Properties of CaF_2 using X-Ray Diffraction and IR Ellipsometry

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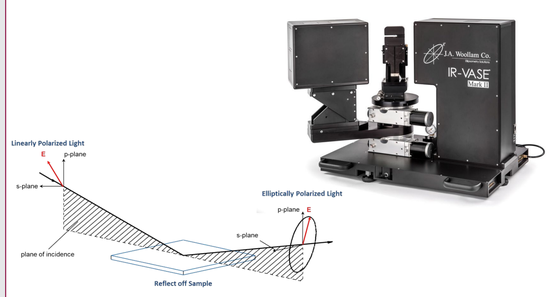
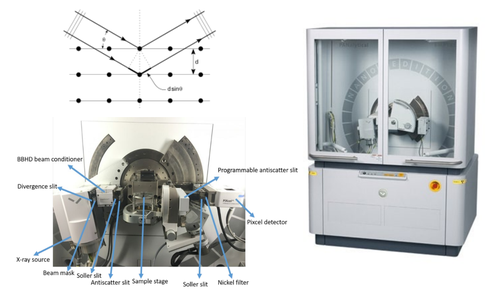
IR Vase Mark II Ellipsometer



Empyrean X-Ray Diffractometer



Abstract

- Calcium fluoride is a desirable substrate for optical devices such as tunable filters based on phase change memory materials.
- Here we will describe the structural and optical properties of calcium fluoride on (100) and (111) bulk substrates.

Methods

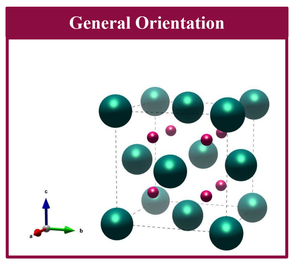
- Determined optical constants using Fourier-transform infrared ellipsometry on the IR-Vase Mark II ellipsometer from J.A. Woollam Company.
- Substrate orientation was determined using the Empyrean x-ray diffractometer from Malvern Panalytical.
- Backside roughening was done with 220 and 80 grit aluminum oxide grain in a sandblaster.

Structure

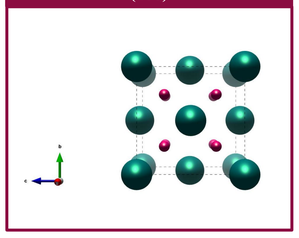
Formula unit:	CaF_2, calcium fluoride
Space group:	$Fm\bar{3}m$ (no. 225)
Cell dimensions:	a = 5.04626 Å
Cell contents:	4 formula units per cell
Atomic positions:	Ca in (4a) $m\bar{3}m$ (0,0,0) +FCC F in (8c) $\bar{4}3m$ (¼, ¼, ¾); (¼, ¼, ¼) +FCC

Fluorine (F^-) Calcium(Ca^{2+})

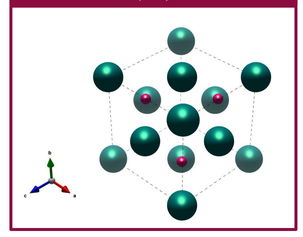
General Orientation



(100)

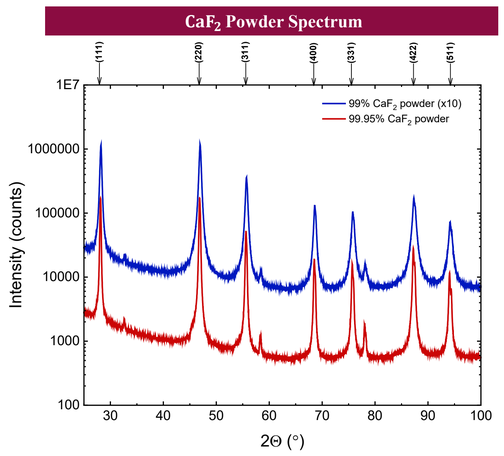


(111)

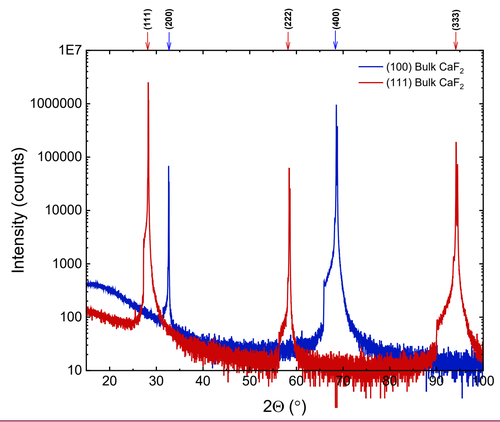


X-Ray Diffraction

CaF_2 Powder Spectrum

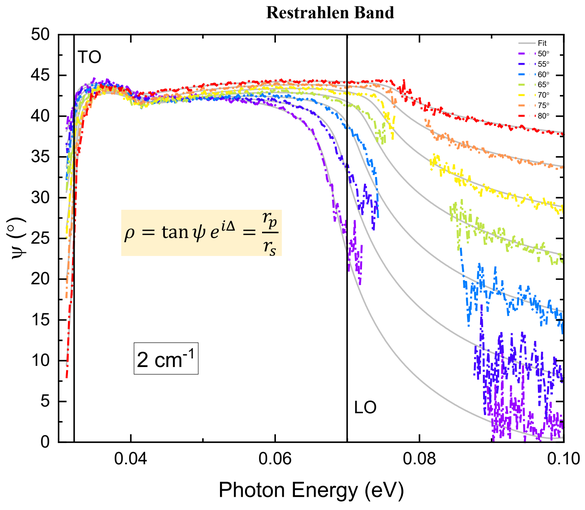


MTI Bulk CaF_2 (100) and (111)

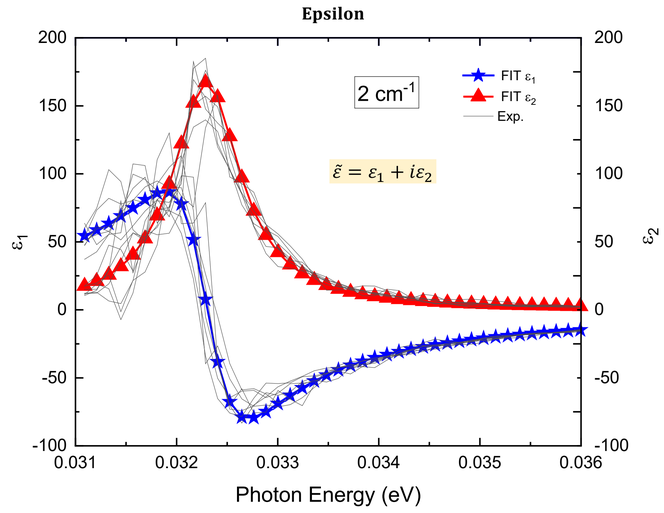


Sydor Optics Bulk CaF_2 (111)

Restrahlen Band



Epsilon



$$\varepsilon(E) = \varepsilon_\infty + \frac{A_{TO}{E_{TO}}^2}{{E_{TO}}^2 - E^2 - i\Gamma_{TO}E} + \frac{A_{2P}E_{2P}(E_{2P} - ibE)}{E_{2P} - E^2 - i\Gamma_{2P}E}$$

Fit Parameters	
MSE	*1.380*
ε_∞	1.990 ± 0.002
A_{TO}	4.240 ± 0.015
E_{TO}	261.0 meV ± 0.109 meV
Γ_{TO}	6.610 meV ± 0.192 meV
A_{2P}	0.265 ± 0.009
E_{2P}	335.0 meV ± 1.080 meV
Γ_{2P}	102.0 meV ± 2.280 meV
b	0.110 ± 0.009

MTI Bulk CaF_2 (111)

$$\varepsilon(E) = \varepsilon_\infty + \frac{A_{TO}{E_{TO}}^2}{{E_{TO}}^2 - E^2 - i\Gamma_{TO}E} + \frac{A_{2P}E_{2P}(E_{2P} - ibE)}{E_{2P} - E^2 - i\Gamma_{2P}E}$$

Fit Parameters	
MSE	1.670
ε_∞	1.970 ± 0.003
A_{TO}	4.110 ± 0.022
E_{TO}	261.0 meV ± 0.148 meV
Γ_{TO}	3.910 meV ± 0.261 meV
A_{2P}	0.330 ± 0.015
E_{2P}	329.0 meV ± 1.690 meV
Γ_{2P}	111.0 meV ± 3.030 meV
b	0.084 ± 0.011

Restrahlen Band

Epsilon

MTI Bulk CaF_2 (100)

Restrahlen Band

Epsilon

$$\varepsilon(E) = \varepsilon_\infty + \frac{A_{TO}{E_{TO}}^2}{{E_{TO}}^2 - E^2 - i\Gamma_{TO}E} + \frac{A_{2P}E_{2P}(E_{2P} - ibE)}{E_{2P} - E^2 - i\Gamma_{2P}E}$$

Fit Parameters	
MSE	*1.190*
ε_∞	1.970 ± 0.003
A_{TO}	4.060 ± 0.019
E_{TO}	261.0 meV ± 0.114 meV
Γ_{TO}	3.820 meV ± 0.204 meV
A_{2P}	0.359 ± 0.016
E_{2P}	327.0 eV ± 1.800 eV
Γ_{2P}	123.0 meV ± 2.940 meV
b	0.045 ± 0.009

Analysis

- CaF_2 is an insulator with an ultra wide bandgap of 12 eV and a large exciton binding energy of 1 eV.
- A wide range of transparency from 125 meV to 10 eV makes CaF_2 an ideal substrate for optical devices.

References

- D. F. Bezuidenhout, in *Handbook of Optical Constants of Solids II*, edited by E. D. Palik (Academic, San Diego, 1998).
- K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data," J. Appl. Crystallogr. **44**, 1272 (2011).