PHYSICAL REVIEW B **72**, 085453 (2005)

Temperature-dependent scanning tunneling spectroscopy of Cr(001): Orbital Kondo resonance versus surface state

T. Hänke, M. Bode,* S. Krause, L. Berbil-Bautista, and R. Wiesendanger
Institute of Applied Physics and Microstructure Research Center, University of Hamburg, Jungiusstrasse 11,
D-20355 Hamburg, Germany

(Received 14 April 2005; published 25 August 2005)

The temperature-dependent surface electronic structure of Cr(001) is investigated by means of scanning tunneling spectroscopy (STS) in the temperature range between 22 and 350 K. Consistent with earlier observations, a sharp peak is found in the tunneling spectra close to the Fermi level E_F. While the binding energy remains unchanged, the peak broadens with increasing temperature. The experimental data are fitted within the framework of two physical models, i.e., in terms of a single-particle band theory and an orbital Kondo effect. Both models lead to a reasonable agreement between the fit and the experimental data. Using the Kondo model, a Kondo temperature T_K of 123 K is obtained. If interpreted in terms of a single-particle band theory, the fit results in an electron-phonon mass-enhancement factor λ, which is 5–10 times larger than the Cr bulk value.

DOI: 10.1103/PhysRevB.72.085453 PACS number(s): 68.37.Ef, 71.38.−k, 72.10.Di, 72.15.Qm

I. INTRODUCTION

The electronic structure of the Cr(001) surface has recently been intensively investigated, mainly due to peculiar magnetic properties of elemental Cr exhibiting antiferromagnetism and a long-period spin density wave. Though the experimental and theoretical data remained contradictory. In a combined experimental and theoretical work, Klebanoff *et al.*[1] found occupied and empty surface states of $d_{xz,yz}$-orbital symmetry, which are energetically located about 1 eV below and above the Fermi level E_F, respectively. Furthermore, a peak close to E_F was observed and explained in terms of a d_{z^2}-like surface state.[2] Later on, Stroscio *et al.*[3] supported this interpretation. By using scanning tunneling spectroscopy (STS), a narrow maximum of the differential conductance dI/dU was observed at 0.05 eV below the Fermi level (occupied states).[3] This maximum was attributed to a spin-polarized Shockley-like surface state with a d_{z^2}-orbital character which—according to band structure calculations in the density functional theory scheme—is a general property of a bcc(001) surface. It has to be mentioned, however, that in all the calculations mentioned above the experimentally observed binding energy could only be reproduced if the Cr surface magnetic moment—which is consistently determined to about $2.5\mu_B$ in both experimental[1] and self-consistent density functional calculations[3]—is arbitrarily reduced (e.g., down to $1.75\mu_B$ in Ref. 3).

In order to unravel this apparent inconsistency, Kolesnychenko *et al.*[4] recently proposed a different interpretation of the density of states peak close to E_F in terms of a Kondo resonance. Owing to a sophisticated preparation procedure that is based on the cleavage of bulk crystals at low temperature,[5] they were able to produce the Cr(001) surface with an unprecedented cleanliness only limited by the concentration of bulk impurities. Scanning tunneling microscopy (STM) experiments performed on these surfaces revealed interference patterns which are inconsistent with a d_{z^2}-like surface state but rather supports a $d_{xz,yz}$-orbital symmetry. In contrast to earlier interpretations, the narrow resonance is explained by an orbital Kondo resonance formed by the above mentioned two degenerated spin-split d_{xz}, d_{yz} surface states located about 1 eV below and above E_F.[4] Similar to the conventional (magnetic) Kondo effect, where the local magnetic moment is screened by a spin-flip mechanism, the orbital Kondo resonance results from the flip of the orbital moment of the d_{xz}, d_{yz} surface state, thereby forming a many-body "orbital singlet."[4]

To get a better data basis for the decision as to which one of the two inconsistent physical interpretations mentioned above is correct, the Shockley-like surface state model within single-particle band theory or the many-body Kondo resonance model, we have performed a temperature-dependent STS study of the spectral shape of the relevant peak. These experiments cover a wide temperature range between 22 K and 350 K, thereby crossing both the magnetic phase transition temperatures of bulk Cr, i.e., the Néel temperature $T_N = 311$ K and the spin-flip temperature $T_{SF} = 123$ K, and the Kondo temperature T_K. While the peak position remains essentially unchanged, our experiments reveal a significant broadening of the peak with increasing temperature. The temperature-dependent spectral shape is fitted within the framework of the two models. While the data can consistently be described within the Kondo model, electron-phonon coupling can only explain the data if the electron-phonon coupling constant λ is one order of magnitude higher than in $\vec{k}$-averaged bulk data.

II. EXPERIMENTAL SETUP AND MEASUREMENT PROCEDURES

The STS experiments were performed in an ultrahigh vacuum (UHV) system with two separate chambers: (i) a preparation chamber for the tip and sample treatment and (ii) an analysis chamber for sample surface characterization by means of low-energy electron diffraction (LEED) and Auger-electron spectroscopy (AES). Furthermore, a satellite of the analysis chamber contains a home-built scanning tunneling microscope which operates at temperatures between 20 K and 350 K. It has a maximum scan range of (8×8) μm^2 at room temperature (RT) and (5×5) μm^2 at 20 K. The core of the scanning tunneling microscope is similar in design to the microscope described in Ref. 6 and is equipped with a tip exchange mechanism, too. In contrast to some commercially available variable-temperature scanning tunneling microscopes, where only the sample is cooled while the tip always remains at RT, the entire microscope including tip and scanner is cooled in our setup by connecting the scanning tunneling microscope via a highly flexible cooper braid to the cold finger of a continuous flow liquid He cryostat. To protect the scanning tunneling microscope from ambient heat radiation, the microscope is situated inside a radiation shield that is connected with a second copper braid to the outer radiation shield of the cryostat being cooled by the exhaust He. For vibration isolation the entire setup is mounted on top of an eddy current damping stage. A resistive heater inside the flow cryostat allows the precise variation of temperature. The base pressure in both chambers is in the low 10^{-11} torr range.

All experiments were performed using a (001)-oriented Cr single crystal, which has the shape of a disk with a 10-mm diameter and 0.8-mm thickness. As already described in previous publications,[7,8] the Cr(001) single crystal was cleaned by prolonged cycles of Ar$^+$-ion etching at elevated temperatures $(T\leqslant 1100$ K) and subsequent annealing for 20–30 min at $T=1150$ K. Compared to earlier results, the amount of residual impurities could be reduced significantly by using an Ar$^+$-ion gun with a mass filter (Wien filter). Eventually, the Cr(001) surface contains about 1% contaminants, which—according to our AES analysis—are mostly carbon (C). All other elements, e.g., O, S, and N, are below the AES sensitivity limit of $\leqslant 1\%$.

STM images were recorded in the constant-current mode at a stabilizing current I_{stab} and a bias voltage U_{stab} applied to the sample. We use polycrystalline W tips, which were electrochemically etched *ex situ* and cleaned *in vacuo* by a high-temperature flash at $T\geqslant 2200$ K. The STM topographic data were plane fitted to compensate for misalignment of tip and sample. We enhanced the contrast of some STM images by mixing the topographic height with its derivative along the fast scan direction.

With both tip and sample held at the same temperature T, spectroscopic information is obtained by adding a small ac modulation voltage $U_{\mathrm{mod}}=5$ mV$_{\mathrm{rms}}$ $(\nu=5.777$ kHz) to the bias voltage U_{stab}. We have confirmed that a further reduction of U_{mod} does not lead to a narrower linewidth. At every point (x,y) of the image, the tip is first stabilized at U_{stab} and I_{stab}. After opening the feedback loop, the bias voltage is linearly ramped from the stabilization value U_{stab} to a final value. Simultaneously, the $dI/dU(U,x,y)$ signal is measured by the lock-in technique. The resulting $dI/dU(U,x,y)$ spectrum is a measure of the sample's local density of states (LDOS) at the position (x,y) below the tip apex with U corresponding to the electron energy with respect to E_{F}.[9–11] The overall spectroscopic energy resolution is given by

$$\Delta E = \sqrt{(3.3\times k_{\mathrm{B}}T)^2 + (2.5\times eU_{\mathrm{mod}})^2}. \qquad (1)$$

To correct for binding energy shifts due to the finite time constant, the spectra were recorded in both directions, i.e., from negative to positive sample bias and vice versa.

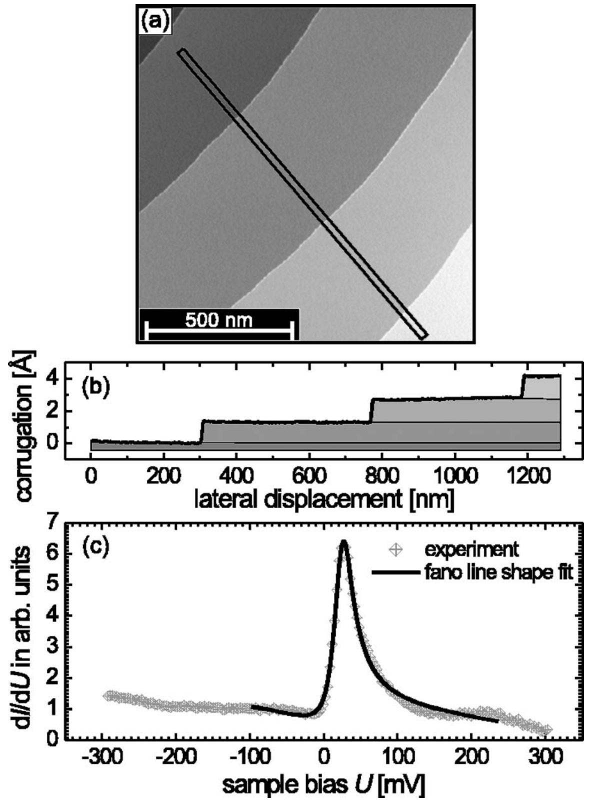

FIG. 1. (a) Topographic STM image of a clean Cr(001) surface (tunneling parameters: $U=-0.12$ V and $I=0.3$ nA). (b) Line section taken along the box in (a). Atomically flat terraces are separated by monatomic steps of 1.44 Å height. (c) Tunneling dI/dU spectrum of Cr(001) measured at 22 K in the middle of a terrace (measurement parameters: $U_{\mathrm{stab}}=-0.3$ V and $I_{\mathrm{stab}}=0.7$ nA). The solid black line is a Fano fit to the data with $\Gamma/2=15.4\pm0.3$ meV, $q=3.9\pm0.16$ meV, and $\varepsilon_0=22.9\pm0.3$ meV.

III. RESULTS AND DISCUSSION

A. The clean Cr(001) surface at 22 K

The surface electronic structure of Cr(001) may strongly depend on the surface quality. Since the Cr(001) surface studied here is prepared by Ar$^+$-ion etching and annealing while a related study used surfaces created by cleavage of bulk crystals[4] we have to verify first that both surfaces exhibit the same electronic properties. This is done at the lowest accessible temperature of our experimental setup, i.e., 22 K. Figure 1(a) shows a typical topographic image of a sputter-cleaned Cr(001) surface. Five terraces can be recognized, which descend from lower right to the upper left edge of the image. Higher resolution STM topographs reveal a surface defect concentration in the order of 1% of the surface atoms in agreement with the AES results mentioned above. The section in panel (b) has been drawn along the black line in Fig. 1(a). Adjacent terraces are separated by monatomic steps of 1.44 Å height. This terrace and step structure, which is found on any real surface, is the result of a slight miscut [locally about 0.04°, averaged over the whole sample surface approximately 0.15° with respect to the ideal (001) surface]. The surface electronic structure can be characterized by STS measurements. Figure 1(c) shows a STS spectrum taken in the middle of a Cr(001) terrace far apart (≈3 nm) from defect sites. A strong and very narrow peak at ~20 mV above the Fermi level can be seen. Qualitatively, our data are in accordance with the results measured on cleaved Cr(001).[4,5] For a more quantitative analysis, we may follow the procedure of Kolesnychenko *et al.*[4] by fitting the measured STS spectra by a Fano resonance[12,13]

$$\frac{dI}{dU} \propto \frac{(q+\varepsilon')^2}{1+\varepsilon'^2}, \quad \varepsilon' = \frac{eU-\varepsilon_0}{\Gamma/2}. \tag{2}$$

Here q reflects the ratio of the matrix elements linking the initial state to the discrete continuum, ε_0 is the energetical position of the resonance, and Γ is the resonance width [full width at half maximum (FWHM)]. The best fit of our data is achieved for $\Gamma/2=15.4\pm0.3$ meV and $\varepsilon_0=22.9\pm0.3$ meV, which is in good agreement with the values of Ref. 4, i.e., 15 meV and 20 meV, respectively. At this point we can conclude that regarding its electronic properties, the sample quality of our sputter-cleaned Cr(001) surface is fully comparable with the surfaces prepared by cleavage at low temperature, despite the fact that it exhibits a slightly higher defect concentration.

B. Temperature-dependent STS

Due to the experimental requirement of a very good temperature stability during the measurement ($\Delta T \leqslant 0.05$ K) and the relatively high reactivity of Cr, it was not possible to measure a complete temperature series within a single experimental run using the same tip and the same sample surface. Instead, we had to perform an experimental run with a newly prepared tip and sample for each particular temperature. For the ease of comparability, we always performed the same experimental course with the stabilization parameters $U_{\text{stab}}=-0.4$ V and $I_{\text{stab}}=0.5$ nA and the same energy resolution employing 400 points in the energy range of ±0.4 V. In each case, 100 spectra were taken in the middle of an atomically flat Cr(001) terrace. Measured tunneling dI/dU spectra (open circles) of 8 selected temperatures (out of a total of 12) covering the range between 22 K and 350 K are shown in Fig. 2(a). Although it broadens significantly with increasing temperature, the peak close to the Fermi level can clearly be recognized throughout the entire temperature range. The peak position remains constant within the limits of our experimental accuracy of a few meV.

In the following, we will discuss the temperature dependence of the spectral shape in the framework of two different models, i.e., Kondo theory and single-particle band theory.

1. Many-body Kondo effect

The Kondo effect is a well-known many-body phenomenon and describes how localized electrons interact with delocalized electrons by the formation of a many-body singlet state, thereby enhancing the LDOS near the Fermi level.[14] Important characteristics of the Kondo effect are the splitting of the Kondo resonance under an applied magnetic field and the broadening and reduction of the Kondo resonance at increasing temperatures.[15–21]

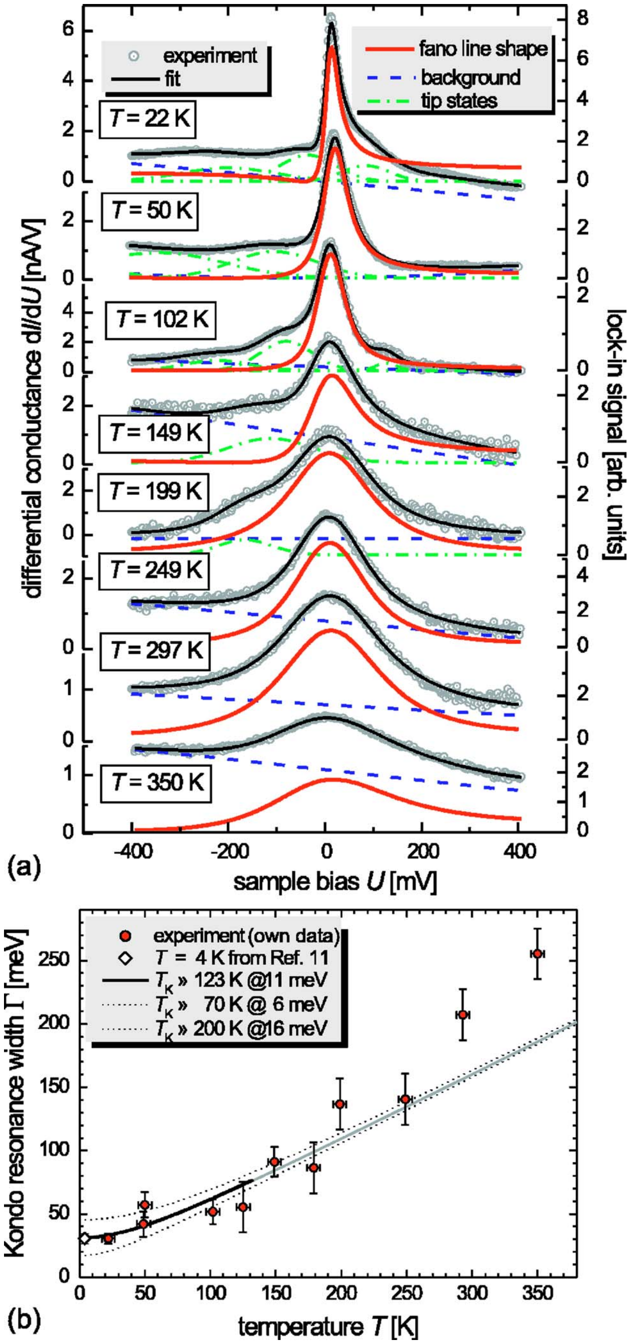

FIG. 2. (Color online) (a) STS spectra of Cr(001) measured at eight different temperatures between 22 K and 350 K (open circles). The experimental data were fitted by a Fano line shape for the peak close to E_F (solid red line), Gaussian peaks to account for tip states (dash-dotted line), and a linear background (dashed line). (b) Width Γ of the Fano peak used to fit the data of (a). The solid and dotted curves show the theoretical temperature dependence given by Eq. (4) for different Kondo temperatures T_K. The best fit is obtained for $T_K=123$ K (≈11 meV).

As recently shown for Ti atoms on Ag(100),[22] it is a nontrivial task, however, to deconvolute the intrinsic temperature-induced variation of the sample's density of states from the temperature-dependent broadening of the tip's Fermi level. As one takes the standard relation for STM dI/dU spectra[23]

$$\frac{dI}{dU}(U,T) = \int_{-\infty}^{+\infty} \rho_t \rho_s(E,T) \frac{d}{dU} F(E - eU, T) dE, \tag{3}$$

where $\rho_s(E,T)$ is the energy-dependent and temperature-dependent local density of states (LDOS) of the surface, ρ_t is the LDOS of the STM tip (assumed to be featureless), and $F(E,T)$ is the Fermi-Dirac distribution, it can be seen that the measured dI/dU signal is always a convolution of the sample LDOS ρ_s and the derivative of the Fermi-Dirac distribution. In order to extract the intrinsic LDOS feature from the spectra at higher temperatures, a Fano resonance line shape given by Eq. (2) (solid gray line) were taken and thermally broadened using Eq. (3) in order to fit the experimental data of Fig. 2. Probably due to tips with pronounced electronic states, it was necessary in some cases (see, e.g., data measured at $T = 102$ K) to add further Gaussian-shaped peaks to the fitting procedure (dash-dotted lines). Furthermore, a linear background (dashed line) was added. Obviously, a reasonable overall agreement between experimental spectra and the fit is achieved.

On the basis of the fitting procedure we can extract the temperature dependence of the width Γ of the dI/dU spectroscopy peak if interpreted in terms of a Kondo resonance [Fig. 2(b)]. The observed behavior of Cr(001) is similar to Ti/Ag(100) (Ref. 22) and also shows a quadratic increase of the width at low temperatures that becomes linear as the temperature is further increased. Following Refs. 21 and 22 in the temperature regime $T \leqslant T_K$ the temperature dependence of the width of a magnetic spin-flip Kondo resonance is given by

$$\Gamma = 2\sqrt{(\pi k_B T)^2 + 2(k_B T_K)^2}. \tag{4}$$

Here T_K is the only fitting parameter that solely allows to adjust the offset at zero temperature. The best result is obtained for $T_K \approx 123$ K ($\cong 11$ meV).[24] Comparison between the experimental data of Fig. 2(b) and a plot of Eq. (4) reveals an excellent overall agreement in the temperature range up to 200 K, i.e., much higher than the actual T_K, which is usually considered as the upper limit of validity of the underlying theory.[22,25] Only above 200–250 K do the experimental data points start to deviate from the theoretical model.

2. Single-particle surface electronic state

The electronic structure and dynamics of surface states has recently attracted substantial attention. Improved experimental and theoretical techniques eventually led to converging results for noble metals,[26] but much less is known about the more complex transition metals. In the following, we will discuss our Cr(001) data in terms of single-particle band theory.

As show in Ref. 27, the lifetime τ of electronic states in nonmagnetic metals is determined by three main contributions: (i) electron-electron (*e-e*) scattering,[28,29] (ii) scattering by impurities or defects, and (iii) electron-phonon (*e-ph*) scattering.[30] If magnetic materials are considered, there is an additional contribution, i.e., electron-magnon (*e-m*) scattering.[31] The (*e-e*)-scattering contribution to the linewidth $\Gamma_{e\text{-}e}$ is given by Fermi liquid theory,[27,28]

$$\Gamma_{e\text{-}e} = 2\beta[(k_B T)^2 + (E - E_F)^2]. \tag{5}$$

Since the factor β is of the order of 1 eV^{-1} and since the results discussed here were measured at a low temperature, the temperature-dependent term in Eq. (5) is very small and can be neglected. Furthermore, the binding energy $E - E_F$ of the Cr(001) peak amounts to a few meV only. Thus, the second term can also be neglected. The impurity scattering contribution is proportional to the impurity concentration, but independent of temperature and binding energy. Therefore, it may only lead to a temperature-independent broadening of the linewidth, visible as an offset at 0 K. For the bulk, the magnitude of the effect is about 10 meV %.[31,32] The only remaining contribution comes from electron-phonon (*e-ph*) scattering. Within the Debye model the inverse lifetime due to (*e-ph*) processes can be calculated from the following formula:

$$\Gamma_{e\text{-}ph}(E,T) = \frac{\hbar}{\tau(E,T)} = \lambda \frac{2\pi}{(\hbar\omega_D)^2} \int_0^{\hbar\omega_D} dE' E'^2 \times [1 - f(E - E') + 2n(E') + f(E + E')], \tag{6}$$

where ω_D is the Debye frequency, λ the electron-phonon mass-enhancement factor, $f(E)$ the Fermi distribution, and $n(E)$ the Bose-Einstein distribution. At high temperatures the phonon scattering $\Gamma_{e\text{-}ph}$ shows a linear dependence $d\Gamma_{e\text{-}ph}/dT \cong 2\pi\lambda k_B$ and is independent of ω_D.

In a recent STS study by Rehbein *et al.*,[33] the temperature-dependent broadening of Gd(0001) surface states was successfully explained by (*e-ph*) scattering and the formal description by Eq. (6). We have applied the same fitting routine to fit the temperature-dependent spectral shape of the dI/dU peak on Cr(001). In general, the fitting procedure is similar to Sec. III B 1 but the Fano line shape, which is adequate to the Kondo effect but not reasonable in the case of (*e-ph*) scattering, is replaced by a Lorentzian function. The result is shown in Fig. 3(a). The extracted linewidth of the Lorentzian (FWHM) is plotted in Fig. 3(b). A quantitative description based on Eqs. (6) and (5) requires the knowledge of three parameters λ, ω_D^{surf}, and $\Gamma_{e\text{-}e}$. As mentioned above, $\Gamma_{e\text{-}e}$ can be estimated by the peak width at zero temperature ($T = 0$ K). Owing to the lack of specific surface parameters for the Debye frequency, we may use the Cr bulk value $\hbar\omega_D^{\text{bulk}} = 52.5$ meV.[34] Using a binding energy of $E_0 = 20 \pm 5$ meV, the fitting procedure results in $\lambda = 1.51 \pm 0.40$ and $\Gamma_{e\text{-}e} = 19.5 \pm 3$ meV. Of course, the surface Debye frequency $\hbar\omega_D^{\text{surf}}$ must not be identical to the bulk value. Even if the experimental data are fitted with two fit parameters, $\hbar\omega_D^{\text{surf}}$ and λ, the values change only slightly and we obtain $\hbar\omega_D^{\text{surf}} = 53$ meV and $\lambda = 1.53 \pm 0.40$.

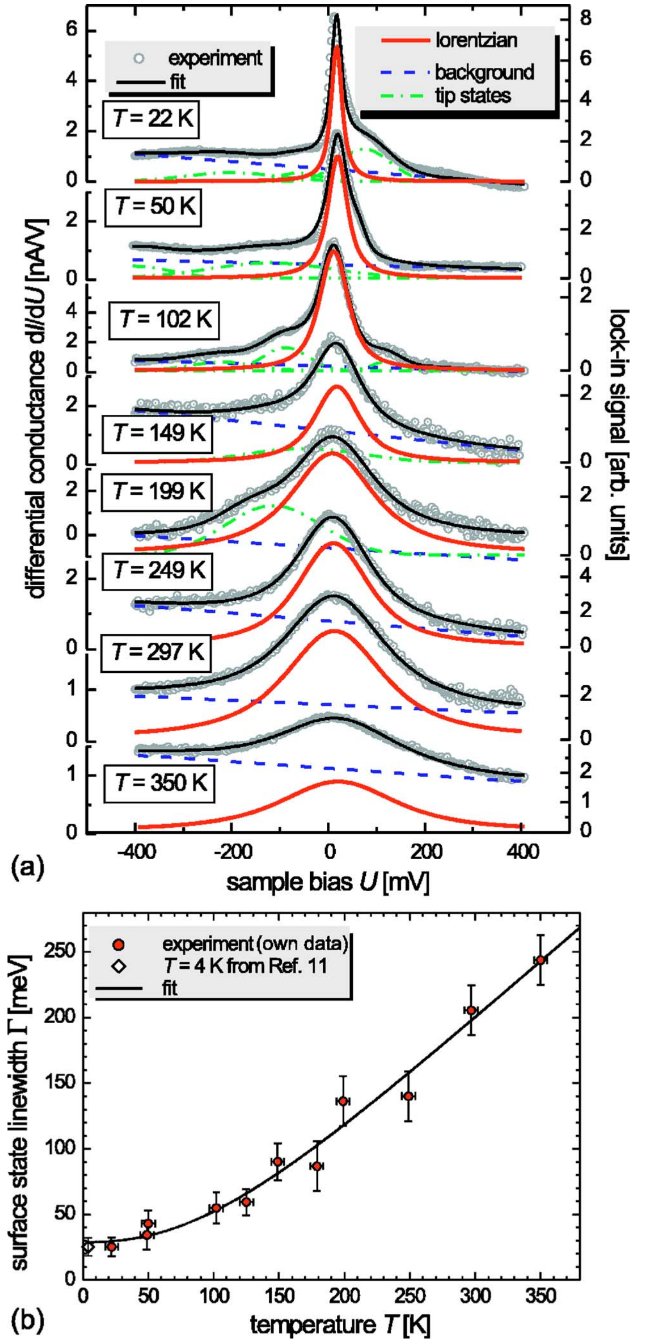

FIG. 3. (Color online) (a) STS spectra of Cr(001) measured at eight different temperatures between 22 K and 350 K (open circles). The experimental data were fitted by a thermally broadened Lorentzian line shape for the peak close to E_F (solid red line), Gaussian peaks to account for tip states (dash dotted line), and a linear background (dashed line). (b) Width Γ of the Lorentzian used to fit the data of (a). The solid curve shows the theoretical temperature dependence given by Eq. (6) for $\hbar\omega_D^{\text{bulk}}=52.2$ meV and $\lambda=1.5$.

C. Discussion

At this point we can recapitulate that our experimental data of the temperature-dependent peak shape of Cr(001) can nicely be fitted within the respective limits of validity of both physical models, i.e., a many-body Kondo effect and single-particle band theory. This is not unexpected as the peak width in both cases rises linear at high temperature. One possibility to estimate which of the two models describes the physical basis of the observations is an evaluation whether the procedures led to reasonable fitting parameters. In each model there is just one fitting parameter, i.e., the Kondo temperature T_K [cf. Eq. (4)] or the mass-enhancement factor λ [cf. Eq. (6)].

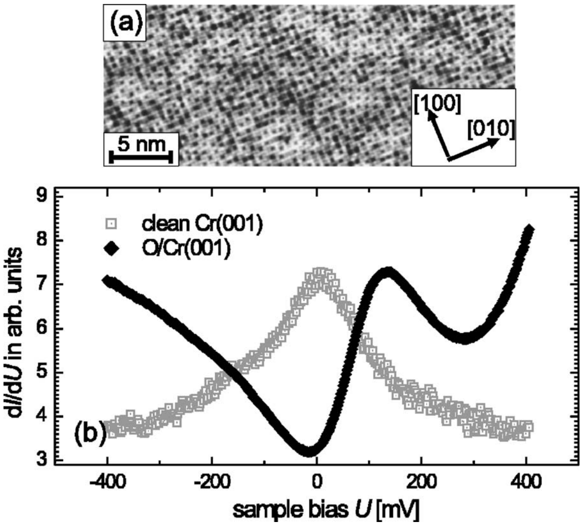

FIG. 4. (a) Topographic STM image of O/Cr(001) measured at $T=200$ K. The sample surface was dosed with 3 L O_2 at a sample temperature of $T=350$ °C. (b) Tunneling dI/dU spectra of clean (gray) and oxygen-covered Cr(001) (black). A considerable peak shift by ≈ 120 meV is observed.

Unfortunately, the Kondo temperature of Cr(001)—if it is a Kondo system—is unknown. But it is a remarkable coincidence that the determined value of $T_K \approx 123$ K is practically equal to the Cr spin-flip temperature T_{SF}. It is well known that the magnetic phase transitions of Cr are accompanied with structural transitions.[35] Due to the magnetoelastic interaction, which is mediated by spin-orbit coupling, the crystalline structure of Cr changes from cubic to orthorhombic at the paramagnetic-antiferromagnetic phase transition and eventually to tetragonal at the spin-flip temperature T_{SF}. One may speculate about possible orbital-order scenarios which have recently attracted considerable interest mainly in context with metal-insulator and normal-superconductor transitions.[36]

In contrast, the electron-phonon mass enhancement factor λ of polycrystalline Cr on a glass substrate was determined experimentally and theoretically. Optical pump-and-probe experiments give $\lambda=0.13\pm0.02$.[37] This value is rather close to the result of strong-coupling theory for paramagnetic Cr ($\lambda=0.25$).[38] The fitting procedure of our STS data, in contrast, yields a value which is 5–10 times larger. At first sight this seems to be inconsistent with earlier results on bulk Cr, thereby excluding the single-particle band model and supporting the Kondo model. Recent experiments on various elements revealed, however, that the surface electron-phonon mass enhancement factor λ may deviate considerably from the $\vec{k}$-integrated bulk value. For example, a strong enhancement of λ at the W(110) surface compared to bulk W was found, which was attributed to the degree of surface localization of the surface electron wave function.[39] Similar observations were made on Be$(10\bar{1}0)$.[40] Furthermore, a strong dependence on the binding energy was observed for Bi(100).[41] Even within one particular electron band λ may vary by more than one order of magnitude, depending on the wave vector $\vec{k}$.[42] Given the fact that our measurement technique (STS) is highly surface sensitive and governed by surface LDOS contributions from the $\bar{\Gamma}$ point of the surface Brillouin zone, a mass-enhancement factor $\lambda = 1.5$ cannot be excluded.

We may conclude that our temperature-dependent STS data of Cr(001) are not sufficient for a definite decision between the two available models. For the Kondo resonance we found a quite good agreement between our experiment and the theoretical prediction, although the theory was formally developed for spin-flip scattering at single magnetic impurity atoms on open surfaces. On the other hand, the analysis in terms of thermally broadened electron bands leads to a rather large mass-enhancement factor λ which is by a factor of 5–10 times larger than the bulk value—a scenario which cannot be excluded at present.

We would like to propose two routes for an *experimentum crucis* being capable of a decisive determination on which of the two hypotheses, the orbital Kondo effect or a surface state, is correct. One possibility is to observe the effect of an increasing adsorbate concentration on the peak position and height. We have performed preliminary experiments with oxygen on Cr(001). As shown in Fig. 4(a) the exposure to 3 L O_2 at $T = 350$ °C leads to a $(\sqrt{5} \times \sqrt{5})R27°$ reconstruction of the Cr(001) surface.[43] The tunneling dI/dU spectrum measured on the oxygen-covered Cr surface is compared to the spectrum of clean Cr(001) in Fig. 4(b). Both spectra were taken with different tips but at the same sample temperature $T = 200$ K. Obviously, the oxygen-treated surface exhibits a peak at ≈135 meV. This peak cannot be related to a Kondo resonance because it is too far apart from the Fermi level. It is, however, not yet clear whether the peak continuously shifts with increasing oxygen concentration or if the Cr-related peak intensity decreases while a new impurity-induced surface state arises as recently found for SiC(100).[44] Further experimental and theoretical effort is necessary to clarify the situation. Another *experimentum crucis* may be a magnetic-field-dependent study of the Cr(001) peak shape. Detailed theoretical predictions of the field-dependent spectral shape of an orbital Kondo resonance are available.[45] Although enormous fields are required to cause a significant effect, recently developed scanning tunneling microscopes,[6] which are able to measure at extremely low temperatures in fields up to 14 T, may be able to bring about a decision.

IV. SUMMARY

In summary, we have performed a temperature-dependent electronic structure investigation of the Cr(001) surface by means of variable-temperature scanning tunneling spectroscopy (STS). Our study covers a wide temperature range ($22\text{ K} \leqslant T \leqslant 350\text{ K}$), which includes the bulk magnetic phase transition temperatures as well as the possible Kondo temperature. We observe a sharp peak close to the Fermi level E_F, which is consistent with earlier STS experiments. While the binding energy remains unchanged, the peak broadens with increasing temperature. Our experimental data are fitted within the framework of two physical models, i.e., single-particle band theory and Kondo theory. Both models lead to an excellent agreement between the fit and the experimental data in the low temperature regime. Using the Kondo model, a Kondo temperature T_K of 123 K is obtained. If interpreted in terms of a single-particle band theory, the fit results in an electron-phonon mass-enhancement factor λ which is 5–10 times larger than the Cr bulk value. In this case the experimental data in the entire temperature range can be nicely reproduced by the theory.

ACKNOWLEDGMENTS

We thank D. Wegner (FU Berlin) and M. Morgenstern (RWTH Aachen) for helpful discussions. Financial support from the DFG Graduate Schools "Spectroscopy of localized atomic systems" and "Design and characterization of functional materials" is gratefully acknowledged.

---

*Corresponding author. Electronic address: mbode@physnet.uni-hamburg.de; URL: http://www.nanoscience.de/bode

[1] L. E. Klebanoff, S. W. Robey, G. Liu, and D. A. Shirley, Phys. Rev. B **30**, 1048 (1984).

[2] L. E. Klebanoff, R. H. Victora, L. M. Falicov, and D. A. Shirley, Phys. Rev. B **32**, 1997 (1985).

[3] J. A. Stroscio, D. T. Pierce, A. Davies, R. J. Celotta, and M. Weinert, Phys. Rev. Lett. **75**, 2960 (1995).

[4] O. Y. Kolesnychenko, R. de Kort, M. I. Katsnelson, A. I. Lichtenstein, and H. van Kempen, Nature (London) **415**, 507 (2002).

[5] O. Y. Kolesnychenko, R. de Kort, and H. van Kempen, Surf. Sci. **490**, 537 (2001).

[6] J. Wiebe, A. Wachowiak, F. Meier, D. Haude, T. Foster, M. Morgenstern, and R. Wiesendanger, Rev. Sci. Instrum. **75**, 4871 (2004).

[7] M. Kleiber, M. Bode, R. Ravlić, and R. Wiesendanger, Phys. Rev. Lett. **85**, 4606 (2000).

[8] M. Kleiber, M. Bode, R. Ravlić, N. Tezuka, and R. Wiesendanger, J. Magn. Magn. Mater. **240**, 64 (2002).

[9] J. Tersoff and D. R. Hamann, Phys. Rev. Lett. **50**, 1998 (1983).

[10] J. Tersoff and D. R. Hamann, Phys. Rev. B **31**, 805 (1985).

[11] M. Morgenstern, D. Haude, V. Gudmundsson, C. Wittneven, R. Dombrowski, C. Steinebach, and R. Wiesendanger, J. Electron Spectrosc. Relat. Phenom. **109**, 127 (2000).

[12] J. Li, W.-D. Schneider, R. Berndt, and B. Delley, Phys. Rev. Lett. **80**, 2893 (1998).

[13] V. Madhavan, W. Chen, T. Jamneala, M. F. Crommie, and N. S. Wingreen, Science **280**, 569 (1998).

[14] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, UK, 1993).

[15] T. A. Costi, A. C. Hewsont, and V. Zlatić, J. Phys.: Condens. Matter **6**, 2519 (1994).

[16] T. Kawasakaa, H. Kasai, W. A. Diño, and A. Okiji, J. Appl. Phys. **86**, 6970 (1999).

[17] A. Schiller and S. Hershfield, Phys. Rev. B **61**, 9036 (2000).

[18] M. Plihal and J. W. Gadzuk, Phys. Rev. B **63**, 085404 (2001).

[19] T. A. Costi, Phys. Rev. Lett. **85**, 1504 (2000).

[20] W. G. van der Wiel, S. D. Franceschi, T. Fujisawa, J. M. Elzerman, S. Tarucha, and L. P. Kouwenhoven, Science **289**, 2105 (2000).

[21] P. S. Cornaglia and C. A. Balseiro, Phys. Rev. B **67**, 205420 (2003).

[22] K. Nagaoka, T. Jamneala, M. Grobis, and M. F. Crommie, Phys. Rev. Lett. **88**, 077205 (2002).

[23] J. Bardeen, Phys. Rev. Lett. **6**, 57 (1961).

[24] Note that in Ref. 4, the peak width Γ was mistakenly labeled T_{K}.

[25] P. Nozières, J. Low Temp. Phys. **17**, 31 (1974).

[26] P. M. Echenique, R. Berndt, E. V. Chulkov, T. Fauster, A. Goldmann, and U. Höfer, Surf. Sci. Rep. **52**, 219 (2004).

[27] B. A. McDougall, T. Balasubramanian, and E. Jensen, Phys. Rev. B **51**, R13891 (1995).

[28] J. J. Quinn, Phys. Rev. **126**, 1453 (1962).

[29] J. J. Quinn and R. A. Ferrell, Phys. Rev. **112**, 812 (1958).

[30] G. Grimmvall, *The Electron-Phonon Interaction in Metals* (North-Holland, New York, 1981).

[31] P. Allen, Comments Condens. Matter Phys. **15**, 327 (1992).

[32] D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1969).

[33] A. Rehbein, D. Wegner, G. Kaindl, and A. Bauer, Phys. Rev. B **67**, 033403 (2003).

[34] C. Kittel, *Introduction to Solid State Physics* (John Wiley and Sons, New York, 1991), 6th ed.

[35] H. Zabel, J. Phys.: Condens. Matter **11**, 9303 (1999).

[36] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).

[37] S. D. Brorson, A. Kazeroonian, J. S. Moodera, D. W. Face, T. K. Cheng, E. P. Ippen, M. S. Dresselhaus, and G. Dresselhaus, Phys. Rev. Lett. **64**, 2172 (1990).

[38] W. L. McMillan, Phys. Rev. **167**, 331 (1968).

[39] E. Rotenberg, J. Schaefer, and S. D. Kevan, Phys. Rev. Lett. **84**, 2925 (2000).

[40] S.-J. Tang, Ismail, P. T. Sprunger and E. W. Plummer, Phys. Rev. B **65**, 235428 (2002).

[41] J. E. Gayone, S. V. Hoffmann, Z. Li, and P. Hofmann, Phys. Rev. Lett. **91**, 127601 (2003).

[42] E. Rotenberg and S. D. Kevan, J. Electron Spectrosc. Relat. Phenom. **126**, 125 (2002).

[43] M. Schmid, G. Leonardelli, M. Sporn, E. Platzgummer, W. Hebenstreit, M. Pinczolits, and P. Varga, Phys. Rev. Lett. **82**, 355 (1999).

[44] R. DiFelice, C. M. Bertoni, C. A. Pignedoli, and A. Catellani, Phys. Rev. Lett. **94**, 116103 (2005).

[45] A. K. Zhuravlev, V. Y. Irkhin, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. Lett. **93**, 236403 (2004).