New magnetic phase in metallic \( V_{2-y}O_3 \) close to the metal insulator transition

S. Klimm, M. Herz, R. Horny, G. Obermeier, M. Klemm, and S. Horn  
Universität Augsburg, 86135 Augsburg, Germany  
(November 1, 2018)

We have observed two spin density wave (SDW) phases in hole doped metallic \( V_{2-y}O_3 \), one evolves from the other as a function of doping, pressure or temperature. They differ in their response to an external magnetic field, which can also induce a transition between them. The phase boundary between these two states in the temperature-, doping-, and pressure-dependent phase diagram has been determined by magnetization and magnetotransport measurements. One phase exists at high doping level and has already been described in the literature. The second phase is found in a small parameter range close to the boundary to the antiferromagnetic insulating phase (AFI). The quantum phase transitions between these states as a function of pressure and doping and the respective metamagnetic behavior observed in these phases are discussed in the light of structurally induced changes of the band structure.

PACS numbers: 75.30.Fv, 75.30.Kz, 72.15.Gd, 71.30.+h

I. INTRODUCTION

The compound \( V_{2-y}O_3 \) shows a complicated phase diagram as a function of temperature, pressure, oxygen stoichiometry and doping on the vanadium site [1]. The pure compound exhibits a metal-insulator (MI) transition at \( T_{MI} = 170 \) K, which separates a metallic paramagnetic from an antiferromagnetic insulating phase. The transition is shifted to lower temperatures by external pressure, Ti doping on the vanadium site and vanadium deficiency \( y \), while Cr or Al doping increases \( T_{MI} \). At sufficiently high Cr and Al doping levels a paramagnetic insulating phase exists at room temperature, which orders antiferromagnetically at \( T_{AF} = 200 \) K. For vanadium deficiencies \( y \geq 0.015 \), a spin density wave (SDW) phase forms at \( T_{SDW} \). The ordering temperature \( T_{SDW} \) is a function of doping slightly decreasing from \( T_{SDW} \approx 11 \) K close to the AFI–SDW boundary down to \( T_{SDW} \approx 8 \) K at \( y = 0.03 \). Neutron scattering measurements revealed the SDW to be of an incommensurate spiral type with wave vector \( q = 1.7 \) \text{c}^* \) along the hexagonal \text{c} axis and the moments lying within the ab-plane. In stochiometric samples \( T_{MI} \) is reduced by the application of hydrostatic pressure with a critical pressure of \( p_c = 2 \) GPa for the complete suppression of the AFI-phase. However, in contrast to doping, the pressure stabilized metallic phase remains paramagnetic down to lowest temperatures. In doped samples external pressure reduces \( T_{SDW} \). The critical pressure increases on doping. A 3-dimensional sketch of the phase diagram is shown in Fig. 1.

Recently it was found [2] that two different SDW phases can be distinguished as a function of pressure and vanadium deficiency \( y \). This indicates that the electronic structure of \( V_{2-y}O_3 \) is still sensitive to pressure and vanadium deficiency in the metallic phase, most likely due to a change of weight or character of the bands at the Fermi energy \( E_F \). A close inspection of the phase diagram of \( V_{2-y}O_3 \) in the vicinity of the phase boundaries may provide an understanding of the important parameters dominating the physics of this classical compound and also the possible role of electronic correlations.

We first demonstrate the existence of two different SDW phases and then discuss the stability of the various phases of \( V_{2-y}O_3 \) based on LDA band structure calculations. We present magnetic susceptibility and electronic transport measurements as a function of vanadium deficiency \( y \), applied pressure \( p \) and magnetic field \( B \) in the vicinity of the phase boundary between the antiferromagnetically ordered insulating and the metallic SDW phase and the boundary between the two different SDW phases.

The electrical resistivity of \( V_{2-y}O_3 \) for different levels...
of doping and as a function of pressure has been investigated earlier, but a systematic investigation including the dependence of the magnetotransport on the crystallographic orientation, which we will show below is essential for a complete picture of the transport properties, has not been done.

II. EXPERIMENTAL

Single crystals of \( V_{2-y}O_3 \) were grown by the chemical vapor transport technique with TeCl4 as transport agent. The stoichiometry was controlled by the composition of the starting materials. X-ray diffraction on powdered single crystals showed the \( V_{2-y}O_3 \) samples to be single phase. Since no non-destructive method with sufficient accuracy to determine the exact stoichiometry of the grown crystals was available, the doping dependence of \( T_{MI} \) or \( T_{SDW} \) as depicted from literature was used to estimate the values of \( y \). In addition the \( c \)-axis parameter of the crystals, which varies almost linearly with \( y \) (Ref. [1], was measured yielding consistent results for the values of \( y \). Although there is a relatively large error in the absolute values of \( y \), the relative position of the various samples on a scale of doping can assumed to be correct. The orientation of the crystals was determined by Laue diffraction. Magnetic measurements were performed using a Quantum Design SQUID magnetometer. Rectangular bars with a typical size of \( 2 \times 0.3 \times 0.3 \text{ mm}^3 \) were cut from the crystals to perform transport measurements along well defined crystallographic directions. The resistivity was measured using a standard 4-probe AC-technique. Experiments under quasi hydrostatic pressure were performed in a CuBe piston-cylinder cell with a manganin gauge and n-pentane – isoamyl (1:1) as a pressure transmitting medium.

III. RESULTS

A. Electrical resistivity

The investigated samples of different stoichiometry will be labeled in the following by the \( y \) value estimated as described above. The temperature dependent resistivity \( \rho \) for different values of doping is shown in the left part of Fig. 2. The curves for different \( y \) are normalized to their respective room temperature resistivity. The absolute value of the room temperature resistivity ranges from 300 to 400 \( \mu \Omega \text{cm} \). At ambient pressure the stoichiometric sample \( (y = 0) \) shows a MI-transition at \( T_{MI} = 160 \text{ K} \) on cooling (175 K on warming up). Above the critical pressure at \( p = 2 \text{ GPa} \) a \( T^2 \) dependence is observed at low temperatures in agreement with existing literature. The residual resistance ratio of \( RRR = 50 \) shows the crystal to be of good quality. As expected the residual resistivity \( \rho_0 \) increases monotonously with increasing vanadium vacancy concentration. The shape of the resistivity curves at intermediate temperatures depends on the current direction with respect to the crystallographic axes, probably reflecting the anisotropic phonon spectrum in this compound. The negative curvature of resistivity is less pronounced for \( j \parallel c \) (not shown here) than for \( j \perp c \) resulting in a more linear temperature dependence.

For \( y > 0.015 \) the transition into the SDW ground state at \( T_{SDW} \) is marked by a minimum in the resistivity for \( j \parallel c \) (along the propagation vector \( q \) of the SDW), while for \( j \perp c \) a less pronounced kink is observed (Fig. 2, right panel) indicating the formation of a gap along the \( c^* \)-direction in reciprocal space. The temperature \( T_{min} \) of the resistivity minimum for \( j \parallel c \) as well as the kink for \( j \perp c \) decreases only slightly on application of an external magnetic field of up to \( B = 12 \text{ T} \). The coefficient \( dT_{min}/dB \approx -0.1 \text{ K/T} \) is almost the same for \( B \parallel c \) as well as for \( B \perp c \).

B. Magnetic susceptibility

The response of the SDW state to an external magnetic field depends on the orientation of the field with respect to the \( c \)-axis and on the level of doping. For \( y > 0.018 \) (deep in the SDW phase) the low field magnetic susceptibility shows an antiferromagnetic cusp at \( T_{SDW} \) for \( B \perp c \) while for \( B \parallel c \) the susceptibility first remains constant below \( T_{SDW} \) and then even slightly increases towards lower temperatures reflecting the response for the hard and easy AF axis, respectively (Fig. 3). This behavior is consistent with the in plane orientation of the
moments in this transverse polarized SDW phase and has already been observed earlier.

Only a weak field dependence of the susceptibility and a slight reduction of $T_{SDW}$ with field is observed for $B \parallel c$. For $B \perp c$, however, the cusp in the susceptibility as a function of temperature, apparent at low fields, transforms into a kink above a critical value $B_{c,\perp} \approx 3$ T. The slope at low temperatures changes from positive to negative with increasing field indicating a reorientation of spins above $B_{c,\perp}$. With an applied field of $B = 3$ T, the transformation is observed as a function of temperature with the susceptibility exhibiting a considerable hysteresis, strongly suggesting a phase transition between two magnetic phases.

Approaching the SDW – AFI phase boundary by reducing $y$, the critical field $B_{c,\perp}$ decreases until for $y = 0.016$ the magnetic transition is observed even at the lowest fields (Fig. 3). Above 8 K the low field susceptibilities for $y = 0.016$ and $y = 0.02$ (Fig. 3) are similar. Below 8 K, however, for $y = 0.016$ the susceptibility for $B \parallel c$ decreases abruptly while for $B \perp c$ it increases. Thus at low temperatures and low doping the hard and easy axes appear interchanged when compared to higher doping levels. For $B \perp c$ an increasing field shifts the transition to higher temperatures, qualitatively similar to the $y = 0.02$ sample, but with the critical field shifted by $\approx 2.5$ T. A magnetic field applied along the $c$-axis, however, shifts the transition of the $y = 0.016$ sample to lower temperatures (Fig. 3, right) and at high fields a behavior as observed for the $y = 0.02$ sample can be restored.

Accordingly, the magnetization behaves differently as a function of applied field in the two phases. This is most clearly seen plotting $\chi_{DC} = M/B$ vs. $B$ (Fig. 3).

Below 8 K, however, for $y = 0.016$ the magnetic transition is observed even at the low-temperature metamagnetic phase (Fig. 4). Above 8 K the low field susceptibilities ($y = 0.016$) shown in Fig. 4. A similar behavior was reported by Bao et al. for a sample with an even higher vanadium deficiency ($y = 0.04$) and was attributed to a spin flop transition. The behavior of the $y = 0.016$ sample is shown in the left panel of Fig. 5. At $T = 2$ K $\chi_{DC}(B)$ does not show a transition for $B \perp c$ since it is already in the second phase. But for $B \parallel c$ a transition occurs at a characteristic field $B_{c,\parallel}$ as expected from the behavior of $\chi(T)$ shown in Fig. 4.

The right panel shows $\chi_{DC}$ of the $y = 0.02$ sample for $B$ parallel and perpendicular to the hexagonal $c$-axis. For $B \parallel c$ $\chi_{DC}$ is almost independent of $B$ while a metamagnetic transition at $B = B_{c,\perp}$ is observed for $B \perp c$ in accordance with the $\chi(T)$ shown in Fig. 3. A similar behavior was reported by Bao et al. for a sample with an even higher vanadium deficiency ($y = 0.04$) and was attributed to a spin flop transition. The behavior of the $y = 0.016$ sample is shown in the left panel of Fig. 5. At $T = 2$ K $\chi_{DC}(B)$ does not show a transition for $B \perp c$ since it is already in the second phase. But for $B \parallel c$ a transition occurs at a characteristic field $B_{c,\parallel}$ as expected from the behavior of $\chi(T)$ shown in Fig. 4.
minimum as the applied magnetic field is varied for both principal field directions. We therefore believe that the metamagnetic behavior observed in the magnetization is not due to a suppression of the SDW phase but rather to a reorientation of the moments or a change of the propagation vector $\mathbf{q}$.

The results presented above suggest the existence of two different magnetic phases within the SDW regime. In the following we will call these phases SDW 1 and SDW 2. SDW 1 designates the well known phase, already characterized by neutron scattering. The newly discovered phase, designated SDW 2, exists in a small range of $y$ close to the SDW – AFI boundary, and is inferred from anomalies observed in the magnetic susceptibility and magnetoresistance. A transition from SDW 1 to SDW 2 with decreasing temperature was observed for a crystal with $y = 0.016$, implying that the phase boundary between the two phases, in the temperature–doping diagram, has a negative slope. Further evidence and a rough estimate for this negative slope is provided by magnetoresistance and susceptibility measurements as a function of magnetic field. A sample which is in the SDW 2 phase at $T = 0.4$ K, has a negative slope. Further evidence and a rough estimate for this negative slope is provided by magnetoresistance and susceptibility measurements as a function of magnetic field. A sample which is in the SDW 2 phase at $B = 0$ transforms into the SDW 1 phase, if a magnetic field above $B_{c,||}$ is applied along the $c$-axis. On the other hand, a field in excess of $B_{c,\perp}$ applied perpendicular to the $c$-axis transforms the SDW 1 phase of a higher doped sample into the SDW 2 phase. Both fields $B_{c,\perp}$ and $B_{c,||}$ are monotonous functions of doping, i.e. they can be used as a measure of the distance of a particular sample to the phase boundary between SDW 1 and SDW 2 phase (on the axis of doping). For given doping $B_{c,||}$ decreases while $B_{c,\perp}$ increases with increasing temperature in the vicinity of this phase boundary. From this doping and temperature dependence of the critical fields $B_{c,\perp}$ and $B_{c,||}$ the slope of the phase boundary between SDW 1 and SDW 2 in the $T – y$ plane can be roughly determined as given in Fig. 4.

![FIG. 6. $T – y$ phase diagram for V$_{2-y}$O$_3$ including the new phase boundary (dotted line).](image)

![FIG. 7. Magnetoresistance of a sample in the SDW 1 phase at $B = 0$.](image)

C. Magnetoresistance

The magnetoresistance (MR) shows a metamagnetic behavior corresponding to that of the magnetic susceptibility. Since we can carry out MR measurements over a larger range of temperature, magnetic field, and hydrostatic pressure we will in the following concentrate on magnetoresistance rather than on magnetization to further characterize the magnetic behavior of V$_{2-y}$O$_3$.

The low temperature region of the PM phase of stoichiometric samples ($p \geq 2$ GPa) exhibits a positive magnetoresistance with a quadratic field dependence. The MR-curves taken at different temperatures scale according to Kohler’s rule, implying a nonmagnetic scattering process. Vanadium deficient samples show a negative contribution to the MR which increases with increasing $y$, indicating the formation of magnetic moments. In the SDW phase Kohler’s rule is not obeyed and magnetic scattering dominates the MR.

In the SDW 1 phase, i.e. for high doping levels, the resistivity for $B \parallel c$ decreases monotonously with increasing $B$ (Fig. 5 right). For a field applied perpendicular to the $c$-axis, however, a dramatically different behavior is observed as shown in the left part of Fig. 5. At a critical field $B$ the resistivity suddenly jumps to a higher value. For clarity only curves with increasing field are shown. On lowering the field below the critical value a hysteresis of about 0.1 T is observed. Since a corresponding anomaly was observed in the magnetization (Fig. 3) we also label the critical field inferred from the MR anomaly as $B_{c,\perp}$. With increasing temperature $B_{c,\perp}$ increases slightly while the size of the jump decreases until it vanishes completely for $T > T_{SDW}$. We attribute this metamagnetic behavior to the transition from SDW 1 to SDW 2, as was already inferred from magnetization measurements. The critical field $B_{c,\perp}$ increases with increasing doping at a slope of $dB_{c,\perp}/dy \approx 4 \times 10^2$ T.
For a sample with composition close to the AFI phase boundary ($y = 0.015$) the MR behaves completely differently (Fig. 5). Here a sudden jump to lower resistivity occurs, with the magnetic field directed along the $c$-axis. The corresponding critical field, taken as the inflection point of this anomaly, decreases with increasing temperature. This critical field has $B_{c,\perp}$ as its counterpart. For $B \perp c$ no anomaly exists. This behavior, which we attribute to the SDW 2 phase, persists in this sample for all temperatures up to $T_{SDW} = 11$ K.

For slightly higher doping ($y \approx 0.016$) a transition from SDW 1 to SDW 2 phase as a function of temperature is observed (Fig. 6) in accordance with our findings from susceptibility measurements (Fig. 3). The transition between the two different behaviors of the MR, characteristic of the two different SDW phases, occurs around $T \approx 6$ K. The characteristic field $B_{c,\parallel}$ at lowest temperature is smaller for the $y = 0.016$ sample than for the $y = 0.015$ sample. Both magnetic field induced transitions, (SDW 1 to SDW 2 and SDW 2 to SDW 1) exhibit a hysteresis shown in Fig. 8 which was omitted for clarity in Fig. 7 and Fig. 8.

The direction of the magnetic field has to be considered for the phase boundary between SDW 1 and SDW 2 in a $T$–$B$ phase diagram, i.e. separate diagrams for the two field directions have to be plotted. This is illustrated in Fig. 10 for various samples of different stoichiometry. The symbols correspond to $B_{c,\perp}$ (right) and $B_{c,\parallel}$ (left), respectively, as determined from the inflection point of the MR curves. Note that the $B_{c,\parallel}$-axis is reversed to account for the opposite effect of $B_{\parallel}$ and $B_{\perp}$ on the stability of the two phases. For the $y = 0.015$ sample the SDW 1 – SDW 2 boundary lies completely in the $B \parallel c$ part of the phase diagram, i.e. the SDW 2 phase is stable in zero field as well as for all values of $B_{\perp}$. The SDW 1 phase can be induced only for large $B_{\parallel}$. On increasing $y$ this phase boundary shifts to the $B \perp c$ side of the phase diagram as indicated by the arrows until above $y \approx 0.017$ the SDW 1 phase is stable down to the lowest temperatures in zero field. Then SDW 2 can only be induced by a sufficiently high $B_{\perp}$ which increases with increasing doping. At the same time the phase boundary becomes steeper until for $y = 0.025$ $dB_{c,\perp}/dT$ even changes sign. Unfortunately a sample with higher doping was not available. The $y = 0.04$ sample investigated by Bao et al. however, shows a negative $dB_{c,\perp}/dT$ confirming the general trend observed in our study. For the $y = 0.016$ sample, which crosses the phase boundary at zero field (square symbols in Fig. 10), the phase boundaries for $B \parallel c$ and $B \perp c$ do not match at $B = 0$. This is due to the large hysteresis on cycling the temperature as already shown in the susceptibility (Fig. 5). In the
temperature range 4 K < T < 8 K both SDW phases apparently coexist in this sample and finite fields $B_{c,1}$ as well as $B_{c,2}'$ are needed to stabilize pure SDW 2 or SDW 1 phase, respectively.

D. Pressure dependence

To clarify whether the transition between SDW 1 and SDW 2 depends only on the hole concentration, the effect of external pressure, which does not change the band filling, should be examined. In general, pressure appears to have the same effect as doping on the $V_{2-y}O_3$ phase diagram. Starting from the stoichiometric compound at ambient pressure, the reduction of $T_{MI}$ by doping and pressure scales with a ratio of $\Delta p / \Delta y \approx 1.4 \times 10^2$ GPa. However, in contrast to the doping induced metallic phase, the pressure induced metallic phase of the stoichiometric sample does not show a transition into a SDW phase down to $T = 0.3$ K (see Fig. 11). If pressure is applied to samples exhibiting a SDW ground state, $T_{SDW}$ is reduced until the PM phase is stabilized down to the lowest temperatures. The sensitivity of the SDW ordering temperature to pressure ($dT_{SDW}/dp$) decreases with increasing doping although $T_{SDW}$ decreases. Thus, except for the absence of a SDW phase in the pressure induced metallic state of the stoichiometric sample, the effects of pressure and doping are similar.

We performed pressure dependent magnetotransport measurements on seven samples with different levels of vanadium deficiency. In the following we only want to discuss information from these measurements relevant to the phase diagram of $V_{2-y}O_3$. For the stoichiometric sample (already discussed above) and for $y = 0.003$, pressure induces a transition from the AFI phase to a paramagnetic metallic ground state. The samples with $y = 0.009$ and $y = 0.014$ show a more complex behavior. This is illustrated in Fig. 11 for the $y = 0.014$ sample. At ambient pressure this sample assumes an AFI ground state ($T_{MI} = 50$ K). At a pressure of 0.1 GPa the sample remains metallic down to lowest temperatures. At this and slightly higher pressures we observe a behavior characteristic for the SDW 2 phase (Fig. 11, left), as it was found, e.g., for the $y = 0.015$ sample (Fig. 8) at $p = 0$. At a pressure of $p = 0.4$ GPa both SDW 1 and SDW 2 behavior can be observed, depending on the temperature. This behavior is reminiscent of the $y = 0.016$ sample, which shows a transition from SDW 1 to SDW 2 as a function of temperature. Increasing the pressure further to 0.6 GPa results in MR features characteristic of the SDW 1 phase (Fig. 11, right). The critical field $B_{c,2}'$, that induces the SDW 2 phase, increases with increasing pressure. Finally, at $p = 2$ GPa no magnetic ordering is observed down to the lowest temperatures.

Hence, the ground state of this sample undergoes three phase transitions as a function of pressure, AFI to SDW 2 phase, SDW 2 to SDW 1 phase and, finally, SDW 1 phase to a paramagnetic metal. For a fixed pressure of 0.4 GPa three phases are observed (SDW 2 – SDW 1 – PM) as a function of temperature.

For the sample with $y = 0.019$, which shows the SDW 1 phase ground state, pressure induces the paramagnetic metallic (PM) phase. The pressure dependent measurements are summarized in the $p – y$ ground state phase diagram ($T = 0.4$ K) in Fig. 12. The newly discovered SDW 2 phase exists only in a small range of doping and pressure close to the AFI phase. Within experimental resolution the SDW 1 – SDW 2 and SDW 2 – AFI phase boundaries appear to be parallel. The situation at the...
IV. DISCUSSION

From our susceptibility and magnetotransport data it can be concluded that two SDW phases exist. Since the different phases of V$_{2-y}$O$_3$ can be observed in a sample with given stoichiometry as a function of pressure we do not believe that disorder introduced by the vanadium deficiency is responsible for the properties of this compound. While the SDW phase at large $y$ (SDW 1) has been extensively studied by neutron scattering the exact nature of SDW 2 remains unclear. However, in the study of Bao et al. an additional incommensurate peak corresponding to a slightly larger $q$ vector was observed at temperatures below 6 K for one sample with a composition close to the AFI – SDW phase boundary. This finding has so far been denoted “unclear”. Taking our new results into account it appears evident that this peak signals the presence of the SDW 2 phase. Since hard and easy axes seem to be interchanged between SDW 1 and SDW 2 the moments are expected to be oriented along the c-axis or at least have an appreciable out of plane component in SDW 2. Unpublished neutron studies of this second phase confirm this assumption. Most likely, the SDW 2 phase is a longitudinal SDW with propagation vector still along the c-axis, but with the e-component of the moments being modulated. Due to this antiferromagnetic coupling of the e-component it is hard to induce a magnetization by a field along the c-axis in SDW 2, while in SDW 1 the antiferromagnetic exchange couples the in plane component of the moments and so a magnetization along the c-axis is more easily obtained. For the same reason, a field applied perpendicular to the c-axis aligns the moments more easily in SDW 2 than in SDW 1. Thus in a sufficiently large field along the c-axis the free energy is lower in SDW 1 compared to SDW 2 and vice versa for B ⊥ c. The assumption of a longitudinal polarization in SDW 2 therefore gives a consistent interpretation of the observed anisotropic response to a magnetic field for both phases.

The MR data show the resistivity is somewhat higher in the SDW 2 than in the SDW 1 phase indicating that an increased portion of the Fermi surface is removed by the formation of SDW 2. This results in a reduced density of free charge carriers and a lower entropy of SDW 2 compared to SDW 1. Thermodynamic considerations therefore predict the SDW 1 phase to become more stable compared to SDW 2 with increasing temperature consistent with the experimentally observed transition in the $y = 0.016$ sample and the corresponding phase diagram (Fig. 10).

Discussing the stability of the different phases with respect to the parameters doping and pressure it is interesting to note, that both external pressure and doping can induce the transition from SDW 2 into SDW 1. Since the SDW formation originates from Fermi surface nesting it follows, that both doping and pressure induces similar changes in the Fermi surface. Band structure calculations predict the bands near $E_F$ to be of $a_{1g}$ and $e_{g}^\pi$ character. Most likely a band with predominant $a_{1g}$ character, which has large dispersion along the c-direction, provides the best nesting conditions and therefore should be responsible for the formation of the SDW.

Hole doping $y$ reduces the band filling. A vanadium deficiency of 1% ($y = 0.02$) changes the filling of the $t_{2g}$ bands by 2.5%. In addition, a volume contraction of $\Delta V/V \approx 0.3\%$ at $y = 0.02$ occurs at room temperature, while the $c/a$ ratio remains almost constant. On the other hand, external pressure does not change the overall band filling, but also causes a volume contraction (of 1% at 2 GPA) accompanied by an 0.35% increase of the $c/a$ ratio in V$_3$O$_7$. Although there is only scanty structural data at low temperatures, it can be assumed that similar changes of volume and corresponding changes of $a$- and $c$-axis parameters occur as a function of doping and pressure in the SDW regime. It should also be noted that there is a substantial increase of the $c/a$ ratio with decreasing temperature of about 0.4% between RT and $T = 77$ K.

In a simplistic band picture, the relative weight of $a_{1g}$ to $e_{g}^\pi$ character can be changed by depopulating one of the bands by hole doping or shifting it to higher energies by pressure. In fact, a sensitivity of band positions in the vicinity of the Fermi energy to pressure and the according structural changes might be expected from changes of the V$3d$–O$2p$ hybridization. Such changes of hybridization are observed at the PM–AFI transition for stoichiometric samples. In addition, dramatic changes of the relative position of the different bands at the Fermi level have been found in recent band structure calculations varying the $c/a$ ratio within the pseudo hexagonal PM phase, resulting in substantial variations of the corresponding Fermi surfaces. Further support for a possible shift of relative band positions of bands with $a_{1g}$ and $e_{g}^\pi$ character in V$_2$O$_3$ is provided by a similar, much more pronounced effect in the isostructural compound Ti$_3$O$_2$. We therefore believe, that relative shifts of bands of $a_{1g}$ and $e_{g}^\pi$ character crossing the Fermi energy are responsible for the observed transition between two different SDW states. In this context we note, that such shifts could also effect the other phases in the complex V$_2$O$_3$ phase diagram, which are, of course, rendered even more complex by the presence of electronic correlations.
V. CONCLUSION

We have shown that, depending on vanadium deficiency $y$, two different SDW ground states exist in V$_2$O$_3$. The transition between the two SDW states as a function of doping and pressure was attributed to changes of the Fermi surface resulting from band filling and structurally induced band shifts, respectively. From magnetic susceptibility and magnetoresistance measurements, the latter performed as a function of pressure, tentative phase diagrams were deduced with parameters temperature, magnetic field, pressure, and doping.

ACKNOWLEDGMENTS

This work was supported by the Deutsche Forschungsgemeinschaft under contract number HO 955/2-1 and SFB 484. We are grateful to P. Riseborough for valuable discussions and to V. Eyert for providing the LDA band structure calculations before publication.

1 M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. 70, 1039 (1998).
2 S. A. Carter, T. F. Rosenbaum, J. M. Honig, and J. Spalek, Phys. Rev. Lett. 67, 3440 (1991).
3 Y. Ueda, K. Kasuge, and S. Kachi, J. Solid State Chem. 31, 171 (1980).
4 W. Bao, C. Broholm, S. A. Carter, T. F. Rosenbaum, G. Aeppli, S. F. Trevino, P. Metcalf, J. M. Honig, and J. Spalek, Phys. Rev. Lett. 71, 766 (1993).
5 S. Klimm, M. Herz, G. Obermeier, R. Horny, M. Klemm, and S. Horn, Bull. Am. Phys. Soc. 45, 909 (2000).
6 D. B. McWhan, A. Menth, J. P. Remeika, W. F. Brinkman, and T. M. Rice, Phys. Rev. B 7, 1920 (1973).
7 S. A. Carter, T. F. Rosenbaum, P. Metcalf, J. M. Honig, and J. Spalek, Phys. Rev. B 48, 16841 (1993).
8 T. F. Rosenbaum, in Metal-Insulator Transitions Revisited, p. 105, eds. P. P. Edwards and C. N. R. Rao, (Taylor & Francis, London, 1995).
9 S. A. Carter, T. F. Rosenbaum, M. Lu, H. M. Jaeger, P. Metcalf, J. M. Honig, and J. Spalek, Phys. Rev. B 49, 7898 (1994).
10 M. Yethiraj, S. A. Werner, W. B. Yelon, and J. M. Honig, Phys. Rev. B 36, 8675 (1987).
11 S. Klimm, G. Gerstmeier, H. Paulin, M. Klemm, and S. Horn, Physica B 230-232, 992 (1997).
12 W. Bao, A. H. Lacerda, J. D. Thompson, J. M. Honig, and P. Metcalf, Phys. Rev. B 63, 052410 (2001).
13 Wei Bao, private communication.
14 T. Wolenski, M. Grodzicki, and J. Appel, Phys. Rev. B 58, 303 (1998).
15 L. F. Mattheiss, J. Phys.: Condens. Matter 6, 6477 (1994).
16 S. Yu. Ezhov, V. I. Anisimov, D. I. Khomskii, and G. A. Sawatzky, Phys. Rev. Lett. 83, 4136 (1999).
17 V. Eyert, private communication.
18 Y. Sato and S. Akimoto, J. Appl. Phys. 50, 5285 (1979).
19 L. W. Finger and R. M. Hazen, J. Appl. Phys. 51, 5362 (1980).
20 O. Müller, J. P. Urbach, E. Goering, T. Weber, R. Barth, H. Schuler, M. Klemm, S. Horn, and M. L. denBoer, Phys. Rev. B 56, 15056 (1997).
21 L. F. Mattheiss, J. Phys.: Condens. Matter 8, 5987 (1996).