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# Epitaxial integration of high-mobility La-doped BaSnO<sub>3</sub> thin films with silicon

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## ABSTRACT

La-doped BaSnO<sub>3</sub> has been epitaxially integrated with (001) Si using an SrTiO<sub>3</sub> buffer layer via molecular-beam epitaxy (MBE). A 254 nm thick undoped BaSnO<sub>3</sub> buffer layer was grown to enhance the mobility of the overlying La-doped BaSnO<sub>3</sub> layer. The x-ray diffraction rocking curve of the BaSnO<sub>3</sub> 002 peak has a full width at half maximum of 0.02°. At room temperature, the resistivity of the La-doped BaSnO<sub>3</sub> film is  $3.6 \times 10^{-4} \Omega \text{ cm}$  and the mobility is  $128 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  at a carrier concentration of  $1.4 \times 10^{20} \text{ cm}^{-3}$ . These values compare favorably to those of La-doped BaSnO<sub>3</sub> films grown by all techniques other than MBE on single-crystal oxide substrates. Our work opens an exciting arena for integrating hyper-functional oxide electronics that make use of high-mobility oxide films with the workhorse of the semiconductor industry, silicon.

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Recently there has been tremendous interest in La-doped BaSnO<sub>3</sub> because of its unusually high mobility at room temperature for a transparent conducting oxide. Mobilities in La-doped BaSnO<sub>3</sub> single crystals<sup>1</sup> and thin films<sup>2</sup> have reached  $320 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  and  $183 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , respectively. The high room-temperature mobility of La-doped BaSnO<sub>3</sub>, in combination with its transparency at optical wavelength, ability to be heavily doped, and oxygen stability<sup>1,3-6</sup> makes it an exciting component for fabricating novel thermally stable devices including power electronics,<sup>7,8</sup> optoelectronic devices,<sup>9-11</sup> thermoelectric devices,<sup>12</sup> solar cells,<sup>13</sup> and field effect transistors.<sup>14,15</sup> Moreover, thanks to the structural and chemical compatibility of BaSnO<sub>3</sub> with functional perovskite oxides that show a plethora of novel and emergent properties, a heterostructure consisting of high-mobility La-doped BaSnO<sub>3</sub>, and other perovskite oxides can potentially enrich the family of functionalities of all-oxide heterostructures and provide opportunities for hybrid devices by exploiting emergent

phenomena of oxide interfaces and heterostructures.<sup>16,17</sup> For example, integration of high mobility La-doped BaSnO<sub>3</sub> with ferroelectrics such as Pb(Zr, Ti)O<sub>3</sub> can potentially realize devices including nonvolatile memories,<sup>18</sup> ferroelectric field-effect transistors,<sup>19</sup> low-power transistors that can beat the 60 mV/decade subthreshold slope limit of conventional semiconductors,<sup>20</sup> and hyper-sensitive temperature or pressure sensors.<sup>21</sup>

While rapid progress has been made on the growth of high-mobility BaSnO<sub>3</sub> thin films during the last few years,<sup>1,2,22-28</sup> most of the La-doped BaSnO<sub>3</sub> thin films have been grown on single-crystal oxide substrates which are currently limited to small size (typically no larger than  $10 \times 10 \text{ nm}$ ). Very limited work on La-doped BaSnO<sub>3</sub> thin films has been carried out on scalable substrates of industrial quality,<sup>29</sup> thus making it difficult to take advantage of the well-developed and efficient fabrication processes in the semiconductor industry.

Specifically, there is no report of growing La-doped BaSnO<sub>3</sub> films on the backbone of semiconductor industry, silicon.

The integration of functional oxides directly on silicon, however, is difficult due to the reactive nature of the (001) Si surface with oxygen to form an amorphous SiO<sub>2</sub> layer that can impede epitaxial growth. Furthermore, most oxides react with silicon. Due to the unknown free energy of BaSnO<sub>3</sub>, we are unable to assess its thermodynamic stability in direct contact with silicon. We note, however, that the binary components of BaSnO<sub>3</sub>-BaO and SnO<sub>2</sub>-are both thermodynamically unstable in contact with silicon.<sup>30</sup> From a simple bond strength perspective, where energies are assigned to M-O bonds (where M is a cation), this would suggest that BaSnO<sub>3</sub> is unstable in direct contact with silicon.<sup>31</sup> The lack of thermodynamic stability does not, however, preclude epitaxial growth. The epitaxial growth of an unstable interface can sometimes be achieved at low temperature, e.g., room temperature as is used to form epitaxial BaO/Si<sup>32</sup> or CeO<sub>2</sub>/Si interfaces,<sup>33</sup> both of which are thermodynamically unstable. Upon heating to about 650 °C, however, reaction is observed at these interfaces following the expectations of thermodynamics.<sup>30,34-37</sup>

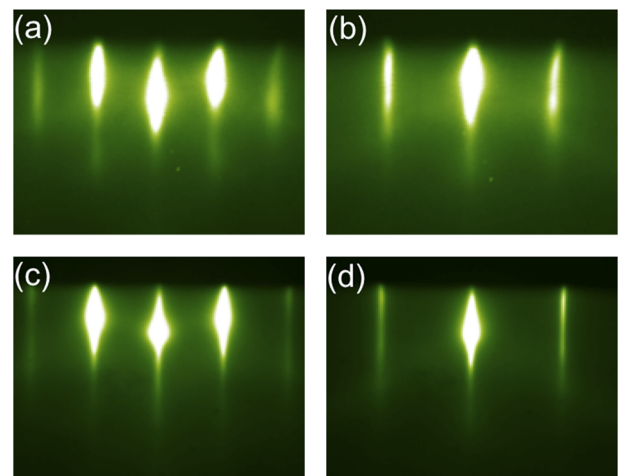
To date, only a few oxides have been epitaxially grown directly on silicon. These include BeO,<sup>38,39</sup> MgO,<sup>40,41</sup> SrO,<sup>36,42</sup> BaO,<sup>32,43</sup> Sc<sub>2</sub>O<sub>3</sub>,<sup>44</sup> Y<sub>2</sub>O<sub>3</sub>,<sup>45</sup> ZrO<sub>2</sub>,<sup>46</sup> HfO<sub>2</sub>,<sup>47</sup> La<sub>2</sub>O<sub>3</sub>,<sup>48</sup> CeO<sub>2</sub>,<sup>33</sup> Pr<sub>2</sub>O<sub>3</sub>,<sup>49,50</sup> Nd<sub>2</sub>O<sub>3</sub>,<sup>51,52</sup> Sm<sub>2</sub>O<sub>3</sub>,<sup>53</sup> EuO,<sup>54,55</sup> Gd<sub>2</sub>O<sub>3</sub>,<sup>56-58</sup> Dy<sub>2</sub>O<sub>3</sub>,<sup>53</sup> Ho<sub>2</sub>O<sub>3</sub>,<sup>53</sup> Er<sub>2</sub>O<sub>3</sub>,<sup>58,59</sup> Tm<sub>2</sub>O<sub>3</sub>,<sup>60</sup> Lu<sub>2</sub>O<sub>3</sub>,<sup>61</sup> Al<sub>2</sub>O<sub>3</sub>,<sup>62</sup> yttria-stabilized zirconia (YSZ),<sup>63</sup> yttria-stabilized hafnia (Y<sub>2</sub>O<sub>3</sub>-HfO<sub>2</sub>),<sup>64</sup> (Ba, Sr)O,<sup>36,43</sup> (La, Y)<sub>2</sub>O<sub>3</sub>,<sup>65</sup> (Pr, Y)<sub>2</sub>O<sub>3</sub>,<sup>66</sup> (La, Lu)<sub>2</sub>O<sub>3</sub>,<sup>67-69</sup> MgAl<sub>2</sub>O<sub>4</sub>,<sup>70</sup> SrTiO<sub>3</sub>,<sup>71,72</sup> La<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>,<sup>73</sup> SrHfO<sub>3</sub>,<sup>74,75</sup> Ba<sub>2</sub>SiO<sub>4</sub>,<sup>37</sup> and La<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub>.<sup>76</sup> Among these, SrTiO<sub>3</sub> is one of the most frequently used epitaxial buffer layers for the growth of functional oxides on (001) Si,<sup>77</sup> thanks to its relatively high crystalline quality on silicon<sup>78-80</sup> and its structural compatibility with various functional perovskite materials.<sup>77,81</sup>

Here we report growth of La-doped BaSnO<sub>3</sub> films on (001) Si using a SrTiO<sub>3</sub> buffer layer grown by molecular-beam epitaxy (MBE). The resulting La-doped BaSnO<sub>3</sub> film on silicon is epitaxial, with a room-temperature mobility of 128 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> and a resistivity of 3.6 × 10<sup>-4</sup> Ω cm, at a carrier concentration of 1.4 × 10<sup>20</sup> cm<sup>-3</sup>. Both the structural perfection and the electrical transport characteristics of the La-doped BaSnO<sub>3</sub> films on silicon rival those of epitaxial La-doped BaSnO<sub>3</sub> films grown on single-crystal oxide substrates.<sup>1,2,5-7,14,22-29,82-84</sup>

The SrTiO<sub>3</sub> buffer layer and the La-doped BaSnO<sub>3</sub> film were grown in a Veeco GEN10 dual-chamber MBE system. Each growth chamber is equipped with an *in situ* reflection high-energy electron diffraction (RHEED) system for monitoring the film growth. Substrate temperature is monitored with a thermocouple for temperatures below 500 °C and an optical pyrometer with a measurement wavelength of 980 nm for temperatures above 500 °C. The silicon substrates (2" diameter, *p*-type, boron doped, and with resistivity larger than 10 Ω cm) were cleaned in an ultraviolet ozone cleaner for 20 min before being loaded into the first growth chamber with a background pressure in the upper 10<sup>-9</sup> Torr range.

An 18 nm thick SrTiO<sub>3</sub> buffer layer was grown on the bare (001) Si. The first 2 nm were grown using the epitaxy-by-periodic-annealing method<sup>85,86</sup> followed by an additional 16 nm grown by codeposition at 580 °C under an oxygen partial pressure of ~ (5 - 8) × 10<sup>-8</sup> Torr. Elemental strontium and titanium beams were generated from a conventional low-temperature effusion cell and a Ti-Ball,<sup>87</sup> respectively. To be specific, two 2.5 unit-cell-thick SrTiO<sub>3</sub> layers were grown by codeposition (strontium, titanium, and oxygen all supplied simultaneously) at 300 °C under an oxygen partial pressure of ~ 5 × 10<sup>-8</sup> Torr, then the substrate temperature was raised to 580 °C under vacuum to enhance the crystalline quality of the as-grown SrTiO<sub>3</sub> film. After forming a 5 unit-cell-thick epitaxial SrTiO<sub>3</sub> film (i.e., two repeats of the epitaxy-by-periodic-annealing step) by this process, the substrate temperature was raised to 580 °C and additional SrTiO<sub>3</sub> was codeposited until the SrTiO<sub>3</sub> film reached a total thickness of 18 nm. RHEED patterns of the 18 nm thick SrTiO<sub>3</sub> film viewed along the [100] and [110] azimuths are shown in Figs. 1(a) and 1(b), respectively. No other phases were detected during or after the growth of the 18 nm thick SrTiO<sub>3</sub> film, indicating that the SrTiO<sub>3</sub> film is a single phase and epitaxial. More detail of the growth of the SrTiO<sub>3</sub> buffer layer on silicon is provided elsewhere.<sup>80</sup>

The (La-doped) BaSnO<sub>3</sub> films are grown in an adsorption-controlled regime, with molecular beams emanating from separate effusion cells containing lanthanum (99.996% purity, Ames Lab), barium (99.99% purity, Sigma-Aldrich), and SnO<sub>2</sub> (99.996% purity, Alfa Aesar).<sup>2</sup> The oxidant used for the growth of the (La-doped) BaSnO<sub>3</sub> films is a mixture of ~10% ozone and 90% oxygen. By growing BaSnO<sub>3</sub> within an adsorption-controlled regime, the stoichiometry of the BaSnO<sub>3</sub> film is ensured by exploiting the volatility of the SnO<sub>x</sub>(g): excess



**FIG. 1.** RHEED patterns viewed along (a) the [100] azimuth and (b) the [110] azimuth of the 18 nm thick (001)-oriented SrTiO<sub>3</sub> buffer layer after growth. (c) RHEED patterns viewed along (c) the [100] azimuth and (d) the [110] azimuth of the overlying 318 nm thick BaSnO<sub>3</sub> film after growth.

$\text{SnO}_x(\text{g})$  leaves the surface of the growing film so that a stoichiometric  $\text{BaSnO}_3$  film is formed.<sup>2</sup> During the growth of the (La-doped)  $\text{BaSnO}_3$ , all components—(lanthanum), barium,  $\text{SnO}_x$ , and the  $\sim 10\% \text{O}_3 + 90\% \text{O}_2$  oxidant—are supplied simultaneously, and the substrate temperature is kept at  $\sim 700^\circ\text{C}$ . RHEED intensity oscillations (Fig. S1) were observed during the initial codeposition growth stage of the  $\text{BaSnO}_3$  film on the  $\text{SrTiO}_3$  buffer layer on silicon, manifesting a layer-by-layer growth mode of the  $\text{BaSnO}_3$  film on  $\text{SrTiO}_3$ -buffered silicon at the initial growth stage.<sup>2</sup> A 254 nm thick undoped  $\text{BaSnO}_3$  buffer layer is deposited on top of the 18 nm thick  $\text{SrTiO}_3$  buffer layer, followed by a 64 nm thick active layer of La-doped  $\text{BaSnO}_3$ . The purpose of the thick undoped  $\text{BaSnO}_3$  layer is to enhance the electron mobility of the active layer.<sup>14,25,83</sup> Further details on the growth of the (La-doped)  $\text{BaSnO}_3$  films can be found elsewhere.<sup>2</sup>

RHEED patterns after the growth of the 64 nm thick La-doped  $\text{BaSnO}_3$  on the 254 nm thick undoped  $\text{BaSnO}_3$  buffer layer are shown in Figs. 1(c) and 1(d). The streaky RHEED patterns indicate that the surface of the La-doped  $\text{BaSnO}_3$  film is epitaxial and relatively smooth on an atomic scale. The  $1 \times 1$  surface reconstruction of the La-doped  $\text{BaSnO}_3$  film observed in RHEED that is sharp and free of diffuse features manifest that the La-doped  $\text{BaSnO}_3$  film is stoichiometric.<sup>2</sup> The surface morphology of the same sample was examined *ex situ* by atomic force microscopy (AFM) using an Asylum Research MFP-3D in tapping mode, as is shown in Fig. S2. The rms roughness of the sample is  $\sim 4 \text{ \AA}$ , which is consistent with the streaky RHEED patterns.

The crystalline quality of the same sample was assessed by *ex-situ* x-ray diffraction (XRD) with a PANalytical X'Pert system utilizing  $\text{Cu K}\alpha_1$  radiation. Figure 2(a) shows the  $\theta$ - $2\theta$  scan of the same heterostructure characterized in Fig. 1. Only 00l reflections of the  $\text{SrTiO}_3$  buffer layer and the  $\text{BaSnO}_3$  film are

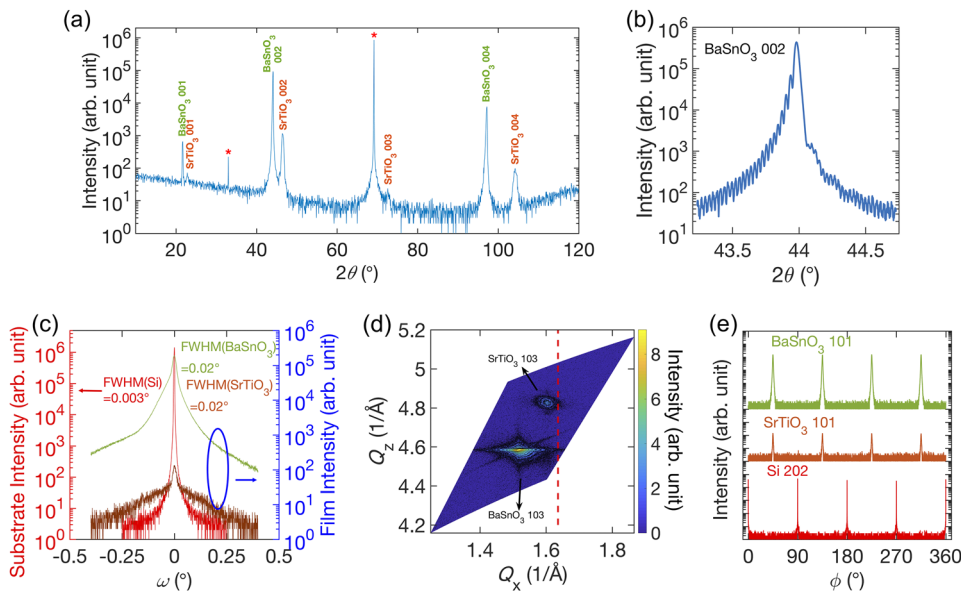
observed in the  $\theta$ - $2\theta$  scan, corroborating that the film is epitaxial and phase pure. A fine  $\theta$ - $2\theta$  scan around the  $\text{BaSnO}_3$  002 peak is shown in Fig. 2(b). Clear thickness fringes around the  $\text{BaSnO}_3$  002 peak manifest that the interfaces of the sample are smooth. Using a Nelson-Riley analysis,<sup>88</sup> the out-of-plane lattice parameter of the  $\text{BaSnO}_3$  film is calculated to be  $4.110 \pm 0.001 \text{ \AA}$ , which is close to, but slightly smaller than the bulk value of  $4.116 \text{ \AA}$ .<sup>89</sup>

We believe the slightly smaller out-of-plane lattice parameter of the  $\text{BaSnO}_3$  film is due to the tensile strain caused by the relatively large difference between the thermal expansion coefficients of  $\text{BaSnO}_3$  (averaging  $9.3 \times 10^{-6} \text{ K}^{-1}$  between room temperature to  $1500^\circ\text{C}$ )<sup>90</sup> and silicon (averaging  $3.7 \times 10^{-6} \text{ K}^{-1}$  between room temperature and  $720^\circ\text{C}$ ).<sup>91</sup> To verify this, we calculate the expected out-of-plane lattice parameter of the  $\text{BaSnO}_3$  film at room temperature ( $a_{\text{out-of-plane},25^\circ\text{C}}^{\text{BaSnO}_3}$ ) and the expected tensile strain under the assumptions that the  $\text{BaSnO}_3$  film is fully relaxed at the growth temperature ( $\sim 700^\circ\text{C}$ ) and that the  $\text{BaSnO}_3$  film is rigidly clamped to the underlying silicon substrate as it is cooled to room temperature.

From

$$a_{\text{in-plane},25^\circ\text{C}}^{\text{BaSnO}_3} - a_{\text{in-plane},700^\circ\text{C}}^{\text{BaSnO}_3} = \frac{a_{\text{in-plane},25^\circ\text{C}}^{\text{silicon}} - a_{\text{in-plane},700^\circ\text{C}}^{\text{silicon}}}{\sqrt{2}}, \quad (1)$$

where  $a_{\text{in-plane},25^\circ\text{C}}^{\text{silicon}} = 5.4305 \text{ \AA}$  is the silicon lattice parameter at room temperature,  $a_{\text{in-plane},700^\circ\text{C}}^{\text{silicon}} = 5.444 \text{ \AA}$  is the silicon lattice parameter at the growth temperature, and  $a_{\text{in-plane},700^\circ\text{C}}^{\text{BaSnO}_3} = 4.142 \text{ \AA}$  is the in-plane lattice parameter of the  $\text{BaSnO}_3$  film at the growth temperature, we can calculate the expected



**FIG. 2.** (a) XRD  $\theta$ - $2\theta$  scan of the same sample characterized in Fig. 1. The asterisks indicate the substrate peaks. (b) An enlarged view of the  $\theta$ - $2\theta$  scan around the  $\text{BaSnO}_3$  002 peak with clear thickness fringes. The  $\theta$ - $2\theta$  scan was measured with an open detector, and the fine scan around the  $\text{BaSnO}_3$  002 peak was measured in a triple-axis geometry. (c) Rocking curves of the  $\text{SrTiO}_3$  and  $\text{BaSnO}_3$  002 peaks, together with that of the Si 004 peak. The FWHM of both the  $\text{SrTiO}_3$  and the  $\text{BaSnO}_3$  002 peaks is  $0.02^\circ$ . The FWHM of the Si 004 peak is  $0.003^\circ$ . (d) RSM around the  $\text{BaSnO}_3$  and  $\text{SrTiO}_3$  103 peaks. (e)  $\phi$  scan of the same sample. The Si 202,  $\text{SrTiO}_3$  101, and  $\text{BaSnO}_3$  101 family of peaks were measured, and the FWHM of the film  $\phi$  scans is  $0.9^\circ$  for both the  $\text{SrTiO}_3$  101 and  $\text{BaSnO}_3$  101 peaks. The  $\phi$  scans are offset from each other along the vertical axis for clarity.

in-plane lattice parameter of the BaSnO<sub>3</sub> film,  $a_{in-plane,25^\circ C}^{BaSnO_3} = 4.132 \text{ \AA}$ .

Using

$$a_{out-of-plane,25^\circ C}^{BaSnO_3} = \frac{2\nu}{\nu-1} a_{in-plane,25^\circ C}^{BaSnO_3} + \frac{1+\nu}{1-\nu} a_{0,25^\circ C}^{BaSnO_3} \quad (2^{92,93})$$

where  $a_{0,25^\circ C}^{BaSnO_3} = 4.116 \text{ \AA}$  is the bulk lattice parameter of BaSnO<sub>3</sub>,  $\nu$  is Poisson's ratio of BaSnO<sub>3</sub> (here we use a value  $\nu = 0.23$  obtained from first-principles calculations),<sup>94</sup> we get  $a_{out-of-plane,25^\circ C}^{BaSnO_3} = 4.106 \text{ \AA}$ , which is close to the out-of-plane lattice parameter we obtained from the XRD measurement ( $4.110 \pm 0.001 \text{ \AA}$ ). Note that the agreement would be improved if some relaxation occurred in the BaSnO<sub>3</sub> film as it is cooled from growth temperature to room temperature.

Using  $a_{in-plane,25^\circ C}^{BaSnO_3} = 4.132 \text{ \AA}$ , we can also calculate the expected tensile strain on the BaSnO<sub>3</sub> film due to the thermal expansion difference. The expected tensile strain is 0.39%. Starting from this expected tensile strain, the expected critical thickness before mechanical cracks form can be calculated<sup>95</sup> using

$$h_c = \frac{a_0(1-\nu)^2}{5\pi \cdot f^2}, \quad (3)$$

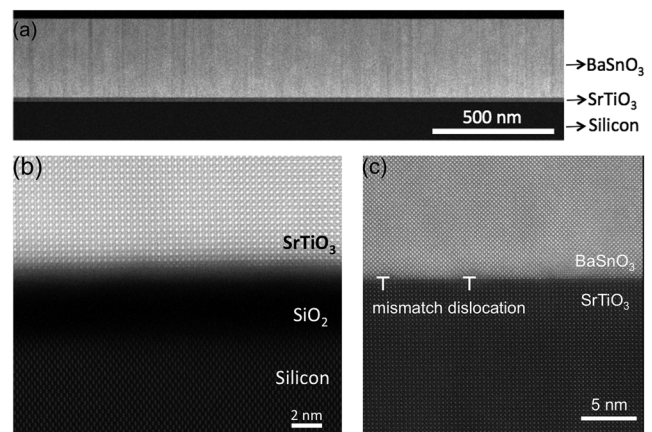
where  $a_0$  is the lattice parameter and  $f$  is the expected tensile strain, 0.39%.  $h_c$  is calculated to be  $\sim 1.0 \text{ \mu m}$ , which is larger than the thickness of our BaSnO<sub>3</sub> film. This is consistent with our observation by AFM that our film is free of cracks.

XRD rocking curves ( $\omega$  scans) of the SrTiO<sub>3</sub> and BaSnO<sub>3</sub> 002 peaks together with that of the Si 004 peak were measured in a triple-axis geometry, and the results are shown superimposed in Fig. 2(c). Despite the large  $\sim 5.4\%$  compressive strain for (001) BaSnO<sub>3</sub> on (001) SrTiO<sub>3</sub>, the crystalline quality of the BaSnO<sub>3</sub> film is similar to that of the SrTiO<sub>3</sub> buffer layer: they both have a full width at half maximum (FWHM) of  $0.02^\circ$  of their rocking curve, which shows a high degree of crystalline perfection for both the SrTiO<sub>3</sub> buffer layer and the BaSnO<sub>3</sub> film. This can be attributed to the optimized growth process of the SrTiO<sub>3</sub> buffer layer<sup>80</sup> and the adsorption-controlled growth of the BaSnO<sub>3</sub> film to maintain its stoichiometry.<sup>2</sup> Figure 2(d) shows reciprocal space maps (RSMs) of the BaSnO<sub>3</sub> and SrTiO<sub>3</sub> 103 peaks. The red line in Fig. 2(d) shows the film in-plane reciprocal space position that the SrTiO<sub>3</sub> and BaSnO<sub>3</sub> films would have if they were commensurately strained to the silicon substrate. Both the in-plane and out-of-plane lattice parameters of the SrTiO<sub>3</sub> buffer layer and the BaSnO<sub>3</sub> film are found to be fully relaxed to their bulk values.

If the strain introduced by defects is highly anisotropic, as is the case for our SrTiO<sub>3</sub> grown on silicon,<sup>80</sup> characterizing them in a single direction (the out-of-plane direction by the 002 rocking curve) is insufficient. The narrow rocking curve of the 002 SrTiO<sub>3</sub> peak is because of the insensitivity of this particular peak to threading dislocations with pure edge character.<sup>80</sup> This conclusion also holds for the 002 BaSnO<sub>3</sub>

peak of these BaSnO<sub>3</sub>/SrTiO<sub>3</sub>/Si films. The threading dislocation density of our SrTiO<sub>3</sub>/Si films is in excess of  $10^{11} \text{ cm}^{-2}$  (Ref. 80) and as shown below so is the threading dislocation density of the BaSnO<sub>3</sub> film grown on the SrTiO<sub>3</sub>/Si. To further characterize the structural perfection of these films in a different direction (in-plane rather than out-of-plane)  $\phi$ -scans were used. These  $\phi$ -scans assess the in-plane mosaic spread of the SrTiO<sub>3</sub> and BaSnO<sub>3</sub> layers as well as establish their epitaxial orientation relationship. The in-plane epitaxial orientation relationship of the heterostructure was confirmed to be cube-on-cube with a  $45^\circ$  in-plane rotation: (001) BaSnO<sub>3</sub>  $\parallel$  (001) SrTiO<sub>3</sub>  $\parallel$  (001) Si and [100] BaSnO<sub>3</sub>  $\parallel$  [100] SrTiO<sub>3</sub>  $\parallel$  [110] Si, as is shown in Fig. 2(e). The FWHM of the film  $\phi$  scan is  $0.9^\circ$  for both the SrTiO<sub>3</sub> 101 peak and the BaSnO<sub>3</sub> 101 peak. Thus, reducing the in-plane mosaic spread remains the biggest challenge to overcome for both the BaSnO<sub>3</sub> and SrTiO<sub>3</sub> layers in this heterostructure.

The microstructure of the same sample including the abruptness of the interfaces was examined by scanning transmission electron microscopy (STEM), using a probe aberration corrected Titan electron microscope operating at 300 keV. Figure 3(a) is a high-angle annular dark field (HAADF) STEM image that shows the film microstructure in cross section. Threading dislocations in the BaSnO<sub>3</sub> film are illustrated from the stripe contrast in the low-angle annular dark field (LAADF) STEM image shown in Fig. S3. The density of the threading dislocation is estimated to be  $\sim 1.3 \times 10^{11} \text{ cm}^{-2}$ , which is similar to the La-doped BaSnO<sub>3</sub> films grown on single-crystal oxide substrates with large lattice mismatch.<sup>2</sup> The threading dislocations come from both the large lattice mismatch between (001) BaSnO<sub>3</sub> and (001) SrTiO<sub>3</sub>, as well as the threading dislocations from the 18 nm thick SrTiO<sub>3</sub> buffer layer on silicon.

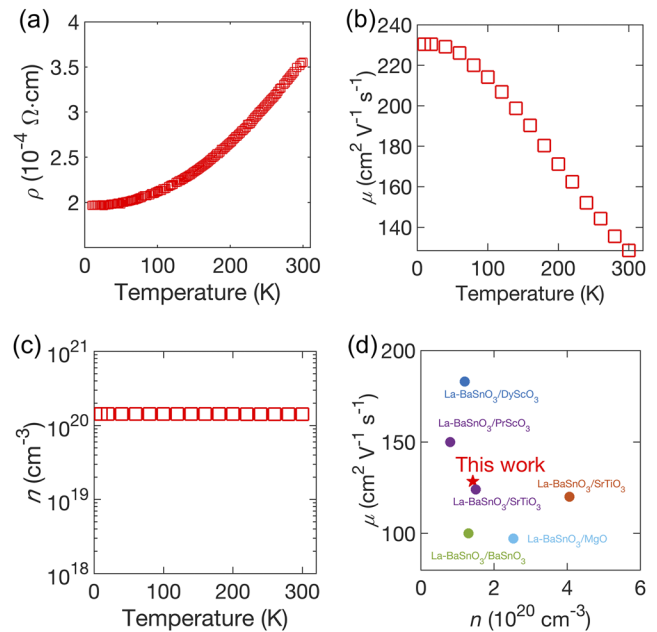


**FIG. 3.** STEM images showing the microstructure of the same sample characterized in Fig. 1. (a) HAADF-STEM image with a low magnification showing the overall sample. (b) The interface between the SrTiO<sub>3</sub> buffer layer and the silicon substrate shows that there is an amorphous SiO<sub>2</sub> layer between the SrTiO<sub>3</sub> buffer layer and the silicon substrate. (c) The interface between the BaSnO<sub>3</sub> film and the SrTiO<sub>3</sub> buffer layer is atomically sharp. Due to the large lattice mismatch between (001) BaSnO<sub>3</sub> and (001) SrTiO<sub>3</sub>, there are misfit dislocations observed in the interface, two examples are marked by the edge dislocation symbols in (c).

The microstructure of the SrTiO<sub>3</sub>/Si and the BaSnO<sub>3</sub>/SrTiO<sub>3</sub> interfaces is shown in Figs. 3(b) and 3(c), respectively. There is a ~4 nm thick amorphous SiO<sub>2</sub> layer between the SrTiO<sub>3</sub> buffer layer and the silicon substrate, which originates from oxygen diffusion through the SrTiO<sub>3</sub> buffer layer during film growth. The extent of interdiffusion across the SrTiO<sub>3</sub>/Si and BaSnO<sub>3</sub>/SrTiO<sub>3</sub> interfaces was investigated by electron energy loss spectroscopy (EELS). As is shown in Fig. S4, there is no observable titanium interdiffusion into the SiO<sub>2</sub> layer. Line profiles of the elemental intensity of silicon, oxygen, and titanium across the SrTiO<sub>3</sub>/Si interface are shown in Fig. S4(f). The HAADF image in Fig. 3(c) shows that the BaSnO<sub>3</sub>/SrTiO<sub>3</sub> interface is abrupt and contains mismatch dislocations. The interface between the BaSnO<sub>3</sub> film and the SrTiO<sub>3</sub> buffer layer is fully relaxed, with an average spacing between edge dislocations of 22 unit cells of SrTiO<sub>3</sub> vs. 21 unit cells of BaSnO<sub>3</sub>, which is consistent with the calculated ratio based on relaxed lattice parameters (~5.4%). EELS mappings of titanium and barium across the BaSnO<sub>3</sub>/SrTiO<sub>3</sub> interface are shown in Fig. S5, and the corresponding line profiles shown in Fig. S5(e) also indicate a clean interface that is free of perceptible interdiffusion.

The transport properties of the same sample was measured in the van der Pauw geometry in a quantum design physical property measurement system (PPMS). Aluminum wires were wire-bonded directly to the La-doped BaSnO<sub>3</sub> film. Figure 4(a) shows the temperature-dependent resistivity. At room temperature, the resistivity is  $3.6 \times 10^{-4} \Omega \text{ cm}$  (corresponding to a conductivity of  $2.8 \times 10^3 \text{ S cm}^{-1}$ ). From 300 K to 10 K, the sample shows weak metallic behavior with no upturn of the resistivity at low temperature. The room temperature mobility of the sample is  $128 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , which is comparable to most La-doped BaSnO<sub>3</sub> films grown on single-crystal oxide substrates.<sup>1,2,5-7,14,22-29,82-84</sup> A comparison of the room temperature mobility of our La-doped BaSnO<sub>3</sub> film on silicon with those of representative La-doped BaSnO<sub>3</sub> films grown on single-crystal oxide substrates is shown in Fig. 4(d). We attribute the high mobility of the La-doped BaSnO<sub>3</sub> film on silicon to its high degree of crystalline perfection.<sup>11</sup> As the temperature decreases, the mobility increases, as is shown in Fig. 4(b). At room temperature, the carrier concentration is  $1.4 \times 10^{20} \text{ cm}^{-3}$ . From an extrapolated measurement of the lanthanum flux, made using a quartz crystal microbalance, and assuming that all of the incident lanthanum is incorporated into the La-doped BaSnO<sub>3</sub> film, the lanthanum concentration in the film is  $(1.6 \pm 0.6)\%$ . Comparing the lanthanum concentration to the measured concentration of mobile carriers ( $1.4 \times 10^{20} \text{ cm}^{-3}$  electrons), the dopant activation percentage is  $(64 \pm 25)\%$ . Figure 4(c) shows that the carrier concentration of the La-doped BaSnO<sub>3</sub> film is almost temperature independent. The temperature-dependent resistivity, mobility, and carrier concentration of our film on silicon closely resemble those of La-doped BaSnO<sub>3</sub> films grown on single-crystal oxide substrates.<sup>1,2,5-7,14,22-29,82-84</sup>

In summary, we have integrated La-doped BaSnO<sub>3</sub> films on silicon using an epitaxial SrTiO<sub>3</sub> buffer layer formed by MBE. The surface morphology, structural perfection, and



**FIG. 4.** Temperature-dependent (a) resistivity ( $\rho$ ), (b) mobility ( $\mu$ ), and (c) carrier concentration ( $n$ ) of the same sample characterized in Fig. 1. The results resemble those of La-doped BaSnO<sub>3</sub> films grown on single-crystal oxide substrates. (d) Comparison of the room-temperature mobility of our La-doped BaSnO<sub>3</sub> film on silicon (red star) with those of representative epitaxial BaSnO<sub>3</sub> films grown on single-crystal oxide substrates in the literature.  $\mu$  is the mobility, and  $n$  is the carrier concentration of the La-doped BaSnO<sub>3</sub> films. The La-BaSnO<sub>3</sub>/DyScO<sub>3</sub> data point is from Ref. 2; the La-BaSnO<sub>3</sub>/PrScO<sub>3</sub> and the purple La-BaSnO<sub>3</sub>/SrTiO<sub>3</sub> data points are from Ref. 24; the brown La-BaSnO<sub>3</sub>/SrTiO<sub>3</sub> data point is from Ref. 7; the La-BaSnO<sub>3</sub>/BaSnO<sub>3</sub> data point is from Ref. 26; the La-BaSnO<sub>3</sub>/MgO data point is from Ref. 84.

electrical properties of our samples are similar to those of La-doped BaSnO<sub>3</sub> films grown on single-crystal oxide substrates. Our results motivate the integration of functional oxide devices utilizing the exceptional properties of BaSnO<sub>3</sub>-based heterostructures (e.g., the possibility of ferroelectric field effect transistors) with the backbone of today's semiconductor industry, silicon.

See [supplementary material](#) for RHEED oscillations of BaSnO<sub>3</sub> on SrTiO<sub>3</sub> on silicon, surface morphology of the sample, and additional STEM images and EELS mappings of the sample.

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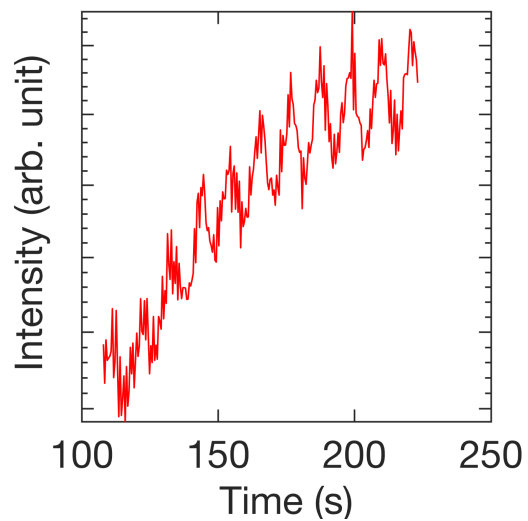


Fig. S1 RHEED oscillations of the BaSnO<sub>3</sub> film grown by codeposition during the initial growth stage on top of the 18 nm thick SrTiO<sub>3</sub> buffer layer on silicon. The oscillations indicate that the growth rate is  $\sim 0.374 \text{ \AA/s}$ .

Fig. S2 Surface morphology revealed by AFM of the same sample characterized in Fig. 1. The rms roughness is  $\sim 4 \text{ \AA}$ .

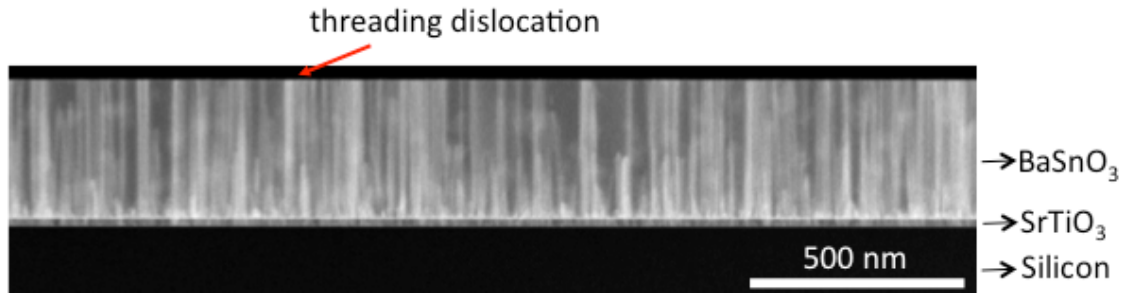


Fig. S3 LAADF-STEM image of the same sample characterized in Fig. 1 showing threading dislocations. The estimated dislocation density is  $\sim 1.3 \times 10^{11} \text{ cm}^{-2}$ .

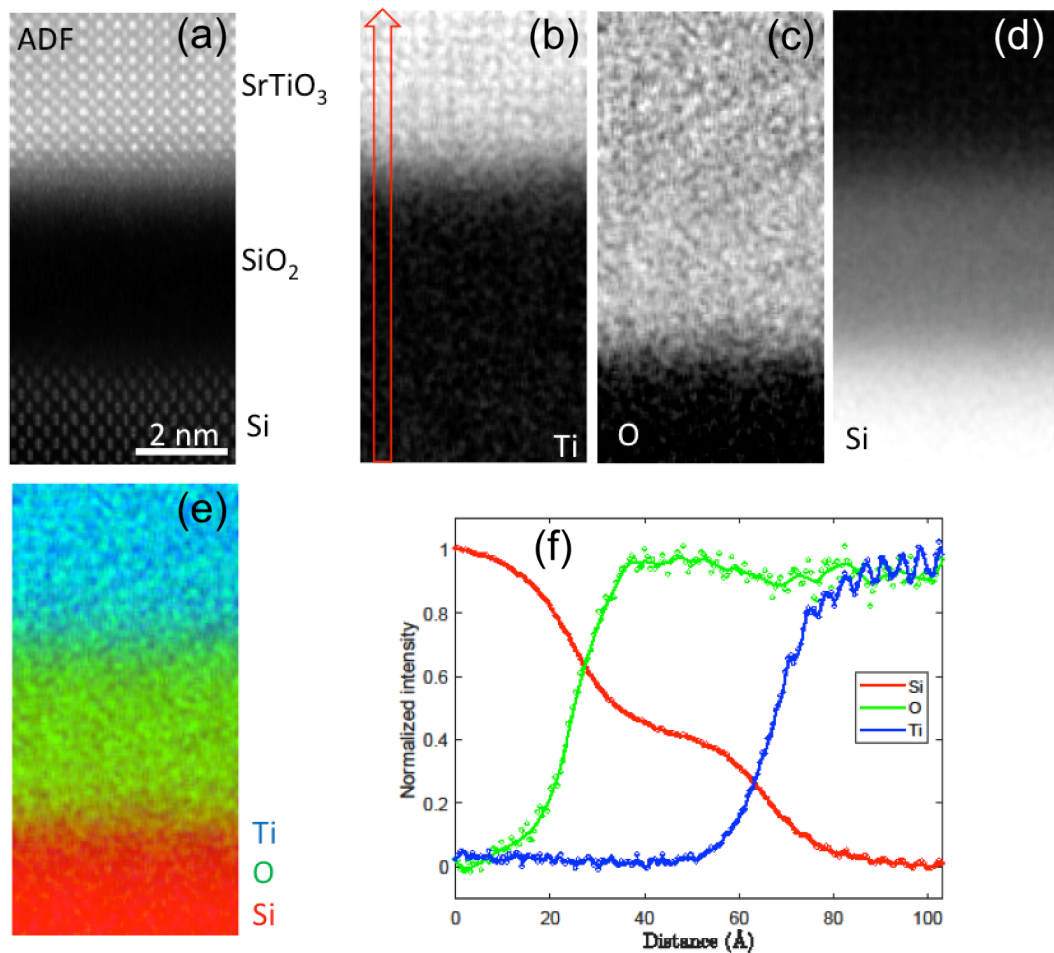


Fig. S4 (a) The HAADF-STEM image of the region in the vicinity of the SrTiO<sub>3</sub>/Si interface of the same sample characterized in Fig. 1. STEM-EELS elemental maps of the same interfacial region for (b) Ti-*L*<sub>2,3</sub>, (c) O-*K*, and (d) Si-*L*<sub>2,3</sub> edges of the same interfacial region. (e) A color-coded elemental map showing that there is no perceptible interdiffusion of titanium into the SiO<sub>2</sub> layer. (f) Line profiles of the elemental intensity of the same region. The zero point of the line profile in (f) corresponds to the bottom side of the arrow shown in (b).

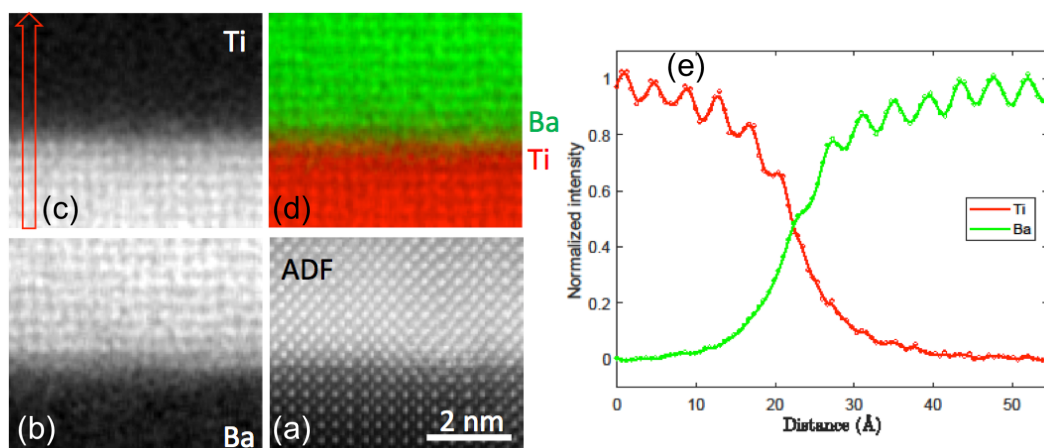


Fig. S5 (a) The HAADF-STEM image in the vicinity of the BaSnO<sub>3</sub>/SrTiO<sub>3</sub> interface of the same sample characterized in Fig. 1. STEM-EELS elemental maps of (b) Ba-*M*<sub>4,5</sub> and (c) Ti-*L*<sub>2,3</sub> edges of the same BaSnO<sub>3</sub>/SrTiO<sub>3</sub> interfacial region. (d) A color-coded elemental mapping showing that there is little perceptible interdiffusion of barium into the SrTiO<sub>3</sub> film. (e) Line profiles of the elemental intensity of the same region. The zero point of the line profile in (e) corresponds to the bottom side of the arrow shown in (c).