4/26/02

Extension of STM to the Spin-Polarized Case (SP-STM)

The following derivation comes from the paper "Resolving Complex Atomic-Scale Spin Structures by Spin-Polarized Scanning Tunneling Microscopy"
D. Wortmann et al., - Phys. Rev. Lett, 86(18), 4132 (2001).

Begins with Bardeen's description:

$$\boxed{\begin{aligned} I(\vec{R}_t, V) = \frac{2\pi e}{\hbar} \sum_{\mu,\nu} \left[f(\varepsilon_\mu^S - \varepsilon_F) - f(\varepsilon_\nu^T - \varepsilon_F) \right] \\ \times\, \delta(\varepsilon_\nu^T - \varepsilon_\mu^S - eV) \left| M_{\nu,\mu}(\vec{R}_T) \right|^2 \end{aligned}}$$

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon - \varepsilon_F)/kT} + 1}$$

$\varepsilon_{\mu/\nu}^{T/S}$ are energies of tip/sample states

$$M_{\nu,\mu}(\vec{R}_T) = \langle \psi_\nu^T | U_T | \psi_\mu^S \rangle$$

U_T = potential of the tip

The tip and sample wavefunctions can have mixtures of spin components. If the tip, for example, has collinear spins, an axis can be found in which the spinor of the tip wave function can be written in terms of pure spin up or spin down ~~states~~, i.e.

$$\psi^T_\nu = \begin{pmatrix} \psi^T_{\nu\uparrow} \\ 0 \end{pmatrix} \quad \text{or} \quad \psi^T_\nu = \begin{pmatrix} 0 \\ \psi^T_{\nu\downarrow} \end{pmatrix}$$

Using this axis, the state of the sample will be:

$$\psi^S_\mu = \begin{pmatrix} \psi^S_{\mu\uparrow} \\ \psi^S_{\mu\downarrow} \end{pmatrix}$$

Ignoring spin-flip during tunneling,

$$\underbrace{M^{\sigma}_{\nu,\mu}(\vec{R}_T)}_{\text{spin-dependent matrix element}} = \langle \psi^T_{\nu\sigma} | U_{T\sigma\sigma} | \psi^S_{\mu\sigma} \rangle = -\frac{2\pi C\hbar^2}{\kappa m}\psi^S_{\mu\sigma}$$

The magnetization of the tip is defined:

$$\vec{m}_T = (n_T^{\uparrow} - n_T^{\downarrow})\,\vec{e}_M^{\,T}$$

Inserting M into the former equation leads to:

$$I(\vec{R}_T, V; \theta) = \frac{8\pi^3 C^2 \hbar^3 e}{K^2 m^2} \int d\epsilon\, g_v(\varepsilon) \sum_{\mu} \delta(\epsilon_\mu - \epsilon)\left[n_T^{\uparrow} \left|\psi_{\mu\uparrow}^{S}(\vec{R}_T)\right|^2 + n_T^{\downarrow}\left|\psi_{\mu\downarrow}^{S}(\vec{R}_T)\right|^2 \right]$$

$$g_v(\varepsilon) = f(\varepsilon - \epsilon_F) - f(\varepsilon + eV - \varepsilon_F)$$

$\theta(\vec{R}_T, V)$ denotes the angle between $\vec{m}_T$ at $\vec{R}_T$ and $\vec{m}_S$ at $\vec{R}_T$

This can be shown to be written as:

$$I(\vec{R}_T, V, \theta) = I_0(\vec{R}_T, V) + I_P(\vec{R}_T, V, \theta)$$

$$= \frac{4\pi^3 C^2 \hbar^3 e}{K^2 m^2}\left[n_T \tilde{n}_S(\vec{R}_T, V) + \vec{m}_T \tilde{\vec{m}}_S(\vec{R}_T, V) \right]$$

n_T and n_S are the local densities of states

$\tilde{n}_S$ is the energy-integrated local density of states of the sample

$\vec{m}_T$ and $\vec{m}_S$ are the local magnetization density of states (vectors)

$\tilde{\vec{m}}_S$ is the energy-integrated local magnetization density of states

$$\vec{m}_s(\vec{R}_T;\varepsilon) = \sum_{\mu} \delta(\varepsilon_\mu - \varepsilon)\, \psi_\mu^{s\dagger}(\vec{R}_T)\, \sigma\, \psi_\mu^{s}(\vec{R}_T)$$

$$\tilde{\vec{m}}_s(\vec{R}_T, V) = \int d\varepsilon\, g_v(\varepsilon)\, \vec{m}_s(\vec{R}_T, \varepsilon)$$

$$n_s(\vec{R}_T;\varepsilon) = \sum_{\mu} \delta(\varepsilon_\mu - \varepsilon)\, \psi_\mu^{s\dagger}(\vec{R}_T)\, \underbrace{u}_{\text{unit matrix}}\, \psi_\mu^{s}(\vec{R}_T)$$

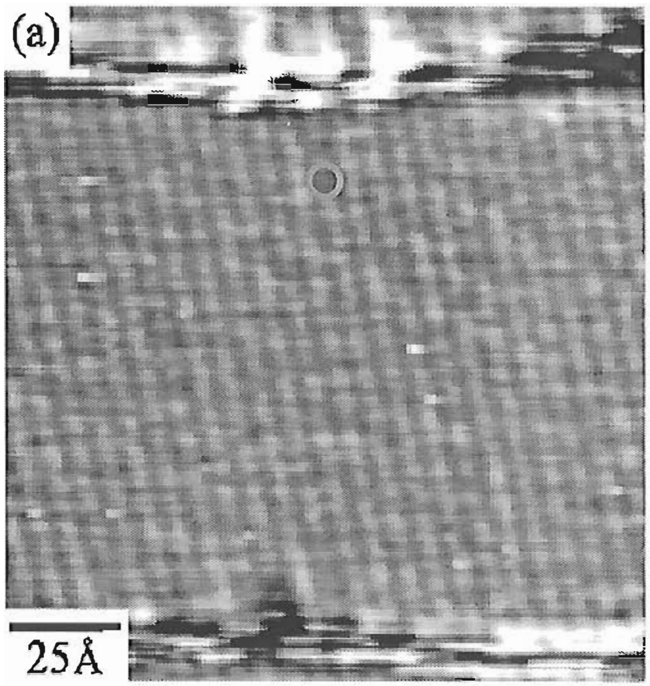
$$\tilde{n}_s(\vec{R}_T, \varepsilon) = \int d\varepsilon\, g_v(\varepsilon)\, n_s(\vec{R}_T, \varepsilon)$$

the above comes from D. Wortmann et al.

PRL 86(18), 4132 (2001)

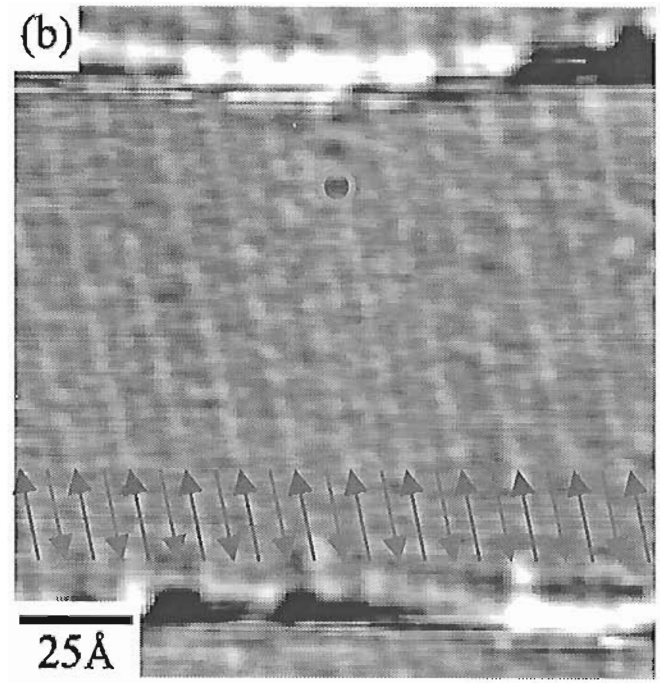
In the first example, the magnetic moment of the tip actually changes between images:

No Spin-Polarized Effect



$V_s = -0.4$ V, $I_t = 0.5$ nA

Spin-Polarized Effect



$V_s = -0.4$ V, $I_t = 0.5$ nA

How can we separate the electronic from magnetic parts?

Method 1. Since the electronic component is periodic with period c/2, deduce the components directly from the data, as follows:

1. Assume the following equation (based on Wortmann *et al.* , *Phys. Rev. Lett.* ***86****(18), 4132 (2001).*)

$$\Delta z \sim \Delta I_t(\mathbf{R}_T, V, \theta) \sim \Delta\ n_T n_S(\mathbf{R}_T, V) + m_T m_S(\mathbf{R}_T, V)\cos\theta$$

2. Form the difference $\Delta z = z(x) - z(x+c/2)$

$$\Delta z \sim n_T[n_S(x) - n_S(x+c/2)] + m_T\{m_S(x)\cos[\theta(x)] - m_S(x+c/2)\cos[\theta(x+c/2)]\}$$

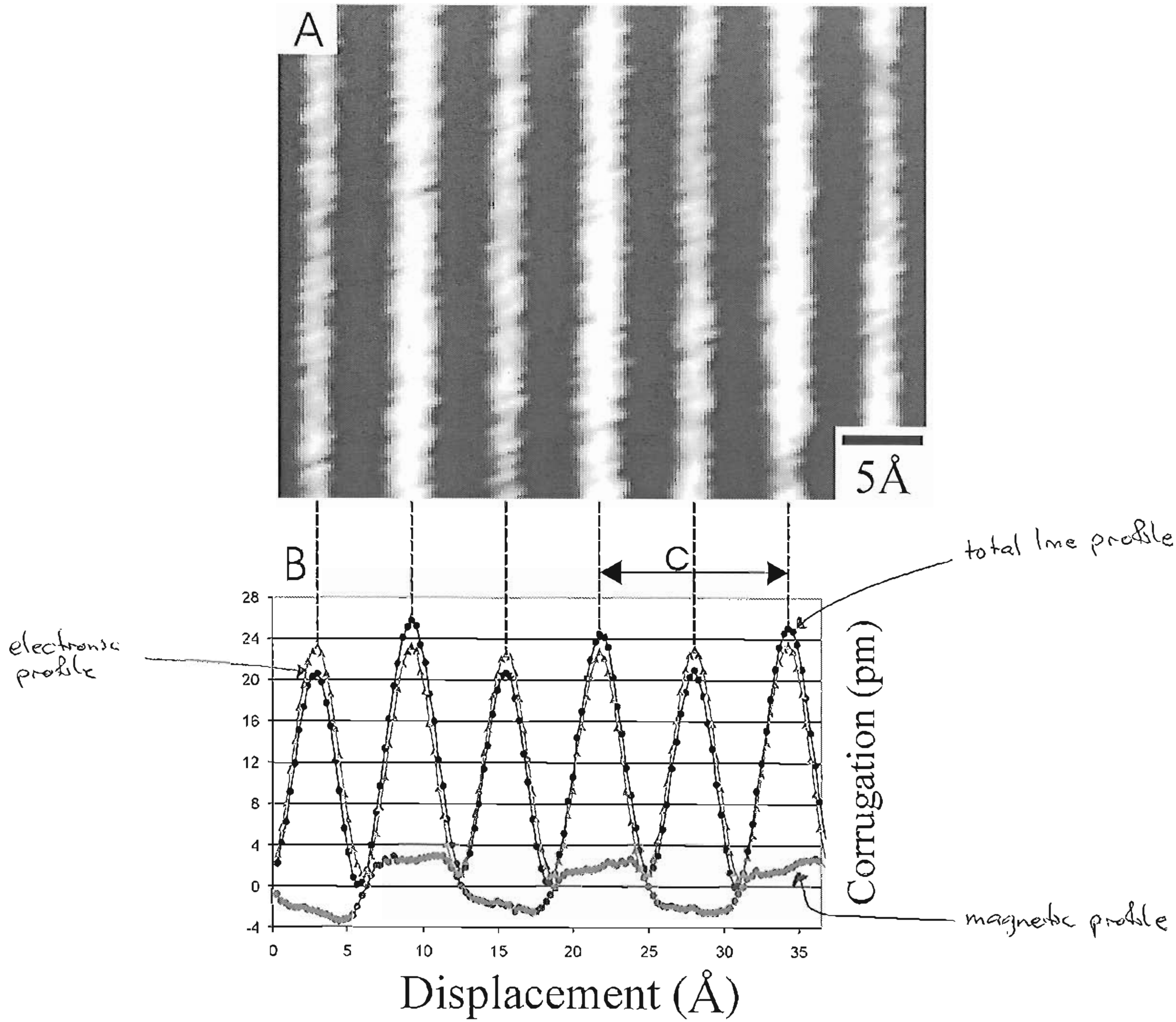
3. Since $n_S(x) = n_S(x+c/2)$, the electronic part cancels out, and the remainder is of purely magnetic origin.

4. Next, if we assume reflection symmetry of the magnetic structure about Mn(1), then $m_S(x) = m_S(x+c/2)$ and $\theta(x+c/2) = \theta + \pi - 2\beta$.
   β = the angle of the tip moment w.r.t. the row, then we get:

$$m_T m_S(x)\{\cos[\theta(x)] + \cos[\theta(x) - 2\beta]\} = z(x) - z(x+c/2)$$

5. Finally, in the case where the spins are not canted w.r.t. the row:

$$\boxed{\begin{array}{c} m_T m_S(x)\cos[\theta(x)] = [z(x) - z(x+c/2)]/2 \quad \text{(magnetic component)} \\ \text{and} \\ n_T n_S(x) = [z(x) + z(x+c/2)]/2 \quad \text{(electronic component)} \end{array}}$$


A
5Å
B
C
electronic profile
total line profile
magnetic profile
Corrugation (pm)
Displacement (Å)
28
24
20
16
12
8
4
0
-4
0
5
10
15
20
25
30
35