FIGURES

Table 1-1. Optical models of bulk and thin film SBT. VASE models specified n and k vs. λ (using Lorentz dispersion) and component % vs. depth (using multiple EMA layers). The Lorentz parameters below generated the dispersion curves in Figure 1b. Regardless of sample preparation method, SBT exhibited primary bandgap absorption in the range $5.2\pm.3$ eV and secondary absorption at $3.75\pm.07$ eV.

SBT sample	sintered bulk	PLD film	MOCVD film	MOD film
substrate		n+ Si (100)	Pt/Ti/SiO ₂ /Si	p Si (100)
model	Lorentz	А	В	С
profile 🔶	SBT	Si SBT	Pt SBT	Si SBT
MSE	6.2	33.2	27.5	33.2
thickness	5 mm	981±8 nm	192±5 nm	493±33 nm
grain size range	2-11 μm	100-300 nm	100-200 nm	50-100 nm
n @ 630 nm	2.37	2.16	2.37	2.10

Structural properties

Lorentz parameters in equation (2)

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SBT sample	sintered bulk	PLD film	MOCVD film	MOD film		
$\epsilon_{o}(*)$	$2.69 \pm .04$	fixed at 1	1.06±.26	$2.61 \pm .02$		
Energy #1 (eV)	5.25±.19	$5.38 \pm .03$	5.16±.07	$4.92 \pm .06$		
Breadth #1 (ev)	$0.95 \pm .01$	0.25±0.06	$0.05 \pm .035$	0.2±3		
Amplitude #1 (*)	69.7±1.5	53±3	97±10	33.3±.07		
Energy #2 (eV)	$3.688 \pm .002$	$3.75 \pm .03$	$3.82 \pm .03$	$3.82 \pm .08$		
Breadth #2 (ev)	$0.009 \pm .006$	$0.22 \pm .05$	$0.44 \pm .06$	0.08 ± 8		
Amplitude #2 (*)	$0.04 \pm .01$	$0.58 \pm .07$	$3.5 \pm .5$	$0.18 \pm .03$		

- In the profile icon, black represents dense SBT, gray is porous SBT, and a white triangle is a linear transition.
- * These variables have the same dimensionless units as n².



Figure 1-1. Comparing SBT refractive index, n, curves from bulk samples and thin films (MOCVD, MOD, & PLD). a) 1-layer VASE models underestimated n in thin films. b) By simulating observed void profiles with EMA layers, models A, B, and C obtained SBT optical properties from thin films that were closer to bulk values.



Figure 1-2. VASE spectra from a bulk polycrystalline SBT sample with 2% voids. Delta and psi spectra were fit by a Lorentz dispersion model with absorbtion at 5.25 ± 0.2 eV and 3.688 ± 0.002 eV, yielding the bulk dispersion curve in Figure 1.



Figure 1-3. SBT/Si film made by PLD. a) Model A fit the VASE spectrum better than a 1-layer model. b) Including a linear transition from SBT to voids, model A accurately predicted the depth of surface roughness, as shown in the AFM cross-section.



Figure 1-4. Comparison of surface empty space profiles from AFM and VASE.
a) Using AFM, the roughness of a SBT/Si film made by PLD was described by a surface height histogram. 98% of the surface was within a thickness of 2FWHM = 101.5 nm.
b) Integrating the AFM surface height histogram yielded an S-shaped empty space profile (solid curve). Using VASE model A, roughness was simulated by a linear increase in empty space (dashed line) over a depth comparable with 2FWHM.



Figure 1-5. SBT/Pt film made by MOCVD. a) The Δ spectrum of this dense film was reasonably modeled as a single layer. b) Model B improved the fit by including surface roughness and voids near the base of the film. c) A sketch illustrates how voids could remain near the Pt substrate between kernal-shaped grains. d) Features seen in a SEM cross-section (dark holes between SBT grains, shallow surface roughness, and overall film thickness) were consistent with VASE model B.



Figure 1-6. SBT/Si film with 3 MOD layers. a) Model C followed the shape of the observed delta spectrum much better than a 1-layer model. b) Model C included porosity between MOD layers, and graded transitions at the top and bottom surfaces. c) Crosssectional TEM confirmed the thickness estimates of dense and porous layers made by VASE in model C. Considering that VASE optically characterized a region 1000 times larger than the area shown by TEM, the profiles showed remarkable agreement.



Figure 1-7. Evolution of a layered model for a SBT/Si film made by MOD. As new layers are added and only layers which improved the fit (i.e. lowered the MSE) were kept, the models gave a more detailed description of how optical constants varied with depth and with λ . However, the fit of VASE spectra could only be improved so far. Of models that approached the minimum MSE, model C was selected based on TEM results, as the simplest model which accurately described the observed void profile.