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Useful Formulae for Spectroscopy

CALCULATION OF MAXIMUM ALLOWABLE PRESSURES ON CIRCULAR WINDOW MATERIALS

Calculation of maximum pressure will depend upon a number of user selectable parameters. For instance, the window material, window size, flange size and a safety factor all may be varied depending upon application.

To calculate maximum allowable pressure, we must assume that the maximum stress in a uniform circular plate is given by the equation:

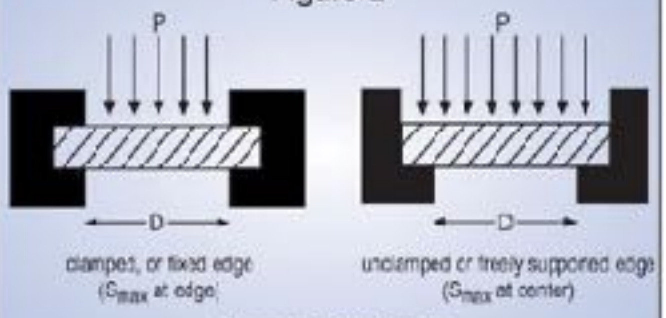
$$\boxed{S_{max} = (k \times D^2 \times P) / (4 \times t^2)}$$

where k is a constant, the value for which depends upon whether or not the window is clamped — use 0.75 for clamped windows and 1.125 for unclamped (See Fig. 2). Smax is the maximum stress, D is the window diameter under pressure (ie, the portion of window not supported by the flange as shown in the schematic in Figure 2), P is the load (expressed in psi), and t is the thickness of the window material. In the formula solving for t, the window diameter D can be expressed in any unit of measure such as mm or inches. To avoid plastic deformation a safety factor must be introduced where SF is a safety factor and Fa is apparent elastic limit for the material itself. Where apparent elastic limit is not available, use yield stress. Allowing for a safety factor (SF), the equations for calculation of maximum allowable pressure and for minimum window thickness (t) where the operating pressure (P) is known are:

$$\boxed{P = 4\,(Fa \times t^2) / (SF \times k \times D^2)}$$

$$\boxed{t = \sqrt{\frac{SF \times P \times K \times D^2}{4 \times Fa}}}$$

Figure 2



To avoid plastic deformation

The apparent elastic limits of some IR optical materials are listed below:

CaF2	5300	KCl	330
BaF2	3900	KBr	160
KRS-5	3800	CsI	810
NaCl	350	MgF2	7200

ATR SPECTROSCOPY

The formulae set forth below are useful for ATR (MIR) spectroscopy.

Penetration Depth

The depth of penetration is defined by the formula:

$$dp = \frac{\lambda}{2\pi n_1 (\sin^2 \Phi - n_{21}^2)^{1/2}}$$

where l is the wavelength of the infrared light, n1 is the refractive index of the ATR crystal, λ is the angle of incidence of the infrared beam at the boundary and n21 is the ratio of the refractive indices of the sample, ns, and ATR crystal,

$$n_c \text{ and } n_{21} = \frac{n_s}{n_c}$$

Since the evanescent wave decreases in intensity exponentially from the surface of the crystal, the penetration depth, dp, is defined as the distance at which the amplitude of this wave has decreased to (1/e) or 37% of its original value.

Effective Angle of Incidence

This is the angle of incidence of the infrared beam internally in the ATR crystal when a variable angle HATR such as the Varimax™ is used for analysis. When the scale angle, Φscale, is not equal to the crystal face angle, Φface, the effective angle, Φ is different than the scale angle due to refraction.

$$\Phi_{actual} = \Phi_{scale} - \sin^{-1}\left[\frac{\sin(\Phi_{scale} - \Phi_{face})}{n_{crystal}}\right]$$

$n_{crystal}$ = refractive index

Number of Reflections

The number of reflections in the crystal gives a measure of the intensity of the resulting spectrum. This number is a function of the effective angle of incidence Φ, and the length, l, and thickness, t, of the crystal.

$$N = \frac{l}{t \cot \Phi}$$

Effective Pathlength

The effective pathlength, Peff, is defined as the product of the penetration depth dp, and the number of bounces, N, the IR beam makes within the crystal:

$$P_{eff} = d_p \times N$$

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