Mechanical Properties of LaGaO$_3$ Single Crystals by Indentation
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1. Introduction

- Doped LaGaO$_3$ is the most recent material for use as a superior thin film electrolyte in intermediate temperature (650-800°C) SOFCs.
- Mechanical properties of these ceramics are still largely unexplored for long-term endurance.
- Why single crystals?
  - Investigation of single crystals could detect anisotropies of physical properties in different crystallographic directions.
  - LaGaO$_3$ single crystals themselves have considerable potential as an electronic substrate material for epitaxial layers of high-temperature superconductors (HTSC).

2. LaGaO$_3$ Single Crystals

- Single-crystals of LaGaO$_3$ were grown by Czochralski technique.
- Crystals up to 2.5 cm diameter and 10 cm length can be grown in the [100] and [001] direction.
- Crystal Structure = Orthorhombic Pbnm space group at 25°C and Rhombohedral R3c at 145°C.
- Molecular Weight = 256.63 gm mol$^{-1}$.
- Density at 25°C = 7.23 gm/cc.
- Melting point 1800°C.
- Crystal growth direction <100>.

3. Vickers Hardness

- Young’s modulus [100] LaGaO$_3$ = 156.5 ± 4.6 GPa.
- Young’s modulus [001] LaGaO$_3$ = 106.35 ± 4.71 GPa.

4. Fracture Toughness

- The modulus values were constant with increasing maximum load.
- Study of the deformation behavior of the LaGaO$_3$ single crystals show an elastic response of the load-displacement and stress-strain curves up to a stress of around 6 GPa.
- At higher stresses both the [100] and [001] LaGaO$_3$ single crystals show increasing irreversible deformation.
- The maximum load for [100] LaGaO$_3$ single crystals is 0.57 ± 0.07 MPa$^{-1/2}$.
- The maximum load for [001] LaGaO$_3$ single crystals in two perpendicular directions is 0.32 ± 0.07 MPa$^{-1/2}$ and 0.91 ± 0.10 MPa$^{-1/2}$.

5. Nano Indentation

- Hertzian Principle
  \[ h_{tot} = \left( \frac{3P}{E^*} \right)^{1/3} \]
- Applied Load $E^*$ - Reduced Modulus $E_r - $ Sample Modulus $E_t - $ Indenter Modulus $v = $ Poisson’s ratio

- Depth-sensing nanoindentation was used to study the deformation behavior of [100] and [001] LaGaO$_3$ single crystals using incremental loading.
- A 13.5 µm spherical tipped diamond indenter was used for all experiments since the spherical indenter gives more reliable modulus values.
- Young’s modulus values of both the [100] and [001] LaGaO$_3$ samples were found to vary slightly with the maximum load applied.
- Average modulus values for the [001] crystal was found to be less than the [100] crystal.

6. Raman Spectroscopy

- Change in intensity ratio for Raman bands 177, 268, 436, 454 cm$^{-1}$ for both crystals have been observed after indentation.
- Possible reason - structure rearrangement (domain switching or phase transformation) induced by indentation.
- Raman mapping was performed on the [100] LaGaO$_3$ surface along the dotted line.
- 337 and 361 cm$^{-1}$ Raman bands were used to create an intensity map of the LaGaO$_3$ [001] surface across a twin.
- Significant decrease (up to full disappearance) of 361 cm$^{-1}$ Raman band was observed inside the twin in a particular case which indicates different orientation of the crystal inside the twin.

7. Conclusions

- Vickers hardness for [100] = 8.04 ± 0.04 GPa.
- Vickers hardness for [001] = 7.89 ± 0.11 GPa.
- Young’s modulus [100] LaGaO$_3$ = 156.5 ± 4.6 GPa.
- Young’s modulus [001] LaGaO$_3$ = 106.35 ± 4.71 GPa.
- The modulus values were constant with increasing maximum load.
- Study of the deformation behavior of the LaGaO$_3$ single crystals show an elastic response of the load-displacement and stress-strain curves up to a stress of around 6 GPa.
- At higher stresses both the [100] and [001] LaGaO$_3$ single crystals show increasing irreversible deformation.
- The maximum load for [100] LaGaO$_3$ single crystals is 0.57 ± 0.07 MPa$^{-1/2}$.
- The maximum load for [001] LaGaO$_3$ single crystals in two perpendicular directions is 0.32 ± 0.07 MPa$^{-1/2}$ and 0.91 ± 0.10 MPa$^{-1/2}$.
- This signifies the anisotropic behavior of [001] single crystals.
- The difference in the $K_{IC}$ values measured from crack lengths propagated in different crystallographic directions is a result of strong anisotropy in the LaGaO$_3$ single crystal. Anisotropy and porosity of the [001] crystal also explains the lower Young’s modulus values.
- Similar anisotropy in coefficient of thermal expansion (CTE) was reported by L. Vasylychko et al. (J. Solid State Chemistry 172 2003 pp 396-411) for Sr and Mg doped LSGM-05 and LSGM-10 single crystals.