Defect memo

Change in refractive index (due to displacement of dopants) can also cause absorption. Scattering can induce loss.

Griscom 1991 :

- **Electron Spin Resonance (ESR) spectrometry**: measure paramagnetic defects → Griscom, 1991. Intrinsic paramagnetic centers so far identified by ESR :
    - E' centers ($\equiv Si \cdot$)
    - Non-bridging oxygen hole centers ($\equiv Si - O \cdot$)
    - Peroxy radicals ($\equiv Si - O - O \cdot$)
    - Self-trapped holes ()

  "Each defect has its own distinctive ESR "sig nature". Thus, if a suitably strong correlation can be established between an optical band and a well characterized ESR signal, then it can be said that one likely source of the band has been identified."

  Intrisic diamagnetic defects not identified:
    - Neutral oxygen vacancy ($\equiv Si - Si \equiv$)
    - 2-coordinated Si ($-O - Si - O -$)
    - Peroxy linkages ($\equiv Si - O - O - Si \equiv$)

  Possibility of diamagnetic trapped-electron centers. Other trapped-electron center also believed to exist is O_2^- molecular ion (paramag but may not be ESR observable)

  Also extrinsic defects due to impurities, hydroxyl (particularly to water radiolysis which can play an important role on post-irradiation growth and decay kinetics if $\geq 100\ ppm\ OH$ in glass) and chloride. → color centers

Girard 2019:

- Nice table with defects and absorption bands
- Three main effects that can affect the fiber transmission : Radiation Induced Attenuation (RIA), Radiation Induced Emission (RIE) and Radiation Induced Refractive Index Change (RIRIC)

  →RIRIC is said to have a big importance under neutron exposure
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Notation : "≡": three bonds, "·": unpaired spin

Type of defect	Study (exp tool)	Absorption peak (eV)	Notes
E' centers ($\equiv Si \cdot$)	ESR (Griscom 91)	5.8 (0.7) (Gi19)	Paramagnetic Unpaired spin in dangling tetrahedral orbital. Located at the oxygen vacancy (G91) % influenced by fiber drawing Formation energy $\sim 3.8eV$ Broken bond picture rather than vacancy $\neq$ types: $E_\beta, E_\delta, E_\gamma, E_\alpha$ (depending on formation mech)
Non-bridging oxygen hole centers (≡Si-O·) **NBOHC**	ESR (Griscom 91)	1.97 (0.17) 4,8 (1.0) 6.4 (1.7)① (Gi19)	Paramagnetic Can come from fission of strained OSi bond (could also interact with other -> charge), from radiolysis of hydroxyl (this one can be observed with ESR
Peroxy radicals ($\equiv Si - O - O \cdot$) **POR**	ESR (Griscom 91)	2.02, 4.08, 5.02, 2.0, 4.8 (Gi19)	Paramagnetic
Self-trapped holes 2 $\neq$: $Si - \dot{O} - Si$ (**STH1**) or · delocalized on 2 bridging O (**STH2**)	ESR (Griscom 91)	STH1 : 2.61 (1.2) + 1.88 (0.2-0.5) (Gi19) STH2 : 2.16 (0.3-0.6) 1.63 (0.3-0.7)	Paramagnetic Begin to bleach above 130K and disappear at around 200K
LTRIA (STH)		0.6-0.7 (non-Gaussian) (Gi19)	
Neutral oxygen vacancy ($\equiv Si - Si \equiv$) = **ODC**(I)		7.6 (0.5–06) (Gi19)	Diamagnetic
ODC(II) ($> Si:$)		5.05 (0.32) and 3.15 (0.30)①6.9 (0.4) (Gi19)	
2-coordinated Si ($-O - Si - O -$)			Diamagnetic
Peroxy linkages ($\equiv Si - O - O - Si \equiv$) **POL**		3.8(0.2), 4.2(0.6), 7.3(0.2), 7.5(0.1) (Gi19)	Diamagnetic
Self-trapped Electron (**STE**)		3.7, 4.6, 6.4 (Gi19)	Not presented in G91
Self-trapped Exciton (**STEX**)		4.2 (1.16) 5.3 (0.78) (Gi19)	Not presented in G91
Impurities		In the 160-200nm (G91)	
Ozone (O_3)		4.8 (0.8–0.86) (Gi19)	
O_2		0.97 (0.013) 1.62 (0.013) (Gi19)	
$Cl0$		3.26 3.65 (Gi19)	
Cl^2		3.78 (0.6) 2.3 (Gi19)	
H(I) ($> Si^* - H$)		Not observed (Gi19)	

Appendix:

- GRISCOM 91:

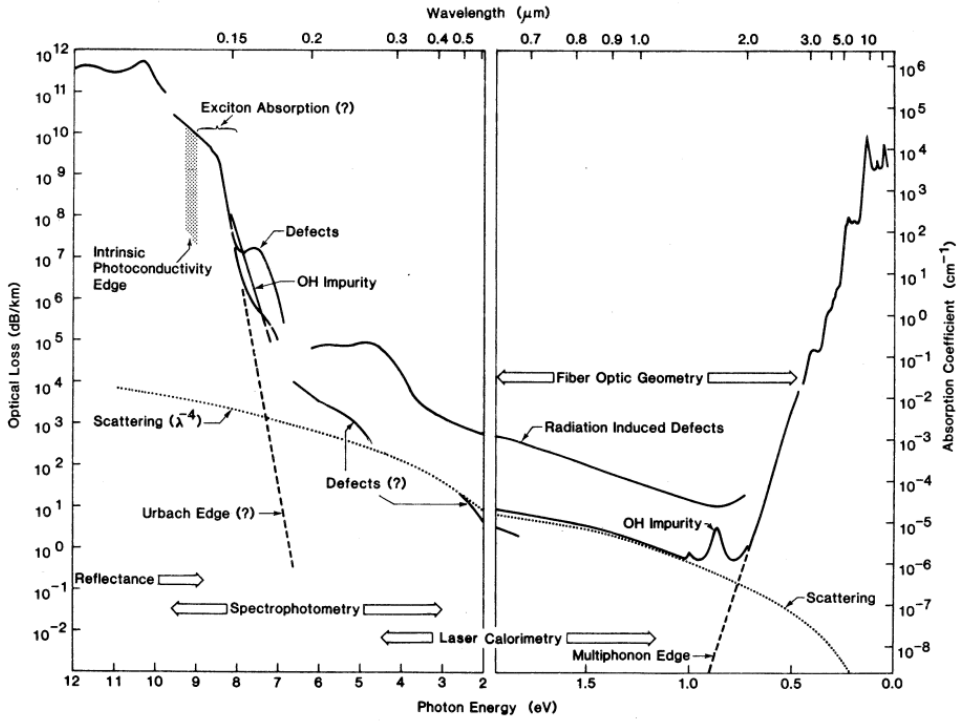


Fig. 1. Optical attenuation spectra of pure fused silica. Radiation-induced spectrum pertains to Suprasil W1. Sources of the original data are cited in Ref. 14.

- GRISCOM 85:

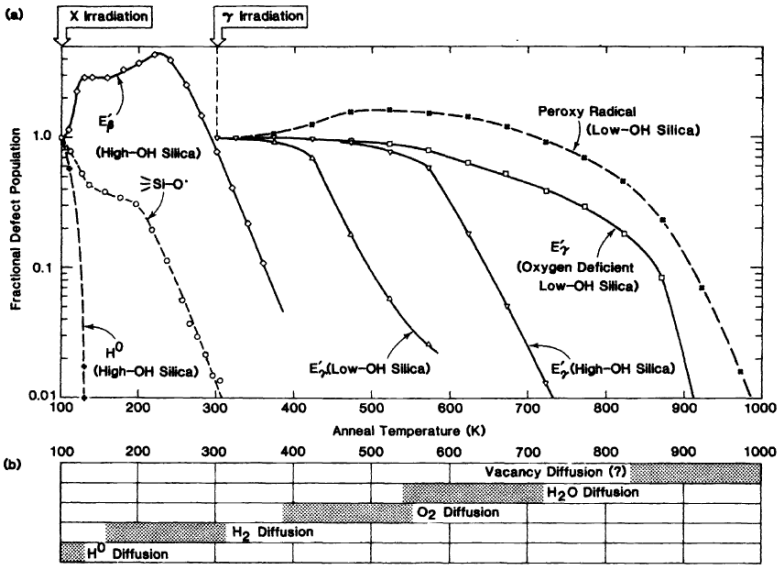
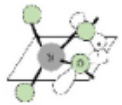
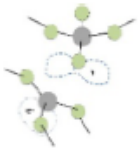


Fig. 5 (a) Isochronal anneal curves (5-10 min anneals) for radiation-induced defect centers in high purity Type-III (1200 ppm OH) and Type IV (< 5 ppm OH) fused silicas and (b) effective temperature ranges for various diffusion-limited anneal mechanisms, after Ref. 31.

Thermally activated post-irradiation processes in a-SiO_2

Table 1
Review of the main optical properties of pure-silica related point defects and those related to chlorine and hydrogen impurities.

Name	Structure	Param	OA peak eV (FWHM eV)	Oscillator strength	Note	PL peak eV (FWHM eV, lifetime RT)	Refs
Oxygen deficient center	>Si:	No	5.05 (0.32)	0.15	S_0-S_1 transition	4.4 (0.4 eV; 4.0 ns)	[16,29,156–159]
					ISC assisted (T_1-S_0 transition)	2.75 (0.34; 10 ms)	
			3.15 (0.30)[①]	$1.60\ 10^{-7}$	S_0-T_1 transition	2.75(0.34; 10 ms)	
ODC(II)			6.9 (0.4)	0.1–0.2	PL features similar bands	4.4 and 2.7	
ODC(I)	≡Si-Si≡	No	7.6 (0.5–06)	0.1–0.2		4.4 (0.4 eV, 1.4 ns)	[16,139,157,159–162]
Non-Bridging Oxygen Hole Centers	≡Si-O•	Yes	1.97 (0.17)	$1.90\ 10^{-4}$	Asymmetric Pekarian-shaped	1.91 (0.17, 10–20 μs)	[16,121,163–169]
			4,8 (1.0)	0.05	5 Gaussian are needed to describe		
			6.4 (1.7)[①]	0.05	the absorption in UV VUV		
NBOHC					see ref [167] for the relative intensity		
E'	≡Si•	Yes	5.8 (0.7)	0.1–0.2		Not observed	[16,156,170–172]
Self-trapped hole		Yes	2.61 (1.2)	0.283[②]	Inherent	None reported	[173–180]
STH_1			1,88 (0.2–0.5)		Strain-assisted (observed in OF)	None reported	[173,177,178]
STH_2		Yes	2.16 (0.3–0.6)	0.283[②]	Inherent	None reported	[173–180]
			1.63 (0.3–0.7)		Strain-assisted (observed in OF)	None reported	[173,177,178]
Peroxy Linkage **POL**	Si-O-O-Si	No	3.8(0.2), 4.2(0.6, 7.3(0.2), 7.5(0.1)	~0.0005–0.003	Computational	None reported	[30]
Peroxy Radical **POR**	Si-O-O•	Yes	2.02, 4.08, 5.02	0.00056, 0.052,0.035	Computational (one SiO_4 H-passivated tetrahedron cluster)	–	[126,132,181]
			2.0, 4.8	0.0004, 0.2	experiment		
Self-trapped Electron			3.7	–	Computational	–	[173,182]
STE			4.6	–	Computational	–	[173,182]
			6.4	–	Computational	–	[173,182]
Self-trapped Exciton		No	4.2 (1.16)	–	Computational	2.85 eV (theory)	Theory [183]
STEX			5.3 (0.78)		Experimental	2.6 −2.8 eV (exp)	Exp [184–189]
Ozone	O_3		4.8 (0.8–0.86)	Cross section $1.2\ 10^{-17}$ cm^2	VUV UV bleaching can induce the O_2 emission [21]		[190,191]
O2	molecular oxygen	Yes	0.97 (0.013)	1.1 10 − 8	T1-S0 transition	0.97 (0.01 eV, 0.4–0.8 s)[②]	[192–198]
			1.62 (0.013)	4.2 10 − 9	T1-S1 transition		
Cl0	Cl0	Yes	3.26	–	–	–	
			3.65	–	–	–	[88,177,199,200]
Cl^2	Cl^2	No	3.78 (0.6)	3.8 cross section $2.58\ 10^{-19}$ cm^2	Vibronic progression T < 110 K	1.2 (0.42, 5 ms at 13 K)	[122]
			2.3				
H(I)	>Si'-H	Yes	Not observed	–	–	Not observed	[14,17,23]
LTRIA	STH	Yes	0.6 – 0.7 eV (non-Gaussian)	–	LTRIA is attributed to inherent STHs	Not observed	[153]

① Peak and FWHM derived from PLE spectra.
② Linear combination Gaussian bands peaking at 2.16 and 2.60 eV.
③ Strong radioluminescence signal under X-rays [103].