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Structure and domain formation in ferroelectric thin films

Vlooswijk, Ard H.G.

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Document Version

Publisher's PDF, also known as Version of record

Publication date:

2009

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Vlooswijk, A. H. G. (2009). *Structure and domain formation in ferroelectric thin films*. [Thesis fully internal (DIV), University of Groningen]. [s.n.].

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Appendix A

Overview of the experimental data on bulk $PbTiO_3$ from literature [13, 41, 161, 162, 163]. Besides general parameters like the Curie temperature and Landau parameters, also lattice parameters and atomic positions of the tetragonal and cubic phase are listed (Pb is fixed at the origin).

critical temperature	T_c [°C]	492.2
Curie temperature	θ [°C]	478.8
Curie-Weiss constant	C [°C]	$1.5 \cdot 10^5$
dielectric stiffness coefficient	α_1 [$\frac{m}{F}$]	$3.8(T-478.8) \times 10^5$
higher-order stiffness coefficient	α_{11} [$\frac{m^5}{FC^2}$]	-7.3×10^7
"	α_{12} [$\frac{m^5}{FC^2}$]	7.5×10^8
"	α_{111} [$\frac{m^9}{FC^4}$]	2.6×10^8
"	α_{112} [$\frac{m^9}{FC^4}$]	6.1×10^8
"	α_{123} [$\frac{m^9}{FC^4}$]	-3.7×10^9
electrostrictive constant	Q_{11} [m^4/C^2]	0.089
"	Q_{12} [m^4/C^2]	-0.026
"	Q_{44} [m^4/C^2]	0.0675
elastic compliance	s_{11} [m^2/N]	8.0×10^{-12}
"	s_{12} [m^2/N]	-2.5×10^{-12}
"	s_{44} [m^2/N]	9.0×10^{-12}

Symmetry-dependent properties		
parameter	25°C	550°C
crystal system	tetragonal	cubic
space group	$P4mm - C(4v)^1$	$Pm3m - O_h^1$
lattice parameter	3.905	3.97
"	4.156	-
tetragonality	1.064	1
z atomic coordinate	0.540	0.5
"	0.612	0.5
"	0.112	0
interatomic distance	2.80; 2.53; 3.20	2.81
"	1.98; 1.78; 2.38	1.99
spontaneous polarization	0.75	0
dielectric constant	124.4	
"	66.6	
piezoelectric coefficient	-23.1	-
"	79.1	-
"	56.1	-
elastic constant	237	
"	60	
"	69	
"	104	
"	90	
"	70	
piezoelectric tensor	2.1	-
"	5.0	-
"	4.4	-
band gap	3.5	

Appendix B

The following Matlab-script is used with a wide grid to estimate the minimum energy followed by a Gauss-Newton iteration to determine the exact energy minimum, as plotted in Figure 5.12:

```
function energy = calc_W(phi, chi, Hn)
%lattice parameters
a = 3.905;
b = 3.945;
c = 4.156;
%Poisson's ratio
mu = 0.3;
%Relative coherency Strain
sr = c*(b-a) / (b*(c-a));

%GRIDS
gx = 2000;
x = linspace(0, -1, gx);
gy = 2000;
y = linspace(0, 1, gy);
```

```

%CALCULATE Q-TERM
%VARIABLES IN Q11
sxp      =      2*pi*(x+1)/chi;
sxp3     =      2*pi*(x+3)/chi;
sxm      =      2*pi*(x-1)/chi;
sx       =      ((2*pi/chi)^2)*x;
sp       =      2*pi*phi;

%Q11(phi,x3) TERMS (equation 17)[5]
cshsxp   =      cosh(sxp);
cshsxm   =      cosh(sxm);
snhsxp   =      sinh(sxp);
snhsxm   =      sinh(sxm);
csp      =      cos(sp);
Q01      =      +(1/2)*log((cshsxp-1)/(cshsxm-1));
Q02      =      +(sxp/2).*(snhsxp/(cshsxp-1));
Q03      =      -(sxp3/2).*(snhsxm/(cshsxm-1));
Q04      =      +sx./(cshsxm-1);
Q110     =      Q01+Q02+Q03+Q04; %Q11(0,x3)
Qd1      =      +(1/2)*log((cshsxp-csp)/(cshsxm-csp));
Qd2      =      +(sxp/2).*(snhsxp/(cshsxp-csp));
Qd3      =      -(sxp3/2).*(snhsxm/(cshsxm-csp));
Qd4      =      +sx.*(cshsxm*csp-1)/((cshsxm-csp).^2);
Q11d     =      Qd1+Qd2+Qd3+Qd4; %Q11(d,x3)
%INTEGRAND
dx       =      1/gx;
Intx3    =      (Q110-Q11d).*(1+x)*dx;
%INTEGRATION
iQ       =      0;
for kx = 1:gx-1
    iQ = iQ+Intx3(kx);
end

```

```

%CALCULATE J-TERM
%VARIABLES IN J
jh      =      4*pi/chi;
jv      =      2*pi*phi*(1-y);

%EQUATION (A4)[5]
J1      =      +(1/(4*pi))*log((cosh(jh)-cos(jv))
      ./ (1-cos(jv)));
J2      =      +(jh*sinh(jh))./(4*pi*(cosh(jh)-cos(jv)));
J3      =      -(jh^2)*(cosh(jh)*cos(jv)-1)
      ./ (8*pi*(cosh(jh)-cos(jv)).^2);
Jt      =      J1+J2+J3;
%INTEGRAND
dy      =      1./gy;
Intv    =      Jt.*y.*dy;
%INTEGRATION
iJ      =      0;
      for ky = 1:gy-1
      iJ =      iJ+Intv(ky);
      end

%calculate W(DH,phi)
%W1, W2 TERMS (NO INTEGRATION)
W1      =      Hn*2*((sr*(1+mu))-1)*phi;
W4      =      2*sqrt(2)./chi;
%W2, W3 TERMS (INTEGRATION REQUIRED)
W2      =      Hn*iQ./(2*pi*chi);
W3      =      Hn.*chi.*(phi).^2*iJ;
energy  =      W1+W2+W3+W4;

```

