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# Width of Infrared Reflection Bands

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The width of strong reflection bands is determined by the oscillator strength, while the width of absorption bands is determined by the damping. The width of the reflection bands of the alkali halides, calculated from the dielectric constant and the normal index of refraction, is in agreement with the experimental data.

THE absorption spectra of the alkali halides were measured by Barnes[1]: for NaCl he found a sharp band at 61.1 $\mu$, of width 4 $\mu$. The reflections pectrum shows a broad band between 39 and 61 $\mu$.[2] This clearly shows that the width of an absorption band can be quite different from the width of the corresponding reflection band. We note that the frequency of the absorption band coincides with the low-frequency limit of the reflection band.

These effects are readily explained by the classical dispersion theory. The complex index of refraction for a cubic crystal containing harmonic oscillators, is given by

$$N^2=(n-i\kappa)^2=n_0^2+\rho/(\nu_0^2-\nu^2),$$

where $\nu_0$ is the resonance frequency of the oscillator, $n_0$ the normal index of refraction, and $\rho$ the oscillator strength. The maximum of the absorption index lies at $\nu_0$: therefore an absorption band at the resonance frequency $\nu_0$ of the oscillator must be expected.

The corresponding reflection curve is given by

$$R=[(n-1)^2+\kappa^2]/[(n+1)^2+\kappa^2];$$

the result is shown in Fig. 1. We notice that an undamped harmonic oscillator gives rise to a region of total reflection between $\nu_0$ and $\nu_l=(\nu_0^2+\rho/n_0^2)^{\frac{1}{2}}$.

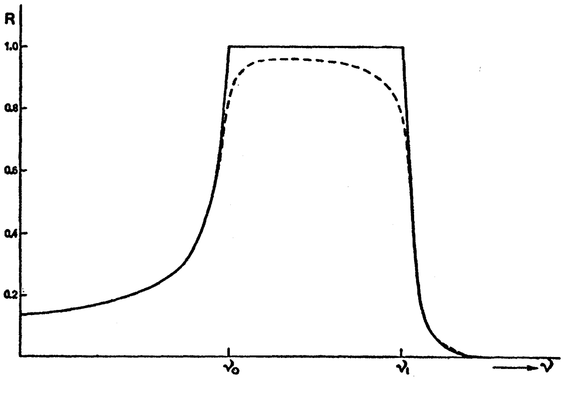

FIG. 1. Reflection band. —— undamped oscillators, - - - - damped oscillators.

The dielectric constant of the alkali halides is $\epsilon=N^2(\nu=0)=n_0^2+\rho/\nu_0^2$. From $\epsilon$, $n_0$, and $\nu_0$ we can calculate the high-frequency limit $\nu_l=\nu_0(\epsilon/n_0^2)^{\frac{1}{2}}$, and hence the width of the reflection band $\nu_l-\nu_0$. For $\nu_0$ we took the values obtained by Barnes from absorption measurements.

In Table I we compare the calculated values of $\lambda_l$ with the short-wavelength limit of the band, which we estimated from the experimental reflection curves. The agreement is satisfactory.

TABLE I. Infrared reflection bands.

| Crystal | $\epsilon$ | $n_0^2$ | $\lambda_0$ | $\lambda_l$ (exp) | $\lambda_l$ (calc) |
|---|---|---|---|---|---|
| KCl | 4.68 | 2.13 | 70.7$\mu$[a] | 46$\mu$[c] | 47.7$\mu$ |
| NaCl | 5.62 | 2.25 | 61.1[a] | 39[c] | 38.7 |
| NaF | 6.00 | 1.74 | 40.6[a] | 23[c] | 21.9 |
| LiF | 9.27 | 1.92 | 32.6[a] | 15[c] | 14.8 |
| MgO | 9.8 | 2.95 | 26[b] | 14[b] | 14.3 |

[a] See reference 1.
[b] Burstein, Oberley, and Plyler, Proc. Indian Acad. Sci. **A28**, 388 (1948).
[c] H. W. Hohls, Ann. Physik **29**, 433 (1937).

Contrary to Lax and Burstein,[3] who suggested that the width of the reflection bands of the alkali halides is a measure of the importance of anharmonic terms, the introduction of a small damping constant is of little influence on the width of the reflection band (Fig. 1); however, the height of the band is determined essentially by the damping.[4–6]

We conclude that: (a) the width of an *absorption* band depends on the damping (anharmonic coupling terms) of the vibration, while (b) the width of a *reflection* band is determined by the oscillator strength.

The foregoing treatment does not take into account the secondary maxima, but it appears, nevertheless, sufficient to show the fundamental relation between the oscillator strength and the width of a reflection band.

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[1] R. B. Barnes, Z. Physik **75**, 723 (1932).
[2] M. Czerny, Z. Physik **65**, 600 (1930).
[3] M. Lax and E. Burstein, Phys. Rev. **97**, 39 (1955).
[4] C. Haas and J. P. Mathieu, J. phys. radium **15**, 492 (1954).
[5] Ketelaar, Haas, and Fahrenfort, Physica **20**, 1259 (1954).
[6] C. Haas, Spectrochim. Acta (to be published).