



Comment on “Lattice deformation and magnetic properties in epitaxial thin films of Sr 1-x Ba x RuO 3 ” [Appl. Phys. Lett. 73, 1200 (1998)]

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COMMENTS

Comment on “Lattice deformation and magnetic properties in epitaxial thin films of $\text{Sr}_{1-x}\text{Ba}_x\text{RuO}_3$ ” [Appl. Phys. Lett. 73, 1200 (1998)]

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Recently, Fukushima *et al.*¹ reported the epitaxial growth of (001) BaRuO_3 films with the perovskite structure on (001) SrTiO_3 substrates. Based on BaRuO_3 films we have grown by both 90° off-axis sputtering and pulsed laser deposition,² however, we believe that the x-ray patterns that they attributed to the growth of the metastable perovskite³ polymorph of BaRuO_3 are actually due to the stable nine layer (9L) hexagonal polymorph of BaRuO_3 ,⁴ with a $(20\bar{2}5)$ orientation. As has been shown for other materials systems,⁵ these polymorphs have nearly degenerate peaks in 2θ , χ , and ϕ

with each other and would give rise to x-ray patterns consistent in both peak positions and peak intensities with those shown by Fukushima *et al.*¹

In studying the epitaxial growth of BaRuO_3 films on (001) SrTiO_3 , we observed very similar θ - 2θ x-ray diffraction (XRD) patterns to those reported by Fukushima *et al.*¹ An example is shown in Fig. 1(a). This θ - 2θ plot alone is inconclusive for phase determination, since the 002 peak of the perovskite polymorph occurs at a nearly identical 2θ value as the $20\bar{2}5$ reflection of the 9L polymorph (see Table I). The small discrepancy between the observed and calculated position of the $20\bar{2}5$ reflection is most likely due to strain and film inhomogeneity.⁷ Additionally, the ϕ scan reported by Fukushima *et al.*¹ is insufficient to discriminate the 101 reflection of the perovskite polymorph from the $11\bar{2}0$ reflection of the 9L polymorph (see Table I). Using four-circle x-ray diffraction and performing a ϕ scan [Fig. 1(b)] at $2\theta \approx 27.2^\circ$ and $\chi \approx 43.0^\circ$ ($01\bar{1}5$ reflection of 9L BaRuO_3) we have found the phase in our films to be consistent with the 9L BaRuO_3 polymorph, and *inconsistent* with the growth of the metastable perovskite polymorph.⁷ This and other ϕ scans, i.e., a scan of the $11\bar{2}0$ reflection of the 9L polymorph, lead us to believe that each of the “very

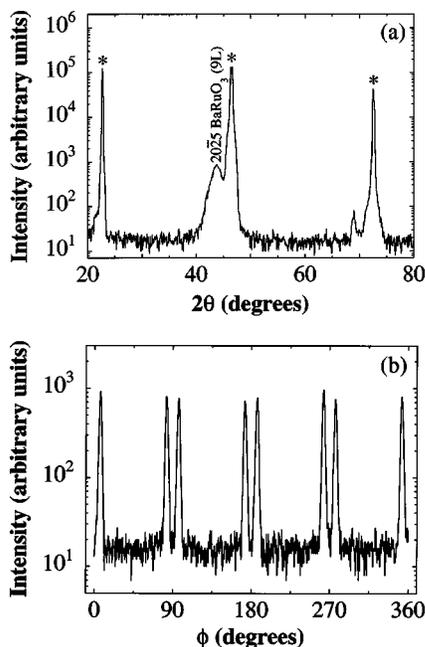


FIG. 1. X-ray diffraction patterns of a film grown under similar conditions as Fukushima *et al.* that is *not* BaRuO_3 with the perovskite structure, but rather the 9L polymorph of BaRuO_3 (see Ref. 7): (a) θ - 2θ at $\chi=90^\circ$ [substrate peaks are labeled as (*)] and (b) ϕ scan of the $01\bar{1}5$ reflection of the 9L polymorph of BaRuO_3 at $2\theta \approx 27.2^\circ$ and $\chi \approx 43.0^\circ$.

TABLE I. Calculated XRD peak positions of the perovskite and the 9L hexagonal polymorph of BaRuO_3 .^a

Phase	Peaks	2θ (deg)	χ^b (deg)	ϕ (deg)
BaRuO_3 (001)-oriented perovskite	002	45.17	90	—
	101	31.51	45	0
	202	65.79	45	0
BaRuO_3 ($20\bar{2}5$)-oriented (nine layer hexagonal)	$20\bar{2}5$	41.83	90	—
	$11\bar{2}0$	31.07	48.62	$\pm 1.4^\circ$
	$22\bar{4}0$	64.79	48.62	$\pm 1.4^\circ$
	$01\bar{1}5$	27.29	41.38	$\pm 6.9^\circ$

^aThe values are based on $\text{Cu } K\alpha_1$ radiation, bulk lattice constants (see Refs. 3 and 4), and $\phi=0^\circ$ chosen to be parallel to the in-plane $[100]$ direction of the (001) SrTiO_3 substrate.

^b $\chi=90^\circ$ is perpendicular to the plane of the substrate.

^cAssuming degenerate epitaxy (see Ref. 6).

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broad peaks of the XRD'' patterns reported by Fukushima *et al.*¹ in their ϕ scan of the ''BaRuO₃(101)^{tetragonal} peak'' may be explained as broad and overlapping 11 $\bar{2}$ 0 peaks of the 9L polymorph (see Table I). Our results are in full agreement with previous unsuccessful attempts to grow metastable BaRuO₃ by epitaxial stabilization on (100) KTaO₃.⁸

It should be noted that the results presented by Fukushima *et al.*¹ are *not* inconsistent with the perovskite polymorph of BaRuO₃, yet they are ambiguous given the demonstrated near overlap of all the peaks reported by them with peaks of the 9L (and 4L) polymorph. Despite our attempts to replicate their work, we cannot synthesize the metastable perovskite polymorph of BaRuO₃ and we would suggest additional, definitive scans for unambiguous corroboration of their interpretation of their results.

¹N. Fukushima, K. Sano, T. Schimiza, K. Abe, and S. Komatsu, Appl. Phys. Lett. **73**, 1200 (1998).

²M. K. Lee, I. W. Scrymgeour, J. Lettieri, D. G. Schlom, and C. B. Eom (unpublished).

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constants of the metastable perovskite polymorph of BaRuO₃ (pseudocubic with $a \approx 4.01$ Å) have been estimated by extrapolating the lattice constants reported in this work for Ba_xSr_{1-x}RuO₃ to $x = 1$.

⁴*Powder Diffraction File* (International Centre for Diffraction Data, Swarthmore, PA, 1995), JCPDS card 45-529. This reference states that the 9L polymorph of BaRuO₃ has lattice constants $a = 5.749$ Å and $c = 21.608$ Å.

⁵J. Lettieri, C. I. Weber, and D. G. Schlom, Appl. Phys. Lett. **73**, 2057 (1998).

⁶S.-W. Chan, J. Phys. Chem. Solids **55**, 1137 (1994).

⁷Our films showed evidence of a mixture of both the four layer (4L) and 9L hexagonal polymorphs. Discrimination of the 4L polymorph from the perovskite phase is equally as difficult since the 20 $\bar{2}$ 3, 11 $\bar{2}$ 0, and 22 $\bar{4}$ 0 reflections of the 4L structure also exhibit a near overlap of peak position and intensity with the perovskite polymorph (and with the 20 $\bar{2}$ 5, 11 $\bar{2}$ 0, and 22 $\bar{4}$ 0 reflections of the 9L polymorph). A ϕ scan of the 01 $\bar{1}$ 5 reflection of the 9L polymorph or the 01 $\bar{1}$ 2 reflection of the 4L polymorph is sufficient to distinguish between these two phases. Nevertheless, in none of our films grown under a wide range of growth conditions by both sputtering and pulsed laser deposition was the perovskite polymorph evident.

⁸H.-M. Christen, L. A. Boatner, J. D. Budai, M. F. Chisholm, L. A. Gea, D. P. Norton, C. Gerber, and M. Urbanik, Appl. Phys. Lett. **70**, 2147 (1997).