PROPERTIES OF MATERIALS FOR SPECTROSCOPY

Material	SWL cm^{-1}	LWL cm^{-1}	RI	S/D	Flatness	Pe Atm	Restrahlen cm^{-1}	Density g/cc	Solubility g/100 g	Melting Point °C	Hardness kg/mm^2
AgBr	22,000	255 292	2.22@10	80/50	5	0.56	88	6.5	1.2E-05	432	7
AgCl	24,500	353 404	1.90@10	80/50	5	0.56	123	5.6	5.2E-02	457	10
Al_2O_3	40,000	1608 1834	1.76@0.6 1.77@0.6	40/20	1/2	6.1	741	4.0	0	2040	1370
AMTIR	11,000	593 625	2.50@10	80/50	1	0.27		4.4	0	370	170
BaF_2	66,600*	691 782	1.45@5	40/20	1/20	0.56	213	4.9	0.17	1280	82
CaF_2	79,500*	896 1025	1.40@5	40/20	1/20	0.77	286	3.2	0.0017	1360	158
CdTe	17,000	313 340	2.67@10	80/50	1	0.08		6.2	0	1092	56
Cleartran™	22,000	690 722	2.20@10	40/20	1/20	2.2	328	4.1	0	1830	240
CsI	42,000	172	1.73@10	80/50	1/10	0.12	69	4.5	44	621	1
Diamond	30,000	<2	2.41@0.6	20/10	1	10.9	None	3.5	0	550[fp]	5700
Ge	5500	432 574	4.00@10	60/40	1/8	1.0	None	5.3	0	936	780
KBr	48,800	345 388	1.52@10	60/40	1/20	0.02	129	2.8	53	730	6
KCl	55,600	385 439	1.45@10	60/40	1/20	0.05	158	2.0	35	776	7
KRS-5	17,900	204 232	2.37@10	60/40	1/1	0.56	74	7.4	0.05	414.5	40
LiF	96,150*	1105 1286	1.39@0.5	40/20	1/10	0.23	400	2.6	0.27	870	105
MgF_2	90,900*	1271 1457	1.38@0.5 1.39@0.5	40/20	1/20	1.0	500	3.2	0.0002	1255	415
NaCl	52,600	457 584	1.49@10	40/20	1/20	0.05	200	2.2	36	801	18
Si	8900	624 969	3.41@10	60/40	1/8	1.8	None	2.3	0	1420	1150
SiO_2	50,000*	2315 2677	1.53@1	40/20	1/20	4.2		2.6	0	1713	460
ZnS	17,000	690 722	2.20@10	40/20	1/20	1.5	328	4.1	0	1830	240
ZnSe	15,000	461 508	2.40@10	40/20	1/20	1.2	219	5.3	0	1526	120
ZrO_2	40,000	1431	2.13@1	60/40	1/8	1.1		5.9	0	2700	1250

Material	Comments	BBAR Coat	Hard Coat
AgBr	Insoluble in water, slightly soluble in sodium hydroxide and some amines. Migrates into base metals. Will blacken under UV radiation. Cold flows and should not be used above 200 °C.	No	No
AgCl	Insoluble in water, slightly soluble in sodium hydroxide and some amines. Migrates into base metals. Will blacken under UV radiation. Cold flows and should not be used above 200 °C.	No	No
Al_2O_3	GRAS. Resistant to strong acids and bases. Birefringent. Very durable and may be used at high temperatures.	Yes 1.05	No
AMTIR	Amorphous material. A chalcogenide glass, which, although relatively hard, is also brittle. Insoluble in water and resistant to acids. It is attacked by alkalis.	Yes 1.3	Yes 2
BaF_2	Hard material suitable for high pressure applications. Extremely vulnerable to thermal shock. Very slightly soluble in water. Attacked by ammonium hydroxide, ammonium salts, complex agents such as EDTA, and acids.	No	Yes 3
CaF_2	Very hard material similar to BaF_2, but almost insoluble in water and less vulnerable to thermal shock. Attacked by nitric acid and strong hydroxides, ammonium salts, and complexing agents such as EDTA. Very desirable for near-IR applications as it has no OH absorption bands.	No	Yes 3
CdTe	Hard but very brittle material. Insoluble in water. Attacked by nitric acid.	Yes 1.35	Yes 2
Cleartran	GRAS. A clear form of ZnS. Properties similar to ZnS.	Yes 1.25	Yes 2
CsI	Soft and hygroscopic. Generally only used for its extended far-IR transmission. Should only be exposed to anhydrous solvents. Never use with alcohols or aqueous solutions. A hard optical coating can be used to provide some protection. In powdered form it can be used to make pellets. Keep stored in a dessicator or heated cabinet.	No	Yes 6
Diamond	GRAS. Hard and chemically resistant. Often used in very high pressure applications. High cost limits size to a few mm. Has a characteristic lattice absorption doublet between 1800 and 2700 cm^{-1}.	Yes 1.25	No
Ge	Hard and brittle. Semiconductor material with low band gap energy. Free electron absorption becomes important at temperatures above about 60 °C and it can become totally opaque at temperatures above 100 °C. Attacked by sulfuric acid and aqua regia. When used as a window it has high reflection losses which can be significantly reduced with BBAR coatings. Used as an ATR prism when low penetration depth is desired.	Yes 2.0	Yes 2
KBr	The most popular IR material. Hygroscopic and can only be used with anhydrous solvents, glycerol or alcohols. Withstands thermal and mechanical shock well. A protective coating can improve its resistance to humidity. Keep stored in a dessicator or heated cabinet.	No	Yes 4
KCl	Hygroscopic and can only be used with anhydrous solvents, glycerol or alcohols. Withstands thermal and mechanical shock fairly well. A protective coating can improve its resistance to humidity. When AR coated can be used as a low cost CO_2 laser window. Keep stored in a dessicator or heated cabinet.	No	Yes 4
KRS-5	Extremely toxic, even with skin contact. KRS-5 should only be handled with protective gloves or finger cots. A relatively soft material, it cold flows and deforms under pressure. This is enhanced at temperatures above 200 °C. It should only be polished by well-trained professionals. Good chemical resistance.	Yes 1.2	Yes 2
LiF	Slightly soluble in water. Hard and brittle. Sensitive to thermal shock. Should not be used above 400 °C.	No	Yes 2
MgF_2	Almost insoluble in water. Can be used at fairly high pressure. Slightly sensitive to thermal shock. Birefringent. Should not be used above 500 °C.	No	Yes 2
NaCl	Harder and less hygroscopic than KBr but can only be used with anhydrous solvents, glycerol or alcohols. Withstands thermal and mechanical shock fairly well. A protective coating can improve its resistance to humidity. Keep stored in a dessicator or heated cabinet.	No	Yes 4
Si	Hard material and resistant to most chemicals except for strong acids. Withstands thermal shock. Has a strong phonon absorption band at 590-630 cm^{-1}. Transmits well at wavenumbers lower than this and well into the far-IR. BBAR coatings are available for the mid-IR region.	Yes 1.7	No
SiO_2	GRAS. Resistant to acids and alkalis. Used in the near-IR. Most forms of SiO_2 have OH absorption bands.	Yes 1.05	No
ZnS	GRAS. Relatively hard material and resistant to thermal and mechanical shock. Insoluble in water but can be attacked by strong acids and bases.	Yes 1.25	Yes 2
ZnSe	Hard and brittle. Attacked by strong acids and bases. Resistance can be improved with the use of a hard coating. The most popular material for ATR applications. When AR coated, can be used as CO_2 laser window.	Yes 1.35	Yes 4
ZrO_2	Hard material with good resistance to chemicals. Cannot be used at high temperatures as a phase change occurs at 1000 °C.	Yes 1.2	Yes 2

Spectral Systems
PRECISION IN OPTICS

NOTES

1. SWL – Highest wavenumber for which transmission is greater than 50% for 1 mm thickness.
2. LWL – Lowest wavenumber for which transmission is greater than 50% for 1 mm thickness and 4 mm thickness.
3. RI – Refractive Index at the indicated wavelength in microns.
4. S/D – Scratch and Dig surface polish achievable with normal polishing techniques. High quality UV-Vis optics are usually 20/10 and IR optics 40/20. Each level is approximately 2 times worse than the lower numbers.
5. Flatness – Routine polishing can yield flatness as measured in wavelengths of 6328Å (HeNe laser).
6. GRAS – US FDA Generally Recognized As Safe. May be used to measure food products.
7. * – UV grade material required to achieve this limit.
8. Pe – Yield strength in atmospheres for a 25 mm × 1 mm thick window with a safety factor of 4. To calculate the thickness required for a given pressure:

   $T/D = 0.034 * \sqrt{P/Pe}$

   T – Window Thickness
   D – Window Diameter
   P – Pressure
9. Restrahlen – Frequencies at which the materials exhibit high resonance reflection. Apparent in reflection measurements.
10. BBAR Coat – Multilayer coating on material to increase energy transmission and/or reduce interference fringing. Number is the approximate gain in signal per window or lens.
11. Hard Coat – Coating to increase abrasion resistance and/or humidity and chemical resistance. Number is the approximate relative increase in abrasion, humidity or chemical resistance.
12. fp – Flash Point.