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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)]

J. Lettieri, I. W. Scrymgeour, and D. G. Schlom

Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802-5005

M. K. Lee and C. B. Eom

Department of Mechanical Engineering and Materials Science, Duke University, Durham, North Carolina 27708

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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 perovskite polymorph\(^3\) of BaRuO$_3$ are actually due to the stable nine layer (9L) hexagonal polymorph of BaRuO$_3$,\(^4\) with a (202) 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 2025 reflection of the 9L polymorph (see Table I). The small discrepancy between the observed and calculated position of the 2025 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 1120 reflection of the 9L polymorph (see Table I). Using four-circle x-ray diffraction and performing a φ scan [Fig. 1(b)] at 2θ = 27.2° and χ = 43.0° (01f5 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.\(^5\) This and other φ scans, i.e., a scan of the 1120 reflection of the 9L polymorph, lead us to believe that each of the \(^{1}\)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 χ = 90° [substrate peaks are labeled as *(*)] and (b) φ scan of the 0115 reflection of the 9L polymorph of BaRuO$_3$ at 2θ = 27.2° and χ = 43.0°.](image)

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![TABLE I. Calculated XRD peak positions of the perovskite and the 9L hexagonal polymorph of BaRuO$_3$.*](table)

<table>
<thead>
<tr>
<th>Phase</th>
<th>Peaks</th>
<th>2θ (deg)</th>
<th>χ° (deg)</th>
<th>φ (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaRuO$_3$</td>
<td>002</td>
<td>45.17</td>
<td>90</td>
<td>—</td>
</tr>
<tr>
<td>(001)-oriented</td>
<td>101</td>
<td>31.51</td>
<td>45</td>
<td>0</td>
</tr>
<tr>
<td>perovskite</td>
<td>202</td>
<td>65.79</td>
<td>45</td>
<td>0</td>
</tr>
<tr>
<td>BaRuO$_3$</td>
<td>2025</td>
<td>41.83</td>
<td>90</td>
<td>—</td>
</tr>
<tr>
<td>(2025)-oriented</td>
<td>1120</td>
<td>31.07</td>
<td>48.62</td>
<td>±1.4°</td>
</tr>
<tr>
<td>(nine layer)</td>
<td>2240</td>
<td>64.79</td>
<td>48.62</td>
<td>±1.4°</td>
</tr>
<tr>
<td>hexagonal</td>
<td>01f5</td>
<td>27.29</td>
<td>41.38</td>
<td>±6.9°</td>
</tr>
</tbody>
</table>

*The values are based on Cu K$_{α1}$ radiation, bulk lattice constants (see Refs. 3 and 4), and φ = 0° chosen to be parallel to the in-plane [100] direction of the (001) SrTiO$_3$ substrate.

$\chi = 90°$ is perpendicular to the plane of the substrate.

$\chi$ Assuming degenerate epitaxy (see Ref. 6).
broad peaks of the XRD patterns reported by Fukushima et al. in their \( \phi \) scan of the ‘‘\( \text{BaRuO}_3(101) \) tetragonal peak’’ may be explained as broad and overlapping 1120 peaks of the 9L polymorph (see Table I). Our results are in full agreement with previous unsuccessful attempts to grow metastable \( \text{BaRuO}_3 \) by epitaxial stabilization on \( (100) \) \( \text{KTaO}_3 \).

It should be noted that the results presented by Fukushima et al. are not inconsistent with the perovskite polymorph of \( \text{BaRuO}_3 \), 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 \( \text{BaRuO}_3 \) and we would suggest additional, definitive scans for unambiguous corroboration of their interpretation of their results.

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3. J. M. Longo and A. J. Kafalas, Mater. Res. Bull. 3, 687 (1968). The lattice constants of the metastable perovskite polymorph of \( \text{BaRuO}_3 \) (pseudocubic with \( a \approx 4.01 \) Å) have been estimated by extrapolating the lattice constants reported in this work for \( \text{Ba}_x\text{Sr}_{1-x}\text{Ru}_3 \) to \( x \approx 1 \).
4. Powder Diffraction File (International Centre for Diffraction Data, Swarthmore, PA, 1995), JCPDS card 45–529. This reference states that the 9L polymorph of \( \text{BaRuO}_3 \) has lattice constants \( a = 5.749 \) Å and \( c = 21.608 \) Å.
7. Our 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 202, 1120, and 2240 reflections of the 4L structure also exhibit a near overlap of peak position and intensity with the perovskite polymorph (and with the 2025, 1120, and 2240 reflections of the 9L polymorph). A \( \phi \) scan of the 0115 reflection of the 9L polymorph or the 0112 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.