $J_0$, and $J_2'$. Judging from the parameters of the model Hamiltonian (see table 1), the main difference between CrO$_2$ and VO$_2$ is in the transfer integrals operating in the NN bond $\langle 01 \rangle$; in CrO$_2$, the transfer integrals between orbitals of the type 1 are considerably weaker than those between orbitals 2 and 3, while in VO$_2$ all three types are comparable. This explains the fact that all three $\uparrow$-spin bands, formed by the orbitals 1–3, are comparable in the case of VO$_2$ (see figure 3), while in CrO$_2$ the band 1 is considerably narrower. Moreover, the crystal field, separating the orbital 3, is considerably stronger in the case of VO$_2$. Therefore, for $n = 2$ in VO$_2$, the $\uparrow$-spin bands 1 and 2 are nearly filled (or half-filled in the non-spin-polarized case), while the band 3 is almost empty. This explains the AFM character of NN interaction $J_1$ at $n = 2$, as the general tendency towards antiferromagnetism near the half-filling (referring to the bands 1 and 2 in the non-spin-polarized case) [26, 27]. However, the decrease of $n$ leads to the partial depopulation of the $\uparrow$-spin bands 1 and 2, which changes the character of the NN interaction $J_1$ towards the FM one due to the DE mechanism. This FM coupling is especially strong around $n = 1.25$. The relative strength of long-range interactions is considerably weaker. Thus these interactions play a less important role in comparison with CrO$_2$.

The mean-field Hartree–Fock (HF) calculations, performed for the FM state of VO$_2$, yield $J_1 = 25.2$ meV and $J_2 = 7.5$ meV. These values are somewhat larger than the ones obtained in DMFT (21.6 and 7.3 meV, respectively) due to the lack of dynamic correlations, which effectively decrease the intraatomic exchange splitting between majority- and minority-spin states near the Fermi level and, thus, additionally strengthens the AFM superexchange interactions in the case of DMFT [8]. Nevertheless, both HF and DMFT calculations support strong FM character of exchange interactions in VO$_2$, if they are calculated near the FM state. It is also important to note that the electronic structure and exchange interactions in VO$_2$ strongly depend on the magnetic state in which they are calculated (and in this sense, VO$_2$ can be regarded as a smart material [31, 32]). For instance, in the HF calculations, the AFM alignment of two V spins in the primitive cell opens the band gap (of about 0.1 eV) and changes the character of NN interactions to the AFM one ($J_1 = −14.6$ meV). This AFM configuration is higher in energy and, thus, cannot be realized as the ground state. However, it can contribute to the thermodynamic average at elevated temperatures. Thus, the FM ground state obtained for the rutile structure of VO$_2$ is not necessarily inconsistent with the negative Curie–Weiss temperature, expected from the high-temperature behavior of magnetic susceptibility [33]: simply, the electronic structure of the paramagnetic state should be very different from the one realized in the FM ground state and, therefore, the magnetic interactions should be also different.

Using parameters of exchange interactions, obtained in DMFT, we again evaluate the ‘mean-field parameter’ $J_0$ and the Curie temperature, using Tyablikov’s RPA. The results are summarized in figure 5. Despite substantial differences in the electronic structure (see figure 3), the Curie temperature exhibits very similar behavior as the function of the band-filling in CrO$_2$ and VO$_2$. In the latter case, $J_0$ and $T_C$ take the maxima at around $n = 1.2$ and 0.8, respectively. The maximal value of $T_C$ is close to 1400 K, i.e. similar to CrO$_2$.

4. Summary and conclusions

By combining first-principles electronic structure calculations with the dynamical mean-field theory, we have investigated the band-filling dependence of interatomic exchange interactions and the Curie temperature in CrO$_2$ and related rutile compounds. We have argued that $T_C$ in the rutile compounds can be substantially increased by controlling the number of the $t_{2g}$ electrons. It appears that, as far as the Curie temperature is concerned, the filling of the $t_{2g}$ band in the stoichiometric CrO$_2$ is not the most optimal one and much higher $T_C$ can be expected for the smaller number of $t_{2g}$ electrons due to the general tendency of the narrow-band compounds towards the ferromagnetism at the beginning of the band-filling [26, 27]. According to our estimates, the optimal number of $t_{2g}$ electrons should be close to $n = 1$, which formally corresponds to the pristine VO$_2$. Thus, if VO$_2$ indeed crystallized in the rutile structure, it could be a good FM material with some of the properties even exceeding CrO$_2$. However, below 340 K, VO$_2$ undergoes the transition to the monoclinic phase, which is accompanied by the dimerization of the V sites and the formation of the nonmagnetic insulating state [33–35]. Actually, the situation when the robust ferromagnetism, expected in some materials, is destroyed by the lattice distortion is rather common in nature. One of the well known examples is LaMnO$_3$, which from the viewpoint of the DE physics is rather common in nature. One of the well known examples is LaMnO$_3$, which from the viewpoint of the DE physics is expected to be a strong ferromagnet with the optimal concentration of electrons in the $e_g$ band [10]. However, this FM state in LaMnO$_3$ is destroyed by the Jahn–Teller distortion, which is responsible for the formation of the layered AFM state [36]. Nevertheless, the FM state can be realized in the thin films, where the crystal structure is controlled by the substrate. Such a possibility for VO$_2$ was indeed demonstrated in [31, 32], where it was argued that by deposing VO$_2$ on different substrates one can achieve the room-temperature ferromagnetism, which can be switched ‘on’ and ‘off’, depending on the treatment conditions. This behavior was attributed to the $V^{3+}$ defects, existing in the thin films of VO$_2$. However, results of our work demonstrate that such behavior can be also intrinsic and related to the general tendency of the narrow-band compounds towards the ferromagnetism at the beginning of the band filling.
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