



Anisotropy of thermal expansion in YAlO_3 and NdGaO_3

Odette Chaix-Pluchery, Bernard Chenevier, J. J. Robles

► To cite this version:

Odette Chaix-Pluchery, Bernard Chenevier, J. J. Robles. Anisotropy of thermal expansion in YAlO_3 and NdGaO_3 . Applied Physics Letters, 2005, 86, pp.251911. 10.1063/1.1944901 . hal-00207926

HAL Id: hal-00207926

<https://hal.science/hal-00207926>

Submitted on 18 Jan 2008

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Anisotropy of thermal expansion in YAlO_3 and NdGaO_3

O. Chaix-Pluchery*, B. Chenevier, J. J. Robles

Laboratoire des Matériaux et du Génie Physique (CNRS UMR 5628),

ENSPG- INPG, BP 46, Saint-Martin d'Hères Cedex, F-38402, France

* Author to whom correspondence should be addressed; e-mail: Odette.Chaix@inpg.fr

Abstract:

YAlO_3 and NdGaO_3 thermal expansion coefficients were measured using in-situ powder X-ray diffraction in the temperature range 28-650°C. They exhibit a clear anisotropy: the expansion, quite similar along the [100] and [001] directions, is much lower along the [010] direction. The formation of cracks observed in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ thin films deposited on YAlO_3 and NdGaO_3 substrates is likely related to the anisotropy. Stress value calculations have been performed in both systems. They indicate the intrinsic components are specifically high in YAlO_3 .

Selecting a substrate for high T_c superconducting film deposition is of crucial importance since it determines the epitaxial relationships, microstructure and, therefore, physical properties of the film. In $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) films, twin boundaries play an important role in the electric transport properties and the twinning geometry is strongly influenced by the substrate. The twinning along the $[110]$ and $[1\bar{1}0]$ directions of YBCO appears as the material passes through the tetragonal to orthorhombic transition. In YAlO_3 and NdGaO_3 substrates, a particular twinning geometry has been shown: the twinning directions of c-axis oriented YBCO films align along a unique direction of the substrate (namely the $[010]$ direction) in contrast to films deposited on conventional substrates such as MgO , LaAlO_3 , SrTiO_3 where the more usual bidirectional twinning is found ^{1,2}. The impact of this unidirectional twinning on the transport properties of YBCO films has been the subject of several studies ^{2,3}.

It appears, through different papers, that the alignment of twin boundaries is strongly correlated to the presence of microcracks in the films ^{4,6}. Cracks are distributed in an array of lines parallel to the substrate a-axis (i.e. propagating perpendicular to the direction of alignment of the twin boundaries), 5-10 μm apart from one another in the case of YAlO_3 substrate, and sometimes more distant in the case of NdGaO_3 ^{4,6}. The sequence between events is not clearly established. In addition, YAlO_3 thermal expansion coefficients along the three directions are not known accurately; values reported in literature are given in Table I and let us assume anisotropy in YAlO_3 ^{9,10} and NdGaO_3 ^{13,14} thermal expansion.

Lattice constant mismatch and differential thermal expansion between film and substrate are the most important factors contributing to stress in films supported on substrates. The YBCO unit

cell diagonal in the (a, b) plane (l_{110}) aligns with the substrate b-axis. This specific orientation minimizes the lattice mismatch between YBCO film and substrate: it is close to 2.3% with YAlO_3 and to 0.8-0.9% with NdGaO_3 at room temperature (lattice parameters are given in Table II, YBCO $l_{110} = \sqrt{a^2 + b^2} = 0.54519 \text{ nm}$ ¹⁶).

To test the possible anisotropy in the thermal expansion of YAlO_3 and NdGaO_3 which could explain the formation of cracks in the thin films, accurate YAlO_3 and NdGaO_3 thermal expansion coefficients are needed. They will thus make possible to estimate the thermoelastic component of the residual stress in both systems. It was the goal of this study. A particularly well-adapted technique to obtain such accurate coefficients is the in-situ high temperature powder X-ray diffraction which permits one to collect reflections from various directions of the reciprocal space as a function of temperature and thus to obtain thermal expansion coefficients as a function of the orientation in the unit-cell.

Fine YAlO_3 and NdGaO_3 powder samples were obtained by grinding a small piece of a single crystal substrate. Samples were then annealed for several hours at 800°C to relax grinding-induced strains. To measure thermal expansion, the samples were progressively heated from room temperature up to 650°C by applying repeated sequences of temperature ramps followed by stabilisation using a high-temperature diffraction stage. Specifications of the heating stage are given in Ref. 23. The typical temperature range between two stabilisations was 50°C. Diffraction patterns were recorded for 800 s at each stabilisation step. The angular position of carefully selected reflections was determined which permitted the lattice parameters to be refined at each annealing temperature. The values thus obtained at 28°C are given in Table II. The results were plotted as a function of temperature and fitted with a simple linear model of thermal expansion. The number of

reflections selected at each temperature was 16 or 17 in the case of YAlO_3 , and varied between 5 and 13 for NdGaO_3 .

The thermal dependence of YAlO_3 and NdGaO_3 lattice parameters is shown in Figs. 1 and 2. A clear anisotropy of thermal expansion in both compounds is observed: expansion is clearly weaker along the [010] direction. The resulting thermal expansion coefficients along the three directions were found to be:

$$\alpha_a = 8.9 (\pm 0.4) \times 10^{-6} \text{ K}^{-1}, \alpha_b = 3.8 (\pm 0.2) \times 10^{-6} \text{ K}^{-1}, \alpha_c = 8.5 (\pm 0.3) \times 10^{-6} \text{ K}^{-1} \text{ in } \text{YAlO}_3$$

$$\alpha_a = 11.3 (\pm 0.8) \times 10^{-6} \text{ K}^{-1}, \alpha_b = 2.3 (\pm 0.5) \times 10^{-6} \text{ K}^{-1}, \alpha_c = 9.1 (\pm 0.8) \times 10^{-6} \text{ K}^{-1} \text{ in } \text{NdGaO}_3.$$

It clearly appears that thermal expansion is sharply anisotropic. $\text{YAlO}_3\text{:Er}^{3+}$, NdGaO_3 and LaGaO_3 thermal expansion coefficients reported in literature are also weaker along the [010] direction, as seen in Table I. However, NdGaO_3 α values are reported to be greater than ours.

All of these compounds crystallize in the orthorhombic distorted GdFeO_3 -type perovskite structure (space group Pbnm)^{12, 15, 18, 19, 21, 22}. This structure is also described as pseudocubic and can be represented as a grid of $[\text{AlO}_6]$ or $[\text{GaO}_6]$ octahedra tilted around the [001], [110] and [111] pseudo-cubic axes (tilt angles equal to 9.46° , 13.45° and 16.39° in NdGaO_3 ²⁵; to 9.32° , 13.65° and 16.48° in YAlO_3 ¹⁹, respectively). The Y and Nd atoms occupy hollows situated between octahedra.

Some peculiarities concerning the thermal behaviour of the b-axis lattice parameter at low temperature also occur in such compounds: anomalies at 50K and 200K in NdGaO_3 , negative thermal expansion in PrGaO_3 at temperatures below 200K²⁶. They have been related to rotational vibrations of the shared anion octahedra which have a negative contribution to the thermal expansion. The balance between rotations and distortions of oxygen octahedra will depend on details of the crystal structure, in particular, on interactions between crystal vibrations and electronic

excitations of rare earth cations. The thermal expansion anisotropy observed at high temperature in YAlO_3 and NdGaO_3 (in LaGaO_3 also) cannot be explained by such interactions because of the absence of such ions with 4f electrons in the case of YAlO_3 and LaGaO_3 .

A careful analysis of the crystal structures indicates no significant difference in the nearest-neighbour interactions along a and b directions. The origin of the sharp difference detected between α_a and α_b remains unclear for the moment. Possible influence of next nearest-neighbours has to be considered.

To understand the development of residual stress at the YBCO / YAlO_3 (NdGaO_3) interface, a σ analysis in terms of intrinsic and thermoelastic stress has been made. As YBCO films are deposited on (001) substrates, the anisotropy in the thermal expansion coefficients is certainly important.

The thermal dependence of YBCO l_{110} is also reported in Fig. 2 for comparison with b parameters of both substrates. The very close values of b_{NdGaO_3} and YBCO l_{110} at a temperature close to YBCO deposition temperature (818°C) make the strains very low whereas they are much larger in the case of YAlO_3 substrate. An anisotropic biaxial stress model is considered ($\sigma = \sigma_{\text{int}} + \sigma_{\text{therm}}$).

The direction dependent thermoelastic components are expressed as $\epsilon_{ii} = \frac{1}{E} \alpha_{ii} - \frac{\nu}{E} \sigma_{jj} = \Delta\alpha_i \times \Delta T$ (i,j=1,2 and i≠j). Here, E and ν are YBCO Young's modulus and Poisson's ratio, respectively ($E=157 \text{ GPa}^{11}$, $\nu=0.3^{27}$), $\Delta\alpha$ and ΔT are the difference in thermal expansion coefficients between film and substrate and temperature change from deposition temperature and room temperature, respectively. Calculations led to:

$$\begin{array}{lll} \sigma_{11\text{therm}} = 0.109 \text{ GPa} & \sigma_{22\text{therm}} = 0.966 \text{ GPa} & \text{in NdGaO}_3 \\ \sigma_{11\text{therm}} = 0.373 \text{ GPa} & \sigma_{22\text{therm}} = 0.860 \text{ GPa} & \text{in YAlO}_3 \end{array}$$

The formation of cracks propagating parallel to the substrate a-axis can be explained by the fact that $\sigma_{11\text{therm}}$ value is much lower than $\sigma_{22\text{therm}}$ value.

The direction dependent intrinsic σ components have been also calculated ($\sigma_{\text{int}} = \varepsilon_{//} \times E/(1-\nu)$). We found:

$$\begin{array}{lll} \sigma_{11\text{int}} = -1.57 \text{ GPa} & \sigma_{22\text{int}} = -0.25 \text{ GPa} & \text{in NdGaO}_3 \\ \sigma_{11\text{int}} = -12.9 \text{ GPa} & \sigma_{22\text{int}} = -7.3 \text{ GPa} & \text{in YAlO}_3 \end{array}$$

Clearly, the YAlO_3 intrinsic components are high and likely accommodated by plastic relaxation via threading dislocations. This part should be further demonstrated by performing high resolution electron microscopy observations.

In conclusion, the careful analysis of YAlO_3 and NdGaO_3 thermal expansion gives evidence of a clear anisotropy. The much weaker contribution along the [010] direction likely facilitates the formation of cracks parallel to the a-axis. Such a sharp difference between α_a and α_b cannot be explained by simple structural considerations. As differential thermal expansion is higher along the [010] direction, thermoelastic energy stored during the cooling process is high and relaxation is needed. Then, cracks formed during relaxation necessarily propagate along the [100] direction. Stress value calculations performed in both systems indicate the intrinsic components in YAlO_3 are high. Plastic accommodation is probably acting to relax the considerable amount of intrinsic stress incorporated during film formation.

References

- 1- C. Dubourdieu, J.P. Sénateur, O. Thomas, F. Weiss, B.P. Thrane, Appl. Phys. Lett. **69**, 1942 (1996).
- 2- C. Villard, G. Koren, D. Cohen, E. Polturak, B. Thrane, D. Chateignier, Phys. Rev. Lett. **77**, 3913 (1996).
- 3- A. Casaca, G. Bonfait, C. Dubourdieu, F. Weiss, J.P. Sénateur, Phys. Rev. B **59**, 1538 (1999).
- 4- J.J. Robles, A. Bartasyte, H.P. Ng, A. Abrutis, F. Weiss, Physica C **400**, 36 (2003).
- 5- H. Yamasaki, Y. Nakagawa, A. Sawa, H. Obara, K. Develos, Physica C **372-376**, 1885 (2002).
- 6- G. Koren, E. Polturak, N. Levy, G. Deutscher, N.D. Zakharov, Appl. Phys. Lett. **73**, 3763 (1998).
- 7- J. Kawashima, Y. Yamada, I. Hirabayashi, Physica C **306**, 114 (1998).
- 8- A. Kulpa, A. C. D. Chaklader, G. Roemer, D. Li Williams, W. N. Hardy, Supercond. Sci. Technol. **3**, 483 (1990).
- 9- M.J. Weber, M. Bass, K. Andringa, R.R. Monchamp, E. Comperchio, Appl. Phys. Lett. **15**, 342 (1969).
- 10- Impex-Hightech data: www.impex-hightec.de
- 11- Y. Yamada, J. Kawashima, J.G. Wen, Y. Niiori, I. Hirabayashi, Jpn. J. Appl. Phys. **39**, 1111 (2000).
- 12- S.B. Ubizskii, L.O. Vasylechko, D.I. Savytskii, A.O. Matkovskii, I.M. Syvorotka, Supercond. Sci. Technol. **7**, 766 (1994).
- 13- F. Sandiumenge, C. Dubs, P. Görnert, S. Gali, J. Appl. Phys. **75**, 5243 (1994).
- 14- A. Senyshyn, L. Vasylechko, M. Knapp, U. Bismayer, M. Berkowski, A. Matkovskii, J. Alloys Compd. **382**, 84 (2004).
- 15- W. Marti, P. Fischer, F. Altorfer, H.J. Scheel, M. Tadin, J. Phys.: Condens. Matter **6**, 127 (1994).

- 16- J. D. Jorgensen, B. W. Veal, A. P. Paulikas, L. J. Nowicki, G. W. Crabtree, H. Claus, W. K. Kwok, Phys. Rev. B **41**, 1863 (1990).
- 17- J. D. Jorgensen, M. A. Beno, D. G. Hinks, L. Soderholm, K. J. Volin, R. L. Hitterman, J. D. Grace, I. K. Schuller, Phys. Rev. B **36**, 3608 (1987).
- 18- R. Diel, G. Brandt, Mat. Res. Bull. **10**, 85 (1975).
- 19- N.L. Ross, Phase Trans. **58**, 27 (1996).
- 20- S. Geller, Acta Crystallogr. **10**, 243 (1957).
- 21- L. Vasylechko, A. Matkovskii, D. Savytskii, A. Suchocki, F. Wallrafen, J. Alloys Compd. **291**, 57 (1999).
- 22- L. Vasylechko, L. Akselrud, W. Morgenroth, U. Bismayer, A. Matkovskii, D. Savytskii, J. Alloys Compd. **297**, 46 (2000).
- 23- O. Chaix-Pluchery, B. Chenevier, I. Matko, J. P. Sénateur, J. Appl. Phys. **96**, 361 (2004).
- 24- J.F. Nye, *Physical Properties of Crystals* (Clarendon, Oxford, U.K., 1985).
- 25- R.H. Mitchell, *Perovskites: modern and ancient* (Almaz Press, Thunder Bay, Ontario, Canada, 2002).
- 26- D. Savytskii, L. Vasylechko, A. Senyshyn, A. Matkovskii, C Bähz, M. L. Sanjuan, U. Bismayer, M. Berkowski, Phys. Rev. B **68**, 024101 (2003).
- 27- A. Goyal, W.C. Oliver, P.D. Funkenbusch, D.M. Kroeger, S.J. Burns, Physica C **183**, 221 (1991).

Figure captions

Fig. 1: Temperature dependence of a- and c-axis YAlO_3 and NdGaO_3 lattice parameters.

Fig. 2: Temperature dependence of b-axis YAlO_3 and NdGaO_3 lattice parameter, and of the YBCO unit cell diagonal in the (a, b) plane (l_{110}), calculated from the YBCO structural data and thermal expansion coefficients given in Table II and Table I, respectively (in orthorhombic system $\alpha_{110} = (\alpha_a a^2 + \alpha_b b^2)/(a^2 + b^2)$, from Ref. 24). The tetragonal to orthorhombic YBCO transition temperature, close to 700°C, is displayed as a dotted line.

Table I

Thermal expansion coefficients of YBCO, YAlO₃, NdGaO₃ and LaGaO₃ as reported in literature and from this study.

Compound	$10^6 \alpha \text{ (K)}^{-1}$	Source
YBa₂Cu₃O_{7-δ} ($\delta=0.08$)	$\alpha_{\text{eff}}=13.4$	Ref. 7
orthorhombic ($\delta=0.18$)	$\alpha_a=11.0$; $\alpha_b=8.7$; $\alpha_c=13.8$	Ref. 8
tetragonal ($\delta=0.68$)	$\alpha_a = \alpha_b=11.0$; $\alpha_c=19.6$	Ref. 8
YAlO₃ crystal	$\alpha_b=2.2$ at 25°C	Ref. 9
YAlO₃ powder	$\alpha_a=8.9$; $\alpha_b=3.8$; $\alpha_c=8.5$	This study
YAlO₃:Er³⁺ (YAP laser crystals)	$\alpha_a=9.5$; $\alpha_b=4.3$; $\alpha_c=10.8$	Ref. 10
NdGaO₃ (110) oriented film	$\alpha_a=10.0$	Ref. 11
NdGaO₃ powder	$\alpha_{110}=8.9$	Ref. 12
NdGaO₃ powder	$\alpha_a=12.5$; $\alpha_b=4.2$; $\alpha_c=9.8$	Ref. 13
NdGaO₃ powder ^a	$\alpha_a=11.7$; $\alpha_b=5.4$; $\alpha_c=11.2$	Ref. 14
NdGaO₃ powder	$\alpha_a=11.3$; $\alpha_b=2.3$; $\alpha_c=9.1$	This study
LaGaO₃ powder	$\alpha_a=12.1$; $\alpha_b=9.7$; $\alpha_c=11.0$	Ref. 15

^a The α coefficients were obtained from a linear fit of NdGaO₃ structural parameters given in Table I in Ref. 14 as a function of temperature. This paper was published during the preparation of ours.

Table II

Lattice parameter values of YBCO, YAlO₃ and NdGaO₃ as reported in literature and from this study.

	a (10⁻¹ nm)	b (10⁻¹ nm)	c (10⁻¹ nm)	Source
YBa₂Cu₃O_{7-δ}				
orthorhombic (δ=0.07)	3.8227(1)	3.8872(2)	11.6802(2)	Ref. 16
tetragonal 818°C (δ=0.6)	3.9018(1)	3.9018(1)	11.9403(5)	Ref. 17
YAlO₃				
^a	5.180(2)	5.330(2)	7.375(2)	Ref. 18
	5.1671(6)	5.3148(8)	7.3538(9)	Ref. 19
^b	5.179(2)	5.327(1)	7.373(2)	This study
NdGaO₃				
	5.426	5.502	7.706	Ref. 20
	5.4276(1)	5.4979(1)	7.7078(2)	Refs. 12, 21,
				22
^b	5.428(4)	5.502(4)	7.707(4)	This study

^a Lattice parameters were converted to Pbnm space group from standardized Pnma space group in Ref. 18.

^b a, b, c refined values were obtained at 28°C from angular positions of the diffraction lines.

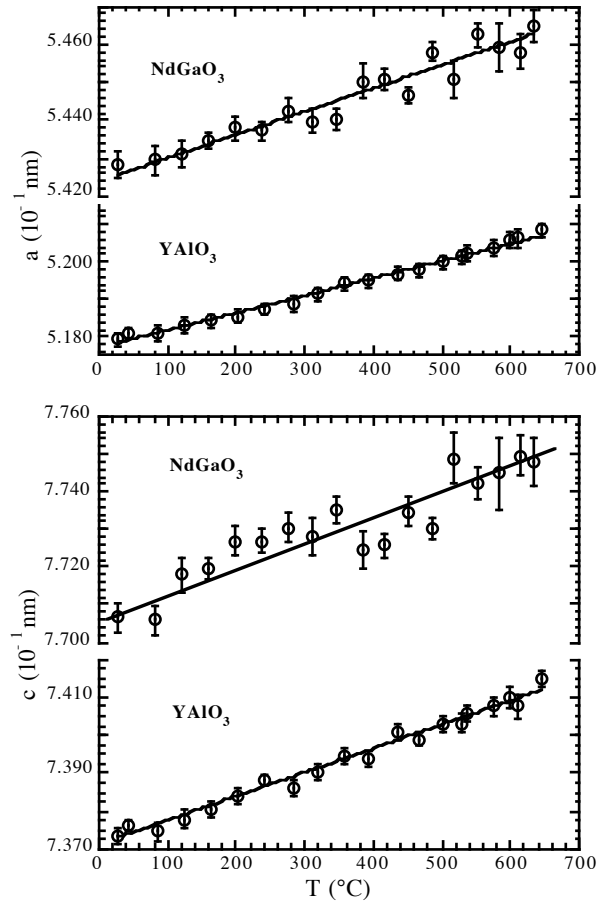


Fig. 1

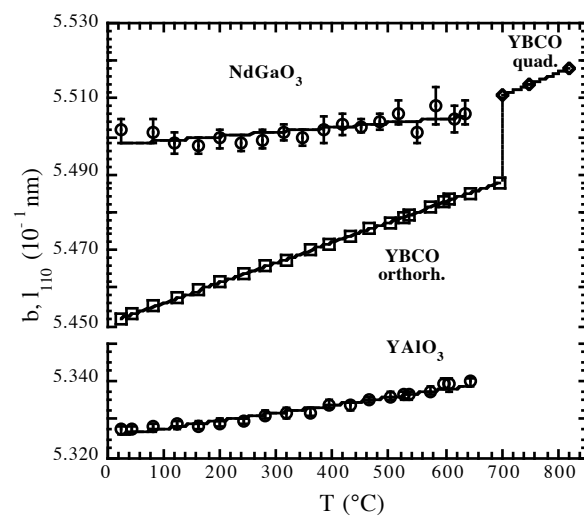


Fig. 2