Optical Constants of Lithium Fluoride in the Far Ultraviolet*

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Lithium Fluoride is a very useful material for ultraviolet work because of its large band-gap. During research into the electronic spectrum of crystalline lithium fluoride, the optical parameters, n and k, were obtained in the course of the data analysis. Although the refractive index has been measured accurately in the transparent region (for example by Gyulai (1) and Schneider (2), very few data are available beyond the transmission ' limit at 12 eV.

In the present work the near-normal-incidence reflectance of freshly cleaved crystals of lithium fluoride was measured from the near ultraviolet to 28 eV. The values of n and k were computed from the reflectivity, r, (where the ratio of the reflected and

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incident light intensities is r^2) through the expressions

$$n = \frac{1 - r^2}{1 + r^2 - 2r \cos \theta}$$
(1)

$$k = \frac{2r \sin \theta}{1 + r^2 - 2r \cos \theta} \qquad (2)$$

The angle, θ , is the absolute phase change on reflection and is related to the reflection spectrum through a Kramers-Kronig integral transform. A detailed discussion of these relationships and the computation of θ has been given elsewhere (3, 4, and references therein).

The error involved in the computation of θ , which relies on an approximation procedure, becomes important near the high energy limit of the reflectance data. The values of n and k are therefore presented only as far as 25 eV. Below this energy the primary source of uncertainty arises from the experimental determination of the reflectance. Errors in the measurements themselves are less than 5%, but it is more difficult to estimate how good the crystal surfaces were. The data given in Table 1 are from surfaces giving the highest reflectance at the 12.8 eV exciton peak (about 40%), since any surface contamination or defects tend to reduce ultraviolet reflectance structure. In practice all the crystals were obtained from the Harshaw Chemical Company, and freshly cleaved surfaces varied only about 5% in peak reflectance.

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The intervals in the photon energies were chosen so as to define the reflectance curve sufficiently well for the Kramers-Kronig analysis. There is some variation in the literature in the use of 'k' as a measure of absorption; in this work it represents the absorption index, and is related to the absorption coefficient, α , through the expression $\alpha = 4\pi k/\lambda$. The spectral variation of n and k is shown in Fig. 1. The electronic transitions responsible for the observed structure will be discussed elsewhere.

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TABLE CAPTION

Table I Optical constants, n and k, of bulk lithium fluoride at 300° K in the range 7 - 25 eV.

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TABLE I								
$\hbar\omega(eV)$	n	k	$\hbar \omega(eV)$	n	k			
7.00	1.46	0.00	13.20	0.81	1.20			
8.00	1.49	0.00	13.25	0.80	1.10			
9.00	1.53	0.00	13.30	0.80	1.01			
10.00	1.60	0.00	13.35	0.80	0.92			
10.50	1.67	0.00	13.40	0.81	0.84			
11.00	1.77	0.00	13.45	0.82	0.76			
11.25	1.84	0.00	13.50	0.84	0.67			
11.50	1.94	0.00	13.55	0.88	0.58			
11.75	2.08	0.04	13.60	0.95	0.50			
12.00	2.28	0.11	13.65	1.05	0.43			
12.20	2.51	0.23	13.70	1.15	0.42			
12.30	2.68	0.33	13.75	1.24	0.46			
12.40	2.93	0.48	13.80	1.29	0.52			
12.50	3.34	1.17	13.85	1.31	0.56			
12.60	2.89	1.90	13.90	1.32	0.59			
12.65	2.57	2.08	13.95	1.32	. 0.62			
12.70	2.24	2.19	14.00	1.32	0.64			
12.75	1.92	2.20	14.10	1.32	0.68			
12.80	1.64	2.13	14.20	1.30	0.71			
12.85	1.42	2.02	14.30	1.27	0.72			
12.90	1.26	1.90	14.40	1.25	0.73			
12.95	1.13	1.77	14.50	1.22	0.74			
13.00	1.04	1.64	14.60	1.19	0.74			
13.05	0.97	1.53	14.70	1.17	0.73			
13.10	0.91	1.43	14.90	1.12	0.71			
13.15	0.84	1.33	15.10	1.08	0.68			

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* ħω(eV)	n	k	ħω(eV)	n	k
15.30	1.04	0.64	. 20.50	1.18	0.6
15.50	1.00	0.59	21.00	1.14	. 0.7
15.70	0.98	0.52	21.40	1.08	0.8
15.80	0.99	0.47	21.60	1.04	· 0.8
15.90	1.02	0.42	21.80	0.99	0.8
16.00	1.06	0.41	22.00	0.91	0.
16.10	1.09	0.39	22.20	0.80	0.
16.20	1.12	0.39	22.40	0.70	0.
16.40	1.16	0.40	22.60	0.62	0.3
16.90	1.20	0.47	22.80	0.55	0.
17.30	1.19	0.51	22.90	0.51	0.
17.40	1.18	0.52	22.95	0.50	0.
17.50	1.16	0.53	23.00	0.48	0.
17.60	1.14	0.52	23.05	0.47	0.
17.70	1.13	0.52	23.10	0.46	0.
18.00	1.11	0.48	23.20	0.45	0.
18.30	1.13	0.45	23.30	0.44	0.
18.40	1.14	0.44	23.40	0.43	0.
18.50	1.15	0.44	23.60	0.43	0.
18.60	1.17	0.44	23.70	0.42	0.
19.00	1.19	0.47	24.00	0.43	0.
19.50	1.21	0.53	24.50	0.44	0.
20.00	1.20	0.58	25.00	0.47	0.

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FIGURE CAPTION

Figure 1 Spectral dependence of the optical parameters, n and k, obtained from a Kramers-Kronig inversion of reflectance data.

