Data Evaluation for Spin-Polarized Scanning Tunneling Spectroscopy Measurements

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Abstract. Spin-polarized scanning tunneling spectroscopy measurements have been done on ultrathin bct Mn films grown on Fe(001)-whiskers. Emphasis is placed on the relationship between the feedback setpoint chosen for the tunneling spectroscopy measurements and the normalization procedures for the data, and the values obtained for the spin polarization of the surface electronic structure.

INTRODUCTION

The first observation of the spectral density of electronic states was made by Giaver [1] in metal-oxide-superconductor tunneling experiments. This work lead to the introduction to the new many-body transfer Hamiltonian approach in tunneling current calculation by Bardeen [2]. The invention of Scanning Tunneling Microscopy (STM) by G. Binnig and H. Rohrer [3] stimulated additional interest in the theory of tunneling. Using the transfer Hamiltonian formalism, tunneling in the STM was studied by Tersoff and Hamann [4] and other authors [5,6]. It was concluded that the tunneling current can be expressed as a simple convolution of the sample Density of States (DOS) and tip DOS with the effective matrix element for tunneling. A simple relation between the tunneling current and the sample DOS can be obtained in the one-dimensional and semiclassical Wentzel, Kramers and Brillouin (WKB) approximation. For a three dimensional problem the calculation of the effective matrix elements for tunneling is still an open question.

From the first experimental observation of the spectral density of the sample electronic states by STM, the first derivative of tunneling current over tip-sample voltage or differential conductivity, dI/dV, was used as measure of the sample DOS. This approach presents two problems, one is the influence of the tip DOS and the other is the effect of the tunneling transmission probability on the observed dependence of the tunneling current on sample voltage. These two problems are still mainly unsolved.

Since its introduction [7] Spin-Polarized Scanning Tunneling Microscopy (SP-STM) and Spectroscopy (SP-STS) has proven very powerful tools for studying surface magnetism with spatial resolution at atomic scale [8,9]. One of the most important issues is to understand the origin of the magnetic contrast in SP-STS images taken with magnetic tips. Although it has been reported that this magnetic contrast is related to the existence of spin-polarized surface states, this relation is not straightforward due to the influence of the tunneling probability.

In this paper we will discuss how to get quantitative information concerning the polarization of the sample and the influence of the setpoint bias voltage.

EXPERIMENTAL

STM and STS measurements were performed in ultra-high vacuum (~5×10^{-11} mbar) at room temperature (RT). Mn layers with a body-centered tetragonal (bct) structure were grown on an Fe(001)-whisker at 370 K. Details of the sample preparation and characterization are given in refs [10,11]. The tips used in the present study were W tips covered with 7-10 nm Fe at RT. The magnetic contrast obtained with these tips depends on the factor $\cos\theta$, where θ is the angle between the magnetization direction of the Fe-coated tip and the Mn layers. In the chamber we cannot apply any magnetic field to the tip or the sample. Therefore, the tip magnetization direction is randomly orientated with respect to the magnetization of the Mn layers and is different from tip to tip. The tip was carefully brought close to the sample to exclude any mass transport between tip and sample. STS measurements were performed at every pixel of a constant current topographic image by opening the STM feedback loop at a given voltage and current (setpoint). dI/dV, $(d\ln I/d\ln V)$ and $(dI/dV)/T$ curves were obtained by numerical calculation from the original I(V) curves.

RESULTS AND DISCUSSION

The growth mode of Mn layers on Fe(001) has been studied before [10,11]. For a Mn nominal thickness of 7 ML there are 4 different layers exposed on the surface, as it is shown in Figure 1a. Previous results showed that the intermixing between Fe and Mn takes place for the firsts Mn layers, but above 3 ML the intermixing of Fe on the Mn film can be neglected. At this surface, I(V) curves were measured with Fe-coated tips at every pixel of the topographic image using a setpoint of V_s=-0.5V and I=0.5nA. Every I(V) curve was numerically differentiated to obtain the dI/dV curve. In order to check the magnetic contrast in the spectroscopy data, dI/dV maps were obtained. Figure 1b shows the dI/dV map at +0.2V, the strong contrast in the spectroscopic image between layers is clear. The contrast oscillates with a periodicity of two layers. This contrast is also present on the step height measured on the topographic image with a sample voltage of +0.2 V as is shown in Figure 1c. This contrast is never observed with clean W tips [10]. With the help of Ab initio calculations the origin of this contrast was trace back to the existence of minority bands at the Γ point above the Fermi level in the surface Density of States (DOS) [12].

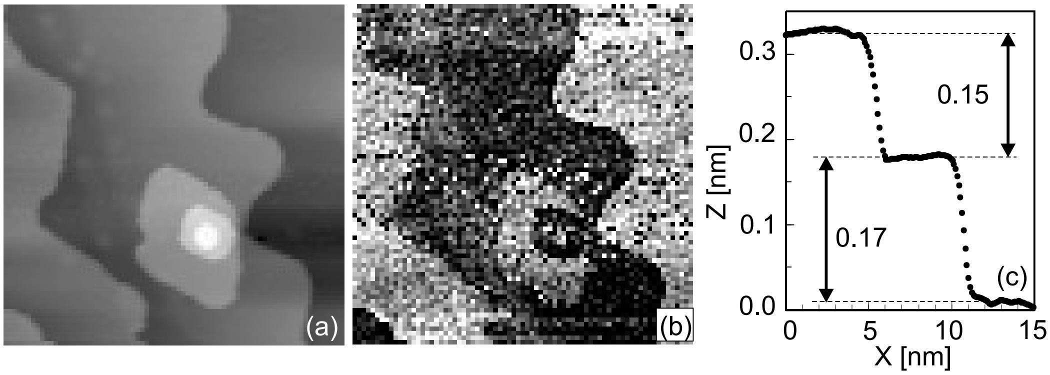

FIGURE 1. (a) STM topography, 70x70 nm^2 of the surface of 7ML Mn film on Fe(001) measured with a Fe-coated tip at a setpoint of V_s=-0.5V, I=0.5 nA. (b) d*I*/d*V* map at +0.2 V of the same area. A I(V) curve was measured in every pixel of the topography shown in (a) and them numerically differentiated. (c) Line profile measured on the Mn layers with an Fe-coated tip.

Various methods for extracting the sample polarization from SP-STS measurements have been reported [13,14]. However, these methods include a certain ambiguity. In all of them is necessary to know the polarization of the magnetic tips used to make the measurements. Other problem is that for a given setpoint voltage the tip-sample distance can change (and so the tunneling probability) between different Mn layers due to changes in the electronic structure. This is not something unexpected due to the spin-polarization of the DOS close to the Fermi level in magnetic materials and therefore, the spin-polarized component of the current changes for the different layers.

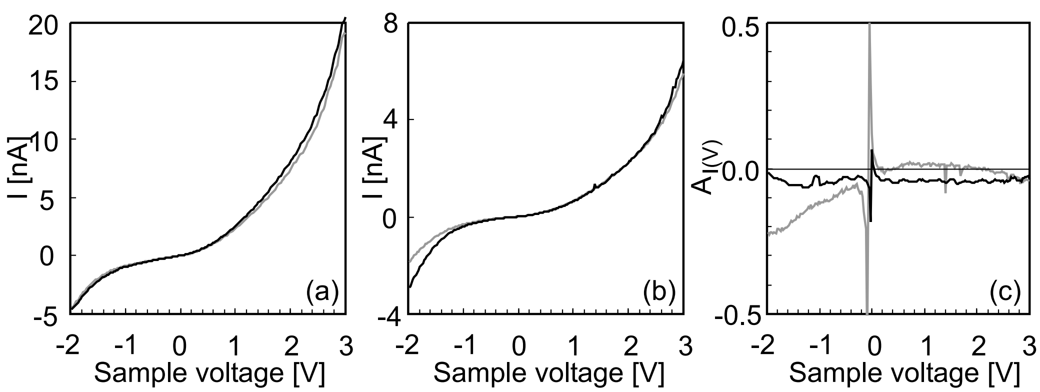

FIGURE 2. (a) I(V) curves measured in the odd (solid black curve) and even (solid grey curve) layers of 7ML of Mn grown on Fe(001) with an Fe-coated tip using a negative sample voltage setpoint (V_s= -0.5V, I= =0.5 nA). (b)) I(V) curves measured in the odd (solid black curve) and even (solid grey curve) layers of 7ML of Mn grown on Fe(001) with an Fe-coated tip using a positive sample voltage setpoint (V_s= +0.5V, I= =0.5 nA). (c) Asymmetry in the I(V) curves. Black solid line if for the I(V) curves measured with a negative voltage setpoint and the grey solid line is measured with a positive voltage setpoint. The asymmetry is defined as $A_{I(V)}=[I(V)_{odd}-I(V)_{even}]/[I(V)_{odd}+I(V)_{even}]$.

Figure 2 shows the I(V) curves measured with a Fe-coated tip on the even and odd Mn layers at negative (Fig. 2a, V_s= -0.5V) and positive (Fig. 2b, V_s= +0.5V) voltage and with the same current (I= 0.5 nA) setpoint. In both cases the I(V) curves show a difference between the even and odd Mn layers as is expected due to the different tunneling probability for the spin-polarized electrons. This difference in the tunneling probability allows us to take magnetic resolve images of the surface as shown in Figure 1b. The problem arises when we try to extract quantitative information about the sample polarization. Figure 2c shows the asymmetry obtained from the I(V) curves measured on different Mn layers. The asymmetry is defined as $A_{I(V)}=[I(V)_{odd}-I(V)_{even}]/[I(V)_{odd}+I(V)_{even}]$. The asymmetry obtained is strongly influenced by the voltage setpoint and can lead to wrong conclusions about the sample polarization.

This dependence is due to different tip-sample distance for the different voltage setpoints and also to the fact that both I(V) curves has the same intensity value for the voltage setpoint. The change in the tip-sample distance with the sample voltage is shown in Figure 1c where the apparent step height measured with a Fe-coated tip changes from terrace to terrace due to the changes in the sample magnetization and its influence in the tunneling transmission probability.

To get rid off this problem we numerically differentiate the I(V) curves. Panels (a) and (b) of Figure 3 show the results. The tunneling conductance also shows differences between the odd and even Mn layers. The shape of the d*I*/d*V* curves does not change depending on the voltage setpoint choose but it is clear that the energy range where the differences between the d*I*/d*V* curves measured in the odd and even layers are present depends strongly on the setpoint voltage.

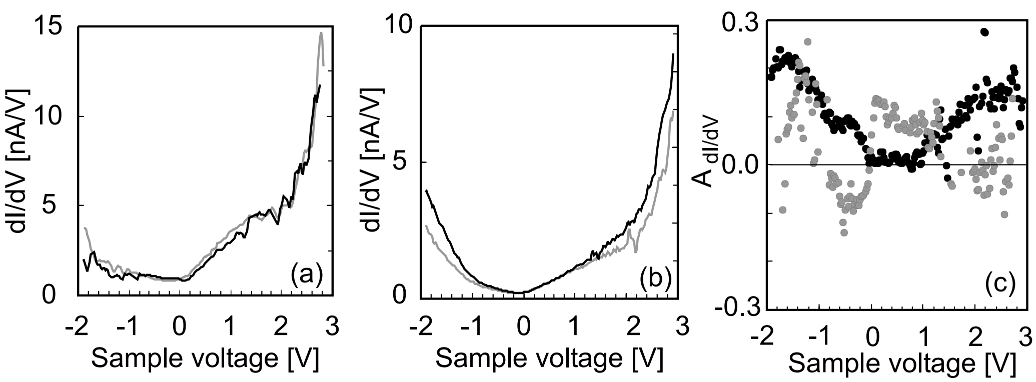

FIGURE 3. (a) d*I*/d*V* curves measured in the odd (solid black curve) and even (solid grey curve) layers of 7ML of Mn grown on Fe(001) with an Fe-coated tip using a negative sample voltage setpoint (V_s= -0.5V, I= =0.5 nA). (b)) d*I*/d*V* curves measured in the odd (solid black curve) and even (solid grey curve) layers of 7ML of Mn grown on Fe(001) with an Fe-coated tip using a positive sample voltage setpoint (V_s= +0.5V, I= 0.5 nA). (c) Asymmetry in the d*I*/d*V* curves. Grey dots are for the d*I*/d*V* curves obtained from measurements taken with a negative voltage setpoint and the black dots are for the positive voltage setpoint. The asymmetry is defined as $A_{dI/dV}=[(dI/dV)_{odd}-(dI/dV)_{even}]/[(dI/dV)_{odd}+(dI/dV)_{even}]$.

In a very simple approximation the tunneling conductance in STS can be related to the DOS of both tip and sample [15]. Figure 3 is a clear example of how this very simple approximation is not enough and it is necessary to take into account the tunneling transmission probability. In panel (c) of the Figure 3 we present the asymmetry of the d*I*/d*V* curves defined in the same way than before. The result on the asymmetry depends strongly on the setpoint chosen to stabilize the feedback in between the I(V) curves.

In general it is accepted that the tunneling conductance can be approximated in term of the DOS of the sample at a voltage V, plus a background term for positive sample voltage. For negative sample voltage the tunneling conductance is dominated by the electronic structure of the tip close to the Fermi level with a background. In both cases the background is given by the tunneling transmission probability that depends exponentially with the bias voltage [16]. In order to get best approximation to the DOS of the sample is necessary to remove the background given by the tunneling transmission probability and prepare tips with a featureless density of states around the Fermi level [17]. In order to remove the exponential background present on the tunneling conductance, Feenstra et al. [18] proposed the use of d$\ln I$/d$\ln V$ as a function that is a relatively direct measure of the DOS of the sample. This method was tested extensively in many experiments and demonstrated reasonable agreement with some experimental and theoretical data.

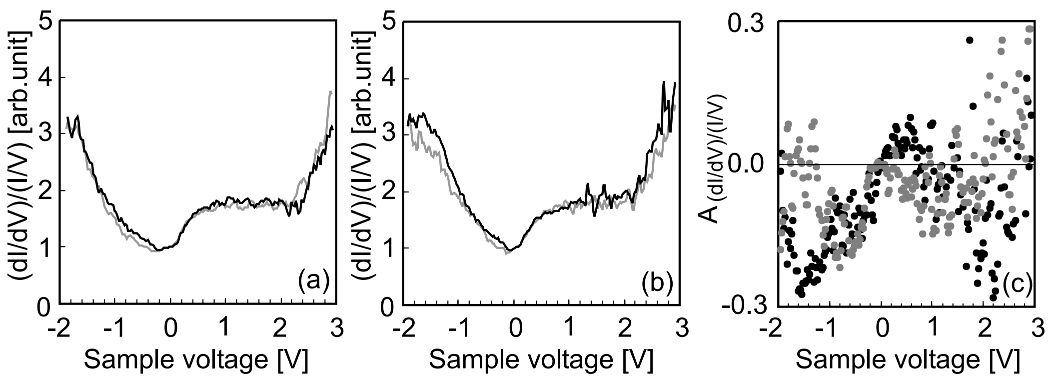

FIGURE 4. (a) (dI/dV)/(I/V) curves obtained on the odd (solid black curve) and even (solid grey curve) layers of 7ML of Mn grown on Fe(001) with an Fe-coated tip using a negative sample voltage setpoint (V_s= -0.5V, I= =0.5 nA). (b)) (dI/dV)/(I/V) curves obtained in the odd (solid black curve) and even (solid grey curve) layers of 7ML of Mn grown on Fe(001) with an Fe-coated tip using a positive sample voltage setpoint (V_s= +0.5V, I= 0.5 nA). (c) Asymmetry in the (dI/dV)/(I/V) curves. Solid line is for the dI/dV curves obtained from measurements taken with a negative voltage setpoint and the dotted line is for the positive voltage setpoint.

In panels (a) and (b) of Figure 4 we show normalized tunneling conductivity (dI/dV)/(I/V) obtained at a negative and positive voltage setpoint. The normalization removes almost completely any dependence of the asymmetry on the voltage setpoint. Unfortunately the asymmetry values obtained are not correct. From previous studies it is known that the electronic structure of the Mn(001) surface above the Fermi level is dominated by three “minority” bands located in energy between the Fermi level and +1.0 eV [12]. These bands produce a broad feature in the tunneling conductance instead of a well define peak. This particular electronic structure makes this normalization procedure unsuitable to recover the surface DOS. It is also well known that the (dI/dV)/(I/V) normalization cannot exclude completely the exponential background [16] and by definition should be 1 at 0 V. These limitations have an influence on the asymmetry obtained from those curves.

To deal with these limitations Ukraintsev [16] proposed in 1996 that normalizing dI/dV with a fitted tunneling probability functions leads to the best recovery of the sample DOS within a one dimensional WKB approach [16]. The tunneling probability function is:

$$T = a_t \exp\left[-2S\left(\frac{2m}{\hbar^2}\left(\overline{\Phi} - V/2\right)\right)^{1/2}\right] + a_s \exp\left[-2S\left(\frac{2m}{\hbar^2}(\overline{\Phi} + V/2\right)^{1/2}\right]$$

The first term of T describes tunneling from the tip Fermi level to unocuupied sample states, and the second term describes the tunneling from the sample Fermi level to unocuupied tip states. a_t and a_s are proportionality coefficients related to the tip-surface effective contact area and are proportional to the tip and the sample DOS at the Fermi level, respectively. $\overline{\Phi}$ is the average of sample and tip work functions, *S* is the tip sample separation and *m* the electron mass. In order to use this normalization procedure is necessary to measure the I(V) curves over a long voltage range to have enough data to make a good estimation of the exponential background. For this reason our I(V) curves are measured in a energy range between -2V and +3V, as shown in Figure 2.

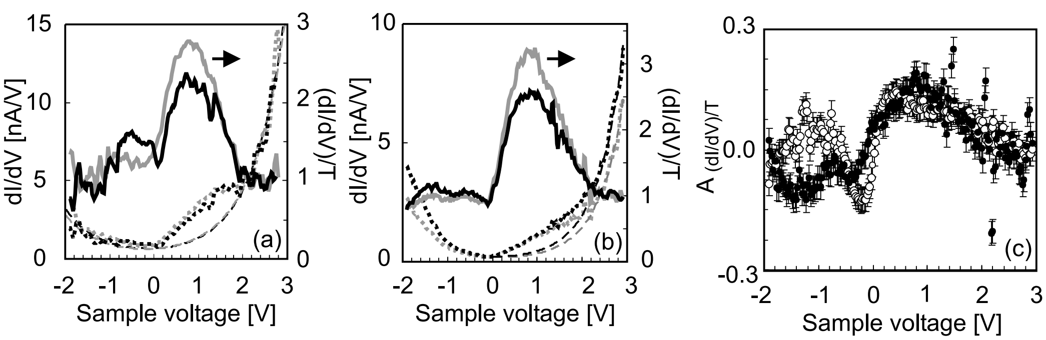

FIGURE 5. (a) d*I*/d*V* curves normalized by T obtained on the odd (solid black curve) and even (solid grey curve) layers of 7ML of Mn grown on Fe(001) with an Fe-coated tip using a negative sample voltage setpoint (V_s= -0.5V, I= =0.5 nA). In dotted lines we show again the d*I*/d*V* curves, the black and grey colors represents different Mn layers and the dashed black line is the function T. (b)) d*I*/d*V* curves normalized by T obtained on the odd (solid black curve) and even (solid grey curve) layers of 7ML of Mn grown on Fe(001) with an Fe-coated tip using a positive sample voltage setpoint (V_s= +0.5V, I= 0.5 nA). In dotted lines we show again the d*I*/d*V* curves the black and grey colors represents different Mn layers and the dashed black line is the function T. (c) Asymmetry in the (d*I*/d*V*)/T curves. The solid dots are for the d*I*/d*V* curves obtained from measurements taken with a negative voltage setpoint and the empty dots are for the positive voltage setpoint.

The result of this normalization is shown in Figure 5a and 5b. In this case the normalized tunneling conductance shows again a clear difference between the curves measured in the even and odd layers (black and grey solid line), the differences are not dependent on the voltage setpoint chosen to stabilize the feedback loop. With new normalization method the normalized conductance resembles better the surface density of states [12]. Above the Fermi level it presents a broad peak centered around +0.8 V that changes its intensity depending on the sample magnetization. Figure 5c shows the asymmetry obtained from these curves. The asymmetry obtained with the different setpoints is identical within the error bars above the Fermi level. Below the Fermi level the results reflects mainly the contribution of the tip DOS [12].

In summary in this paper we have explored the influence of the setpoint chose to stabilize the feedback loop during Spin-Polarized Scanning Tunneling Spectroscopy measurements. We have shown that the setpoint has a strong influence and we discussed the different approach to the analysis of I(V) curves in order to recover the surface DOS.

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REFERENCES

1. I. Giaver, *Phys. Rev. Lett.* **5**, 147 (1960); **5**, 464 (1960).
2. J. Bardeen, *Phys. Rev. Lett.* **6**, 57 (1961).
3. G. Binnig and H. Rohrer, *Helv. Phys. Acta* **55**, 726 (1982).
4. J. Tersoff and D.R: Hamann, *Phys. Rev. Lett.* **50**, 1998 (1983); *Phys. Rev. B* **31**, 805 (1985).
5. N. Garcia, C. Ocal and F.Flores, *Phys. Rev. Lett.* **50**, 2002 (1983).
6. N.D. Lang, *Phys. Rev. Lett.* **55**, 230 (1985); **55**, 2925 (1985); **56**, 1164 (1986).
7. R. Wiesendanger, H.-J. Güntherodt, G. Güntherodt, R.J. Gambino and R. Ruf, *Phys.Rev. Lett.* **65**, 247 (1990).
8. S. Heinze, M. Bode, A. Kubetzka, O. Pietsch, X. Nie, S. Blügel and R. Wiesendanger, *Science* **288**, 1805 (2000).
9. O. Pietzsch, A. Kubetzka, M. Bode and R. Wiesendanger, *Sicence* **292**, 2053 (2001).
10. T.K. Yamada, M.M.J. Bischoff, T. Mizoguchi and H. van Kempen, *Surf. Sci.* **516**, 179 (2002).
11. M.M.J. Bischoff, T.K. Yamada, T. Mizoguchi and H. van Kempen, *Surf. Sci*. **501**, 155 (2002).
12. T.K. Yamada, M.M.J. Bischoff, G.M.M. Heijnen, T. Mizoguchi and H. van Kempen, *Phys. Rev. Lett.* **90**, 056803 (2003).
13. Wiesendanger and M. Bode, *Solid State Commu.* **119**, 341 (2001).
14. S.N. Okuno, T. Kishi and K. Tanaka, *Phys. Rev. Lett.* **88**, 066803 (2002).
15. C.J. Chen, *"Introduction to Scanning Tunneling Microscopy"*, Oxford University Press, New York (1993), pp 21-26.
16. V.A. Ukraintsev, *Phys. Rev. B* **53**, 11176 (1996).
17. A.L. Vázquez de Parga, O.S. Hernan, R. Miranda, A. Levy Yeyati, A. Martin-Rodero, N. Mingo and F. Flores, *Phys. Rev. Lett.* **80**, 357 (1998).
18. R.M. Feenstra, J.A. Stroscio and A.P. Fein, *Surf. Sci.* **181**, 295 (1987).