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Strain and composition effects in epitaxial ferroelectrics

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Appendix A

Matlab script for simulating experimental CTR profiles

The MATLAB code used to calculate the truncation rods of $PbTiO_3$ films on $SrTiO_3$ is shown. The equations used in this program are described in chapter 3. Figures 3.13 and 4.4. The script refers to a number of other scripts that contain the atomic scattering factors and the calculation of the unit cell structure factors.

```
%X-ray simulation file.
clear;
%File control

dir = ’directory\’;
file = ’filename’;
fid = [dir file ’.xrdml’];

% Film parameters
N_avg = 50; %Thickness (Number of unit cells)
s_pto = 2; %RMS Film Roughness
s_sto = 0; %RMS Substrate Roughness
dist = 2.5; %thickness Distribution FWHM
bg = 0; %constant background
x =0.75; %Domain fraction up
```

```
d = 0.0; %Expansion at interface
a_sto = 3.903; %Cubic STO lattice  parameter
c_pto = 4.115;  %Out of plane PTO lattice parameter
S = 10*10^6; %scaling factor

% Constants
R = 2.82E-5; %Thomson radius of electron
lambda = 1.540; %X-ray wavelength, Cu k-alpha radiation

%load data files
ASF %Atomic Scattering factors
DATA_PTO %PTO coordinates, DW factors, Absorption
DATA_STO %STO coordinates, DW factors, Absorption

%load experimental data
t = XRDMLread(fid);
tt_exp = t.Theta2;
I_exp = t.data;
theta_exp = tt_exp/2;

%Simulation
q_001_pto = 2*pi/c_pto;
q_001_sto = 2*pi/a_sto;
a_pto = a_sto; %coherent epitaxial thin film
m = 1;
p = pdf('Normal',-2:2,0,dist); %gaussian distribution of thicknesses
for theta = theta_exp, I = I_exp;
    q = 4*pi/lambda*sin(theta*(2*pi/360));
    SF_PTO %PTO structure factors
    SF_STO %STO structure factors

    %STO substrate
    F_ctr_STO = F_sto /(1-exp(-a_sto*(i*q + e_sto/q)));
    for n = [1,2,3,4,5]
    P = p(n);
```

```
    N = N_avg + (n-3);

    %PTO film
    F_ctr_film_up = F_pto_up*(1-exp(-c_pto*(N)*(i*q + e_pto/q)))/
    (1-exp(-c_pto*(i*q + e_pto/q))) + F_pto_pbo_up*exp(i*c_pto*q);
    F_ctr_film_down = F_pto_down*(1-exp(-c_pto*(N)*(i*q + e_pto/q)))/
    (1-exp(-c_pto*(i*q + e_pto/q))) + F_pto_pbo_down*exp(i*c_pto*q);

    %Reflectances
    r_ctr_sub = (i*4*pi*R/(a_pto^2*q))*F_ctr_STO;
    r_sub = (2*r_ctr_sub/(1+(1+(2*r_ctr_sub)^2)^1/2))*
    exp(-0.5*s_sto^2*(q-q_001_sto)^2);
    r_ctr_film_up = ((i*4*pi*R/(a_pto^2*q))*F_ctr_film_up)*
    exp(-0.5*s_pto^2*(q-q_001_pto)^2);
    r_ctr_film_down = ((i*4*pi*R/(a_pto^2*q))*F_ctr_film_down)*
    exp(-0.5*s_pto^2*(q-q_001_pto)^2);
    r_tot_up = r_ctr_film_up + r_ctr_sub*
    exp(-c_pto*(N+d)*(i*q + e_pto/q));
    r_tot_down = r_ctr_film_down + r_ctr_sub*
    exp(-c_pto*(N+d)*(i*q + e_pto/q));
    r_tot_up_p(n) = P*r_tot_up;
    r_tot_down_p(n) = P*r_tot_down;
    end
    r_TOT_up = sum(r_tot_up_p);
    r_TOT_down = sum(r_tot_down_p);

    %Intensities
    I_sim(m) = S*(abs(x*r_TOT_up + (1-x)*r_TOT_down))^2;
           %Simulated intensity
    diff(m) = log10(I(m)) - log10(I_sim(m));
           %Difference between experiment and simulation
    m = m+1;
end

%Plotting
```

```
axes(’Fontsize’, 14)
subplot(3,1,[1 2])
semilogy(tt_exp, I_exp, ’+’, ’color’,[0,0,0], ’LineWidth’,2);
hold on
semilogy(tt_exp, I_sim, ’-’, ’color’,[0.4,0.4,0.4], ’LineWidth’,2);
ylabel (’Intensity (counts/s)’,’FontSize’,14)
hold off
subplot(3,1,3)
plot(tt_exp, diff, ’color’,[0,0,0], ’LineWidth’,2);
line(tt_exp,0,’color’,[0,0,0],’LineWidth’,3)
xlabel(’2{\theta}(\circ)’,’FontSize’,14)
ylabel (’diff. (a.u.)’,’FontSize’,14)
```

Appendix B

Landau Coefficients for $PbTiO_3$ and $SrTiO_3$

Landau coefficients used for the Landau-Ginzburg simulations in this thesis.

Coefficient	$PbTiO_3$ [34]	$SrTiO_3$ [129]	Units
α_1	3.8·(T-752)	$7.45 \cdot (T - 51.64)$ [102]	10^5 J m / C^2
α_{11}	-0.7252	1.04	10^8 J m^5 / C^4
α_{12}	7.5	0.746	10^8 J m^5 / C^4
α_{111}	2.606	0	10^8 J m^9 / C^6
α_{112}	6.1	0	10^8 J m^9 / C^6
Q_{11}	8.9	4.96	10^{-2} m^4 / C^2
Q_{12}	-2.6	6.75	10^{-2} m^4 / C^2
Q_{44}	6.75	1.9	10^{-2} m^4 / C^2
s_{11}	8.0	3.52	10^{-12} m^3 / J
s_{12}	-2.5	-0.85	10^{-12} m^3 / J
s_{12}	9	7.87	10^{-12} m^3 / J
c_{11}	1.746	3.36	10^{11} J / m^3
c_{12}	0.794	1.07	10^{11} J / m^3
g_{11}	1.14	1.25	10^{10} J m / C^2
g_{12}	0.0463	-0.108	10^{10} J m / C^2

Table B.1: