

Radiation Hardness of
Insulating Materials and
Semiconductors

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31. 08. 2005

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The Problem:

What determine the Sensitivity of Solids to Radiation?

- a) **The electronic configuration of the atoms**
- b) **The crystal structure**

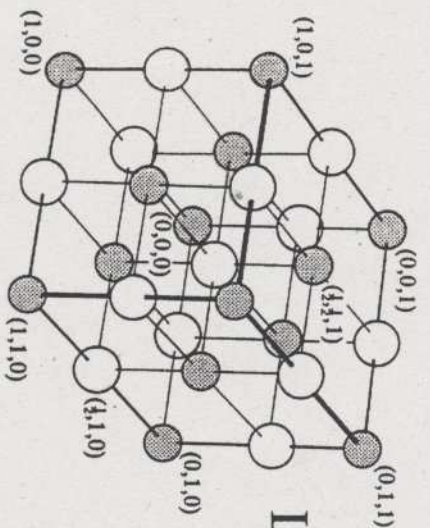
**I. Damage creation in Dielectrics
Two classes of insulating materials**

II. Semiconductors Si; SiC

III. Peculiarities of Damage creation under heavy ion irradiation

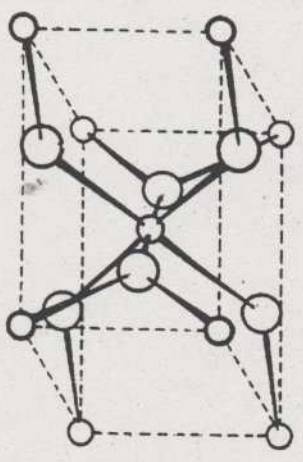
**I. Damage Creation in Dielectrics by the Decay of Electronic
Excitations [1, 3, 5, 6, 12]**

Crystal structure

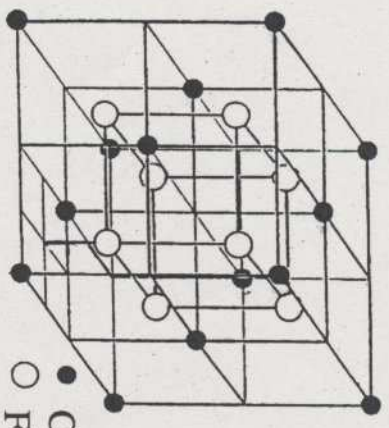
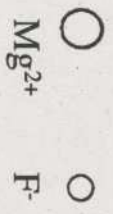


CaF₂ (cubic)
 $a = 5.463 \text{ \AA}$
 $\rho = 3.18 \text{ g/cm}^3$
 $\text{F}^- \quad r = 1.33 \text{ \AA}$
 $\text{Ca}^{2+} \quad r = 0.99 \text{ \AA}$
 $E_g = 11.2 \text{ eV}$

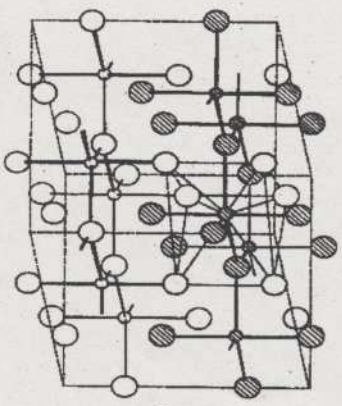
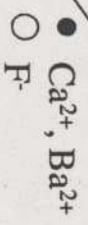
LiF (cubic)
 $a = 4.028 \text{ \AA}$
 $\rho = 2.635 \text{ g/cm}^3$
 $\text{F}^- \quad r = 1.33 \text{ \AA}$
 $\text{Li}^+ \quad r = 0.74 \text{ \AA}$
 $E_g = 14.6 \text{ eV}$



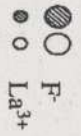
MgF₂ (tetragonal)
 $a = 4.623 \text{ \AA} \quad c = 7.354 \text{ \AA}$
 $\rho = 3.18 \text{ g/cm}^3$
 $\text{F}^- \quad r = 1.33 \text{ \AA}$
 $\text{Mg}^{2+} \quad r = 0.72 \text{ \AA}$
 $E_g = 11 \text{ eV}$



BaF₂ (cubic)
 $a = 6.200 \text{ \AA}$
 $\rho = 4.89 \text{ g/cm}^3$
 $\text{F}^- \quad r = 1.33 \text{ \AA}$
 $\text{Ba}^{2+} \quad r = 1.34 \text{ \AA}$
 $E_g = 8.3 \text{ eV}$



LaF₃ (hexagonal)
 $a = 4.148 \text{ \AA} \quad c = 7.354 \text{ \AA}$
 $\rho = 5.9 \text{ g/cm}^3$
 $\text{F}^- \quad r = 1.33 \text{ \AA}$
 $\text{La}^{3+} \quad r = 1.1 \text{ \AA}$
 $E_g = 10.5 \text{ eV}$

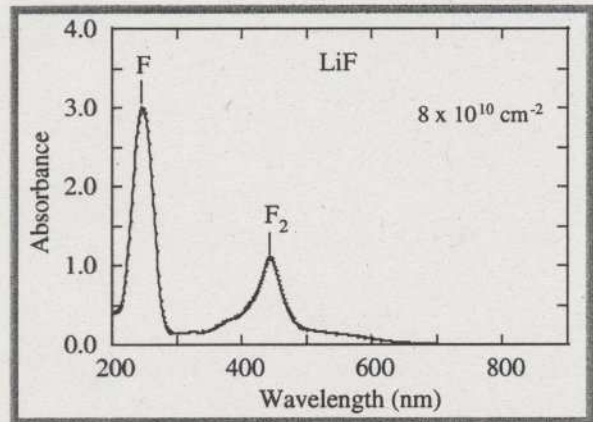
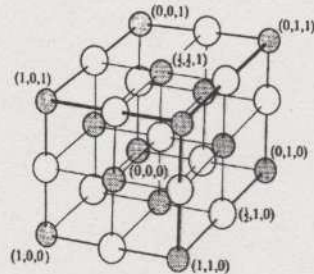


other fluoride crystals

U (5.9 MeV/u)

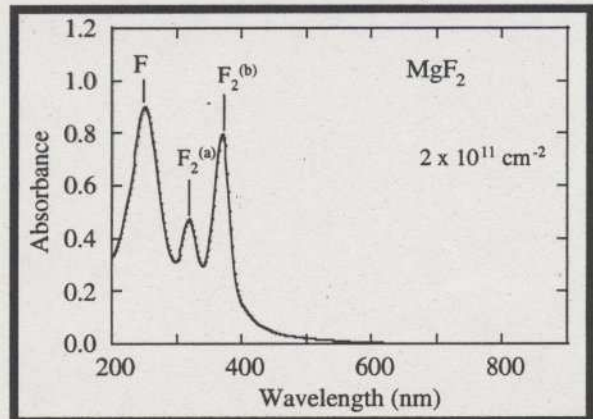
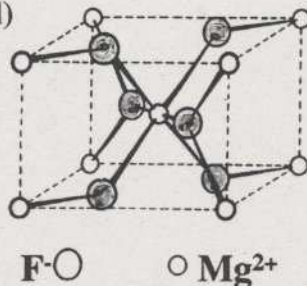
LiF (cubic)

$a = 4.028 \text{ \AA}$
 $\rho = 2.635 \text{ g/cm}^3$
 $F^- \text{ } r = 1.33 \text{ \AA}$
 $Li^+ \text{ } r = 0.74 \text{ \AA}$
 $E_g = 14.6 \text{ eV}$



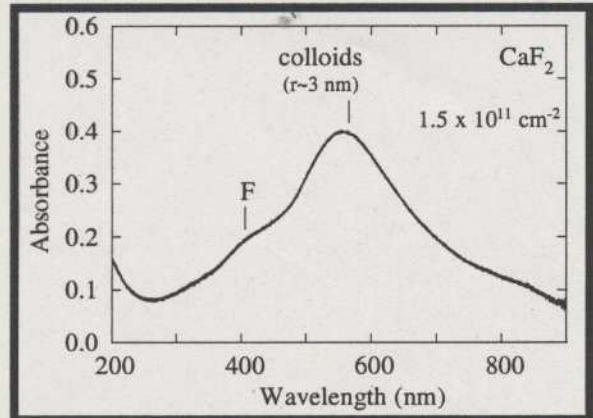
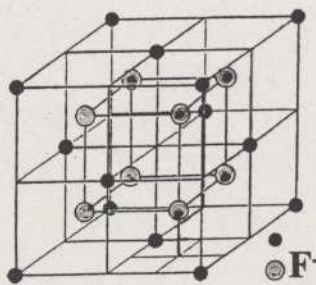
MgF₂ (tetragonal)

$a = 4.623 \text{ \AA}$
 $c = 7.354 \text{ \AA}$
 $\rho = 3.18 \text{ g/cm}^3$
 $F^- \text{ } r = 1.33 \text{ \AA}$
 $Mg^{2+} \text{ } r = 0.72 \text{ \AA}$
 $E_g = 11 \text{ eV}$



CaF₂ (cubic)

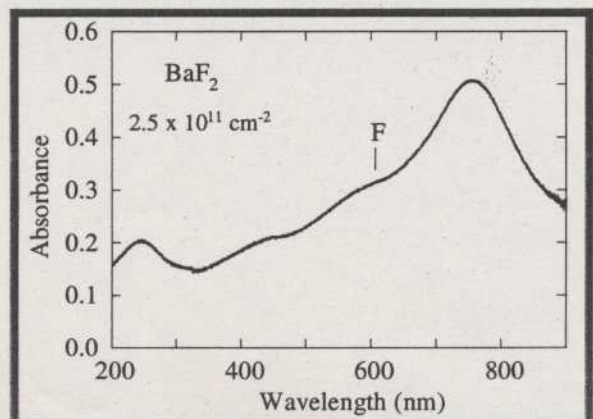
$a = 5.463 \text{ \AA}$
 $\rho = 3.18 \text{ g/cm}^3$
 $F^- \text{ } r = 1.33 \text{ \AA}$
 $Ca^{2+} \text{ } r = 0.99 \text{ \AA}$
 $E_g = 11.2 \text{ eV}$



BaF₂ (cubic)

$a = 6.200 \text{ \AA}$
 $\rho = 4.89 \text{ g/cm}^3$
 $F^- \text{ } r = 1.33 \text{ \AA}$
 $Ba^{2+} \text{ } r = 1.34 \text{ \AA}$
 $E_g = 9.1 \text{ eV}$

Ca²⁺, Ba²⁺

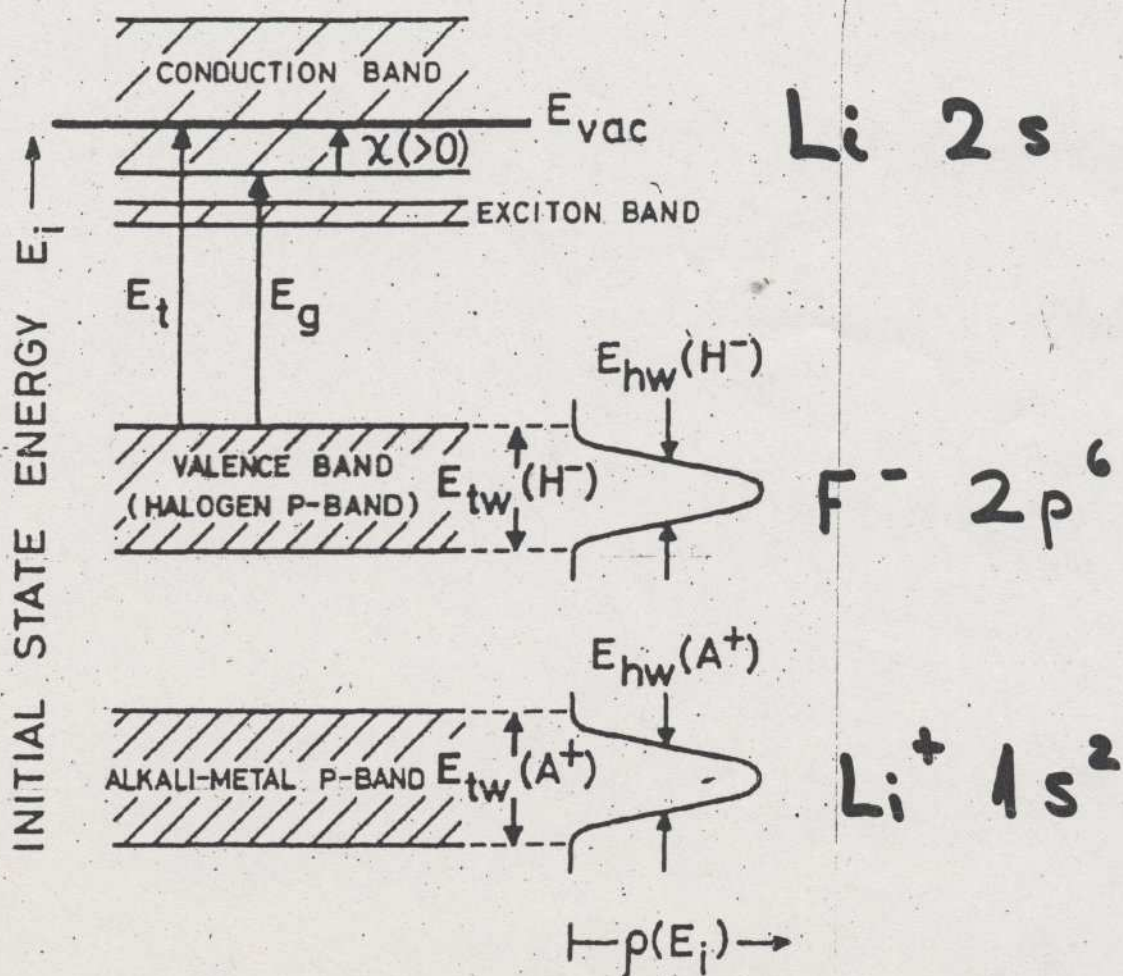


Electronic Band Structure of LiF

R. T. Poole et al. Phys. Rev. B 11 (1975) 5179

CB Li 2s VB Li⁺ 1s²[He]

VB F⁻ 2p⁶ [Ne]



Electronic structure:

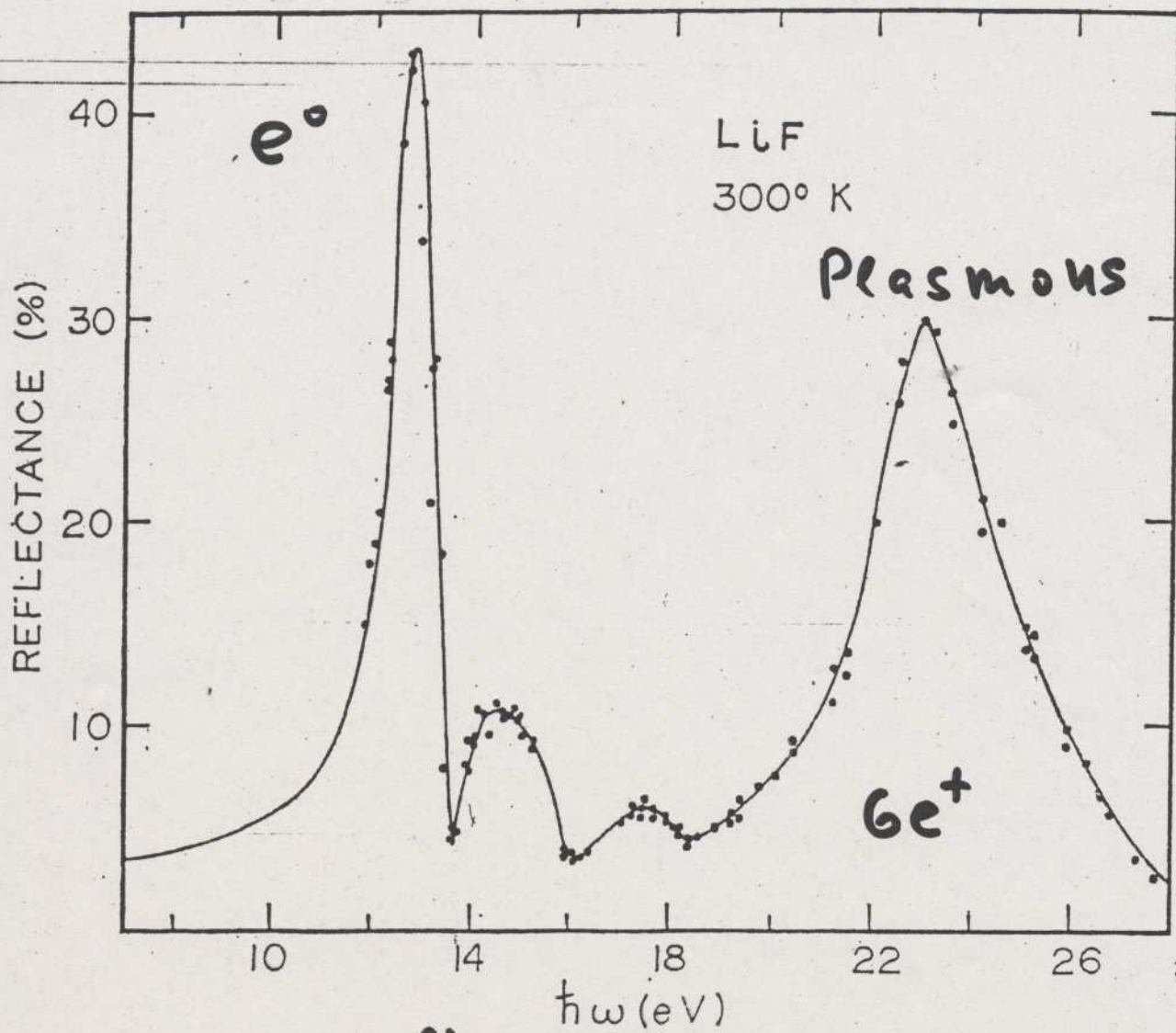
Anion Exciton 13.6 eV

Gap $E_g = 14.2$ eV

Plasmons 25 eV

Cation Exciton 63 eV

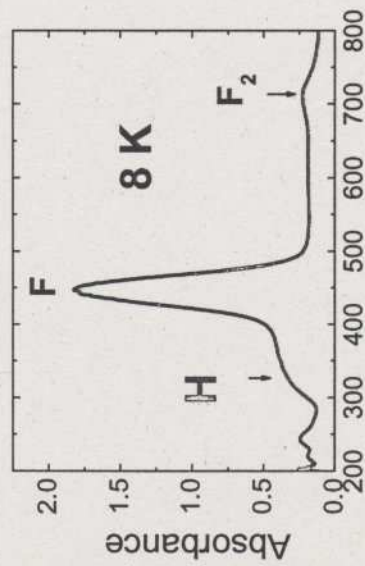
D. M. Roessler, W. C. Walker,
J. Phys. Chem. Solids 28 (1967) 1507



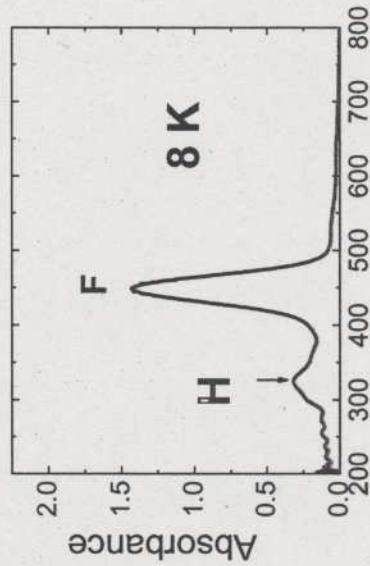
\sim
14.2 eV
 E_g

Appearance of H centers at 8 K Irradiation

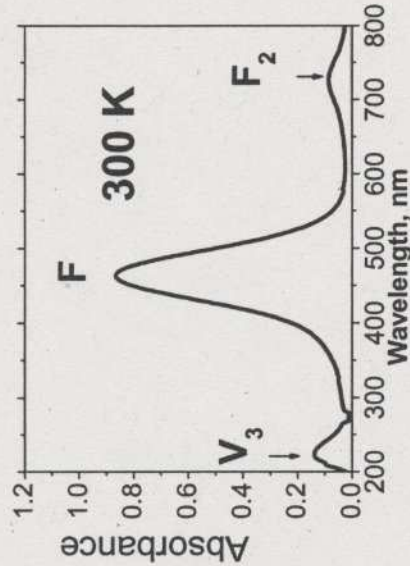
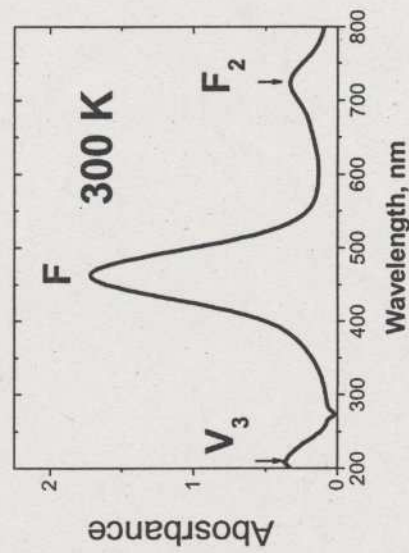
^{238}U



^{12}C

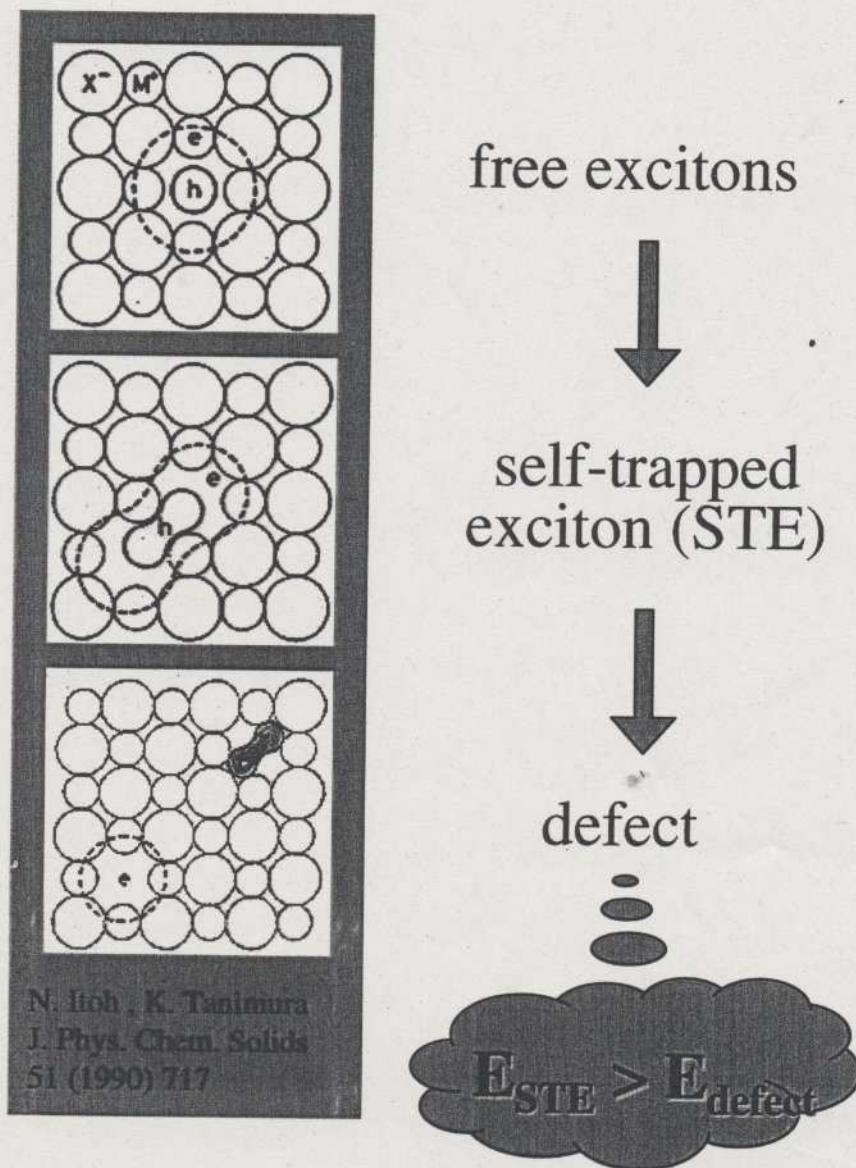


NaCl



H centers are not stable at $T > 70\text{ K}$

Exciton mechanism



The discovering of exciton mechanism in 60ths

Ch.B. Lushchik et al., Sov. Phys. Solid State 6 (1965) 1789

H.N. Hersh, Phys. Rev. 148 (1966) 928

D. Pooley, Proc. Phys. Soc. 87 (1966) 245

Ch.B. Lushchik et al., Sov. Phys. Uspekhi 20 (1977) 489 (review)

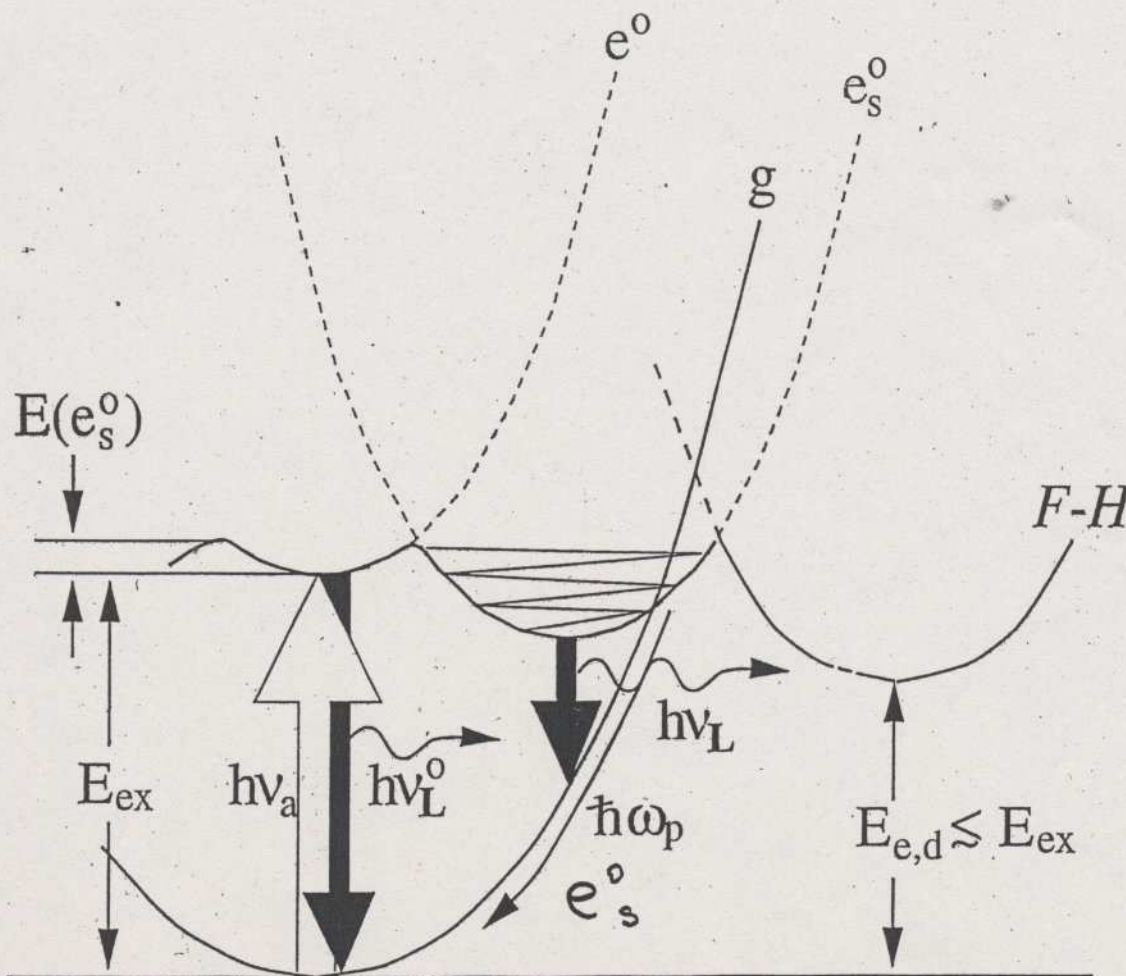
Exciton Processes in Dielectrics

$E(e^0)$ free Exciton Energy

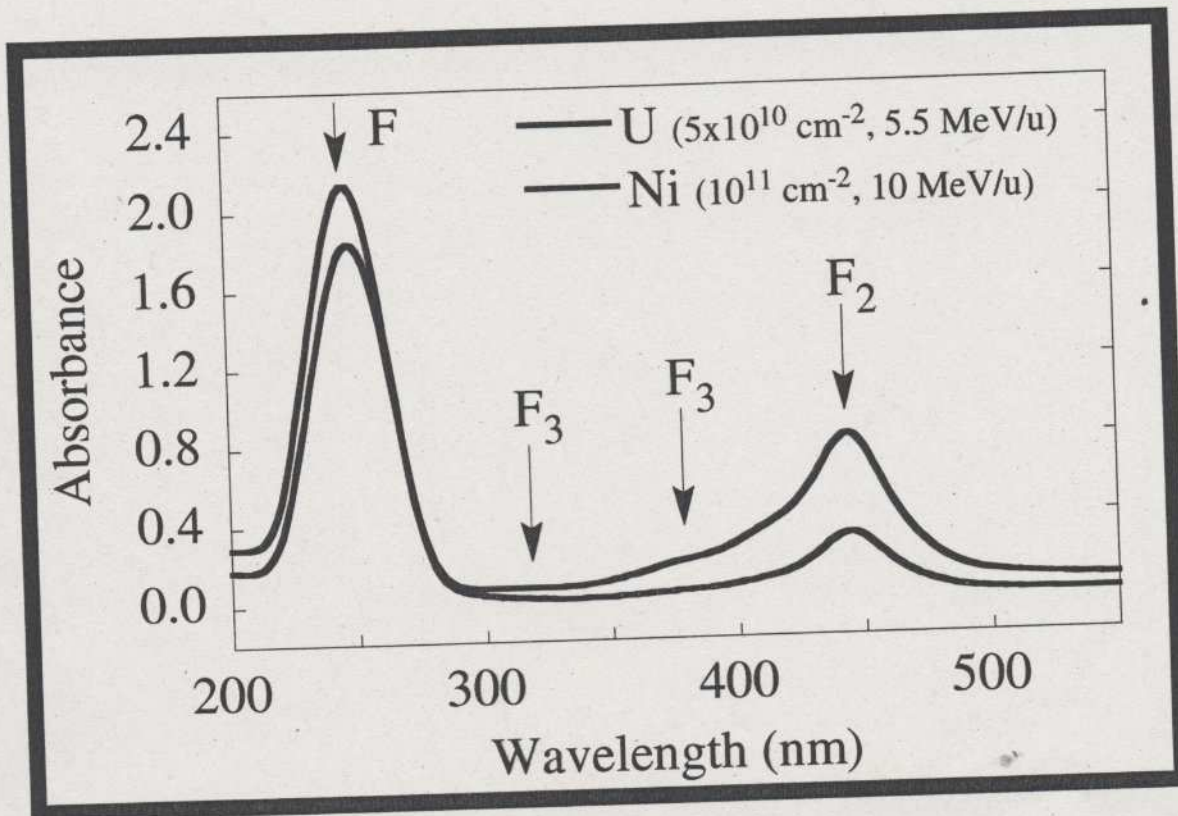
$E(e_s^0)$ self trapped Exciton Energy

Frenkel Pair F - H

Luminescence $h\nu_L$



Efficiency of F-center creation in LiF



	photons	gammas	light ions (C, S, Ni)	heavy ions (Au, Pb, U)
energy / F-center	42 eV ~3E _g	400 eV	500-600 eV	900-1200 eV
F-centers / track			10 ⁵	10 ⁶

Electron-Hole Pair Creation Energies

R. C. Alig and S. Bloom, *Phys. Rev. Let.* 55 (1975) 1522

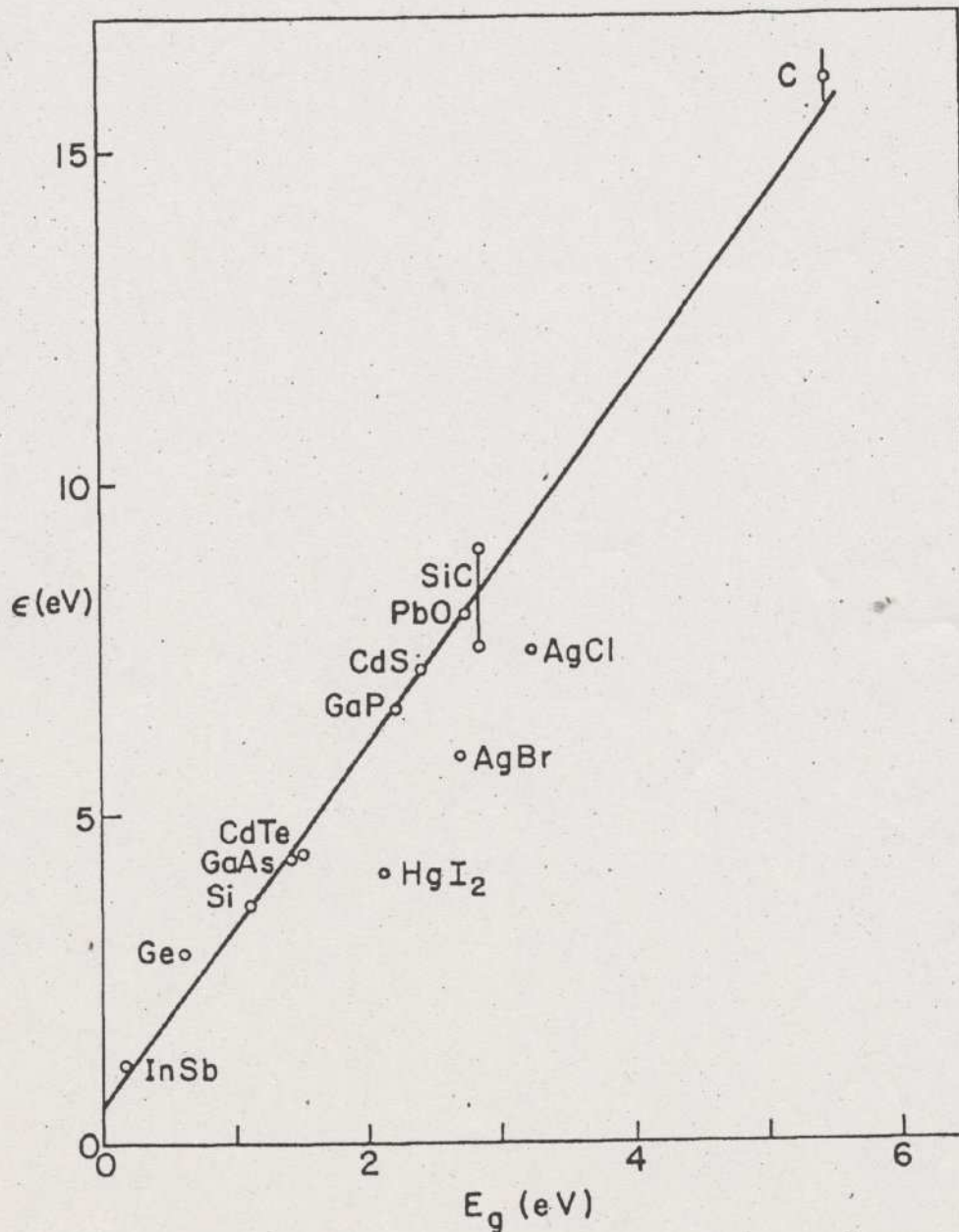
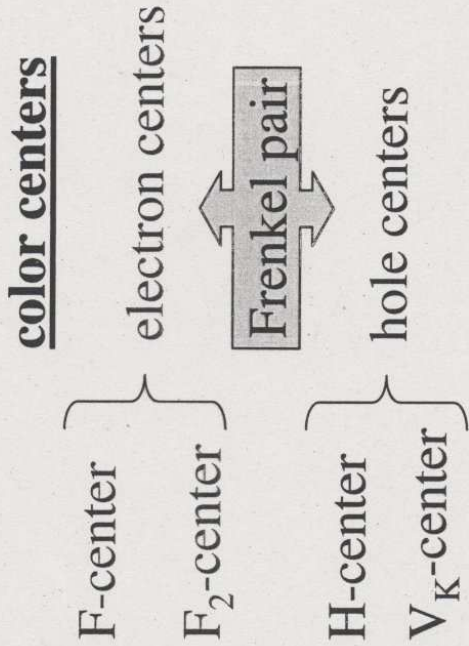
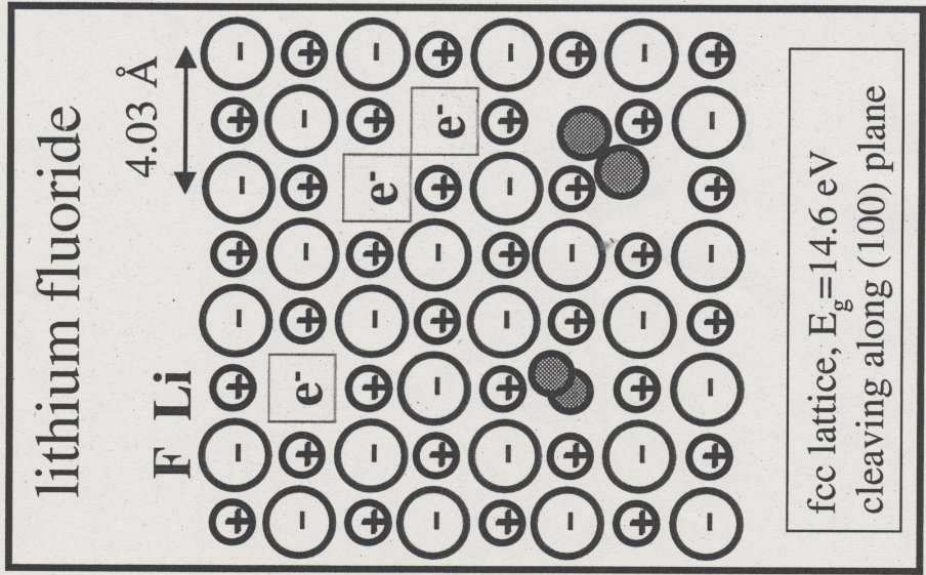


FIG. 1. The measured pair-creation energies ϵ of several semiconductors, versus the fundamental semiconductor band gap E_g . A straight line has been fitted to selected points on this plot.

Defect creation in ionic crystals

LiF, NaCl, KCl, MgF₂, CaF₂, BaF₂

non-amorphisable !!



**II. Damage Creation in Dielectrics by Elastic Collisions [1, 2, 4,
7, 8, 10, 11]**

Radiation Hardness and Self Trapping

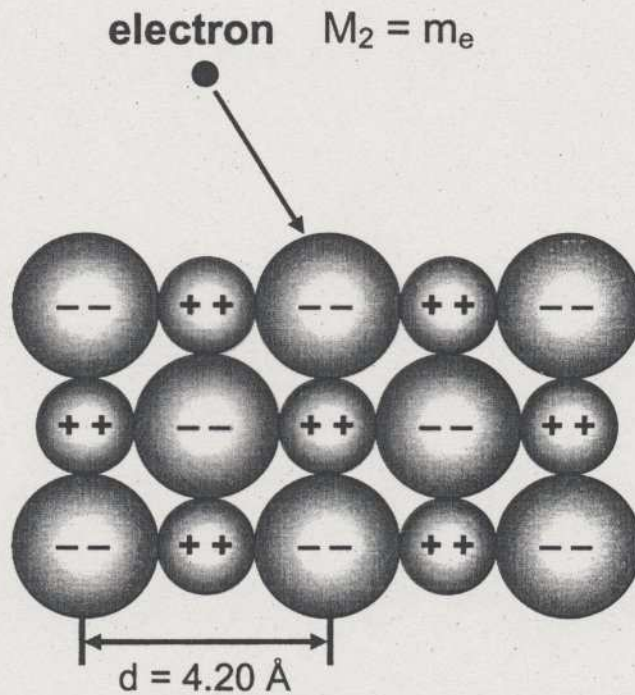
N. Itoh, NIM B 122 (1997) 405 - 409

Table 1

Presence and absence of self-trapping of carriers in major materials

Material	Electrons	Holes	Excitons
Diamond, silicon, germanium	no	no	no
III-V compounds	no	no	no
II-VI compounds	no	no	no
Se			yes
As ₂ S, As ₂ Se			yes
Copper halides	no	no	no
Thalious halides	no	no	no
Alkali halides with NaCl structure	no	yes	yes
Alkali halides with CsCl structure	no	yes	yes
Alkaline earth fluorides	no	yes	yes
PbCl ₂	yes	yes	
PbI ₂	no	no	no
MgO	no	no	no
ZnO	no	no	no
SiO ₂	no	no	yes

Defect production in MgO



$$r_{O^-} = 1.40 \text{ \AA} \quad E_d(O^-) = 59 \text{ eV}$$

$$r_{Mg^{++}} = 0.74 \text{ \AA} \quad E_d(Mg^{++}) = 64 \text{ eV}$$

$$M_1 = A_1 \text{ or } A_2$$

$$O^- \quad A = M_1 = 16$$

$$\Delta E_{tr} = \frac{4 \cdot M_1 \cdot M_2}{(M_1 + M_2)^2} \cdot E_0$$

$$\Delta E_{tr} = E_d(O^-) = 59 \text{ eV}$$

$$M_2 = 1/1840$$

$$E_0^{\min} = \frac{\Delta E_{tr} \cdot (M_1 + M_2)^2}{4 \cdot M_1 \cdot M_2} \sim 430 \text{ keV}$$

Damage Creation in MgO

W. A. Sibley, NIM B 1 (1984) 419 - 426

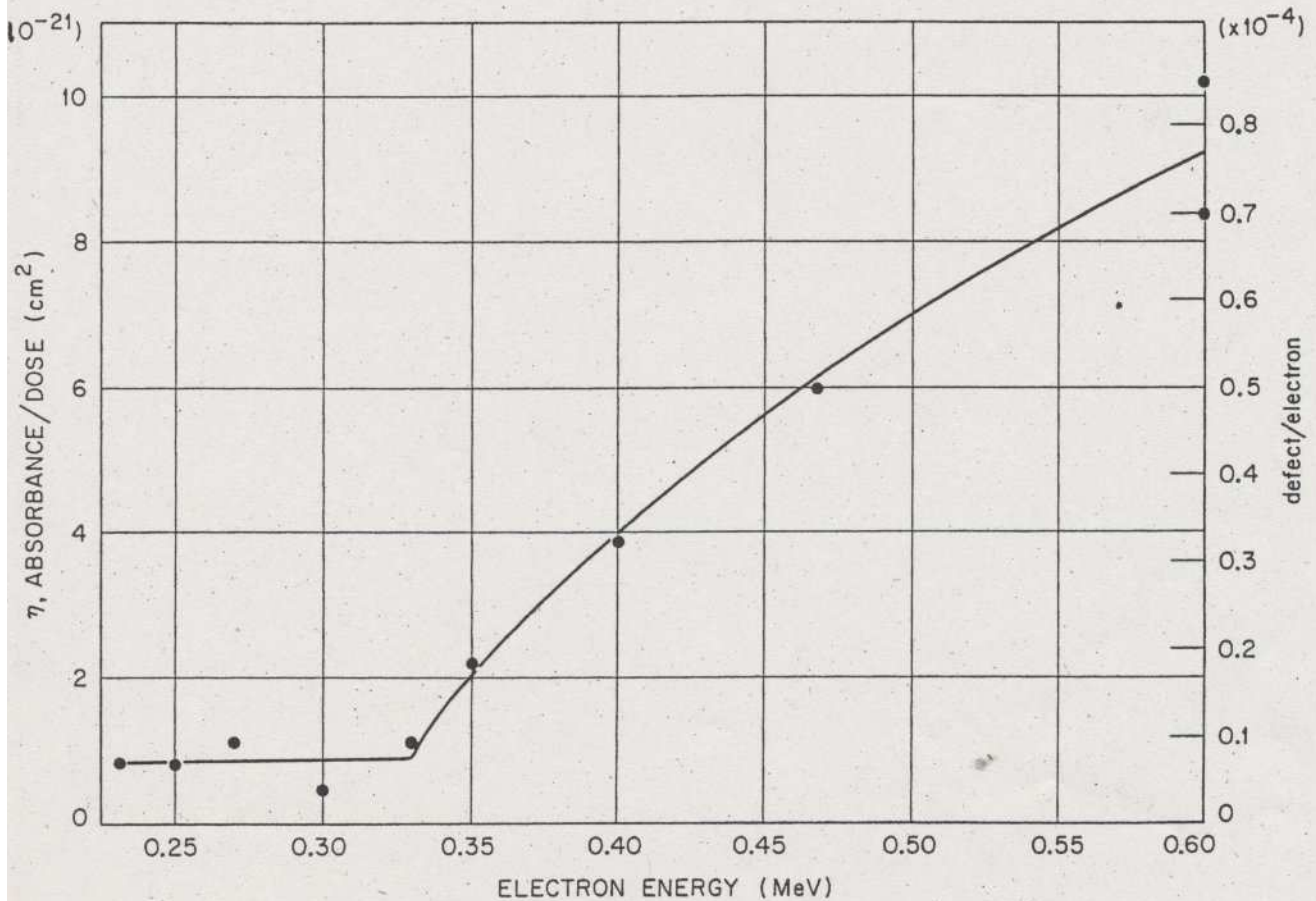


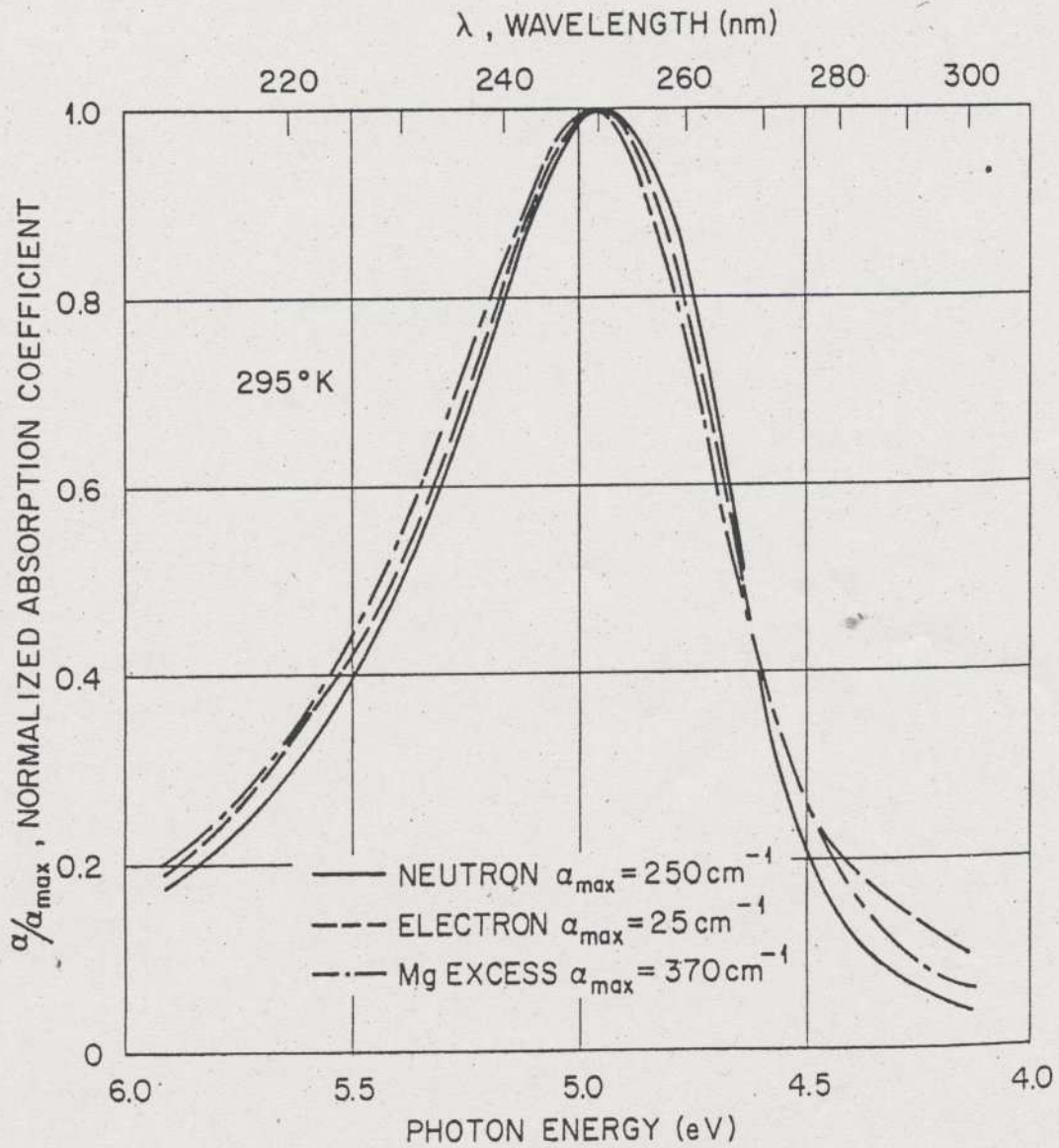
Fig. 4. Defect production rate as a function of irradiation energy for MgO crystals (after ref. 10).

Threshold Effect
 $\Delta E(\text{LiF}) / \Delta(\text{MgO}) \sim 0.001$

Damage Creation in MgO

W. A. Sibley, NIM B 1 (1984) 419 - 426

F center absorption



$$\Delta E(\text{LiF}) / \Delta(\text{MgO}) \sim 0.001$$

Table 2

Displacement energies for some non-metals near room temperature

Material	T^d (eV)	Material	T^d (eV)
C (graphite)	28–31	SiC	45–90
C (diamond)	80	MgO	64(Mg) 60(O)
Si	11–22	Al ₂ O ₃	18(Al) 76(O)
Ge	12–30	MgAl ₂ O ₄	56(O)
GaAs	9(Ga) 9(As)	ZnO	40(Zn) 57(O)
ZnS	10(Zn) 15(S)	UO ₂	40(U) 20(O)
CdS	7(Cd) 9(S)	BeO	76(O)

Radiation Damage and Stress Effects in Superconductors: Materials for High-Field Applications

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Silicon carbide: synthesis and processing

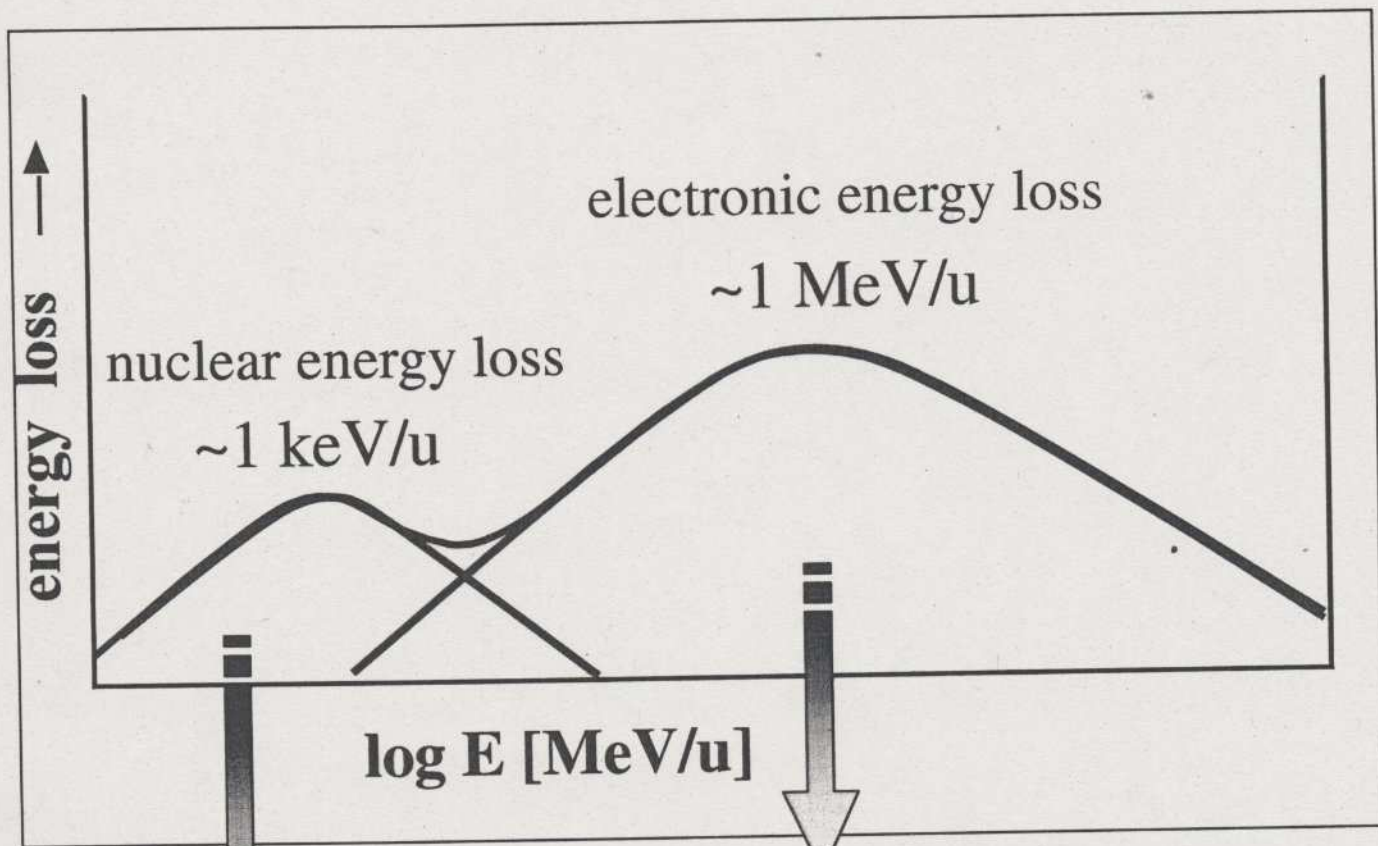
W. Wesch

Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, D-07743 Jena, Germany

Table 2
Comparison of selected semiconductor properties

	Si	GaAs	6H-SiC	4H-SiC	3C-SiC	Diamond
Bandgap [eV] ^a	1.1	1.42	3.0	3.3	2.3	5.5
Melting point [°C]	1420	1238		sublimes > 1800		phase change 20
Thermal conductivity [W cm ⁻¹ K ⁻¹]	1.5	0.5	4.9	4.9	5.0	
Electron mobility at 10 ¹⁶ cm ⁻³ [cm ² V ⁻¹ s ⁻¹]	1100	6000	370	800	750	(2200)
Hole mobility at 10 ¹⁶ cm ⁻³ [cm ² V ⁻¹ s ⁻¹]	420	320	90	115	40	(1600)
Breakdown field at 10 ¹⁷ cm ⁻³ [MV cm ⁻¹]	0.6	0.6	3.2	3	4	(10)

**III. Peculiarities of Damage Creation in Dielectric Materials
under Heavy Ion Irradiation [1, 5, 6]**



collision processes

primary electrons $10^{-17} - 10^{-16}$ s

δ - electrons $10^{-15} - 10^{-14}$ s

lattice excitations
excitons
electrons and holes $10^{-13} - 10^{-3}$ s

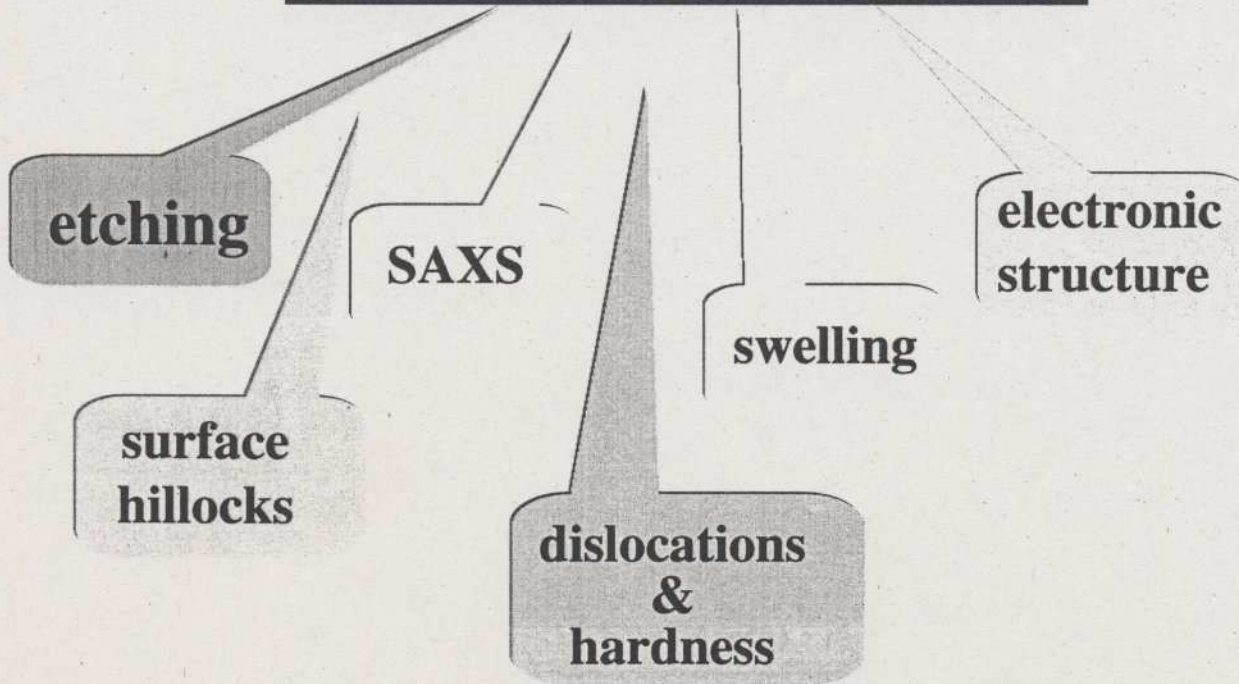
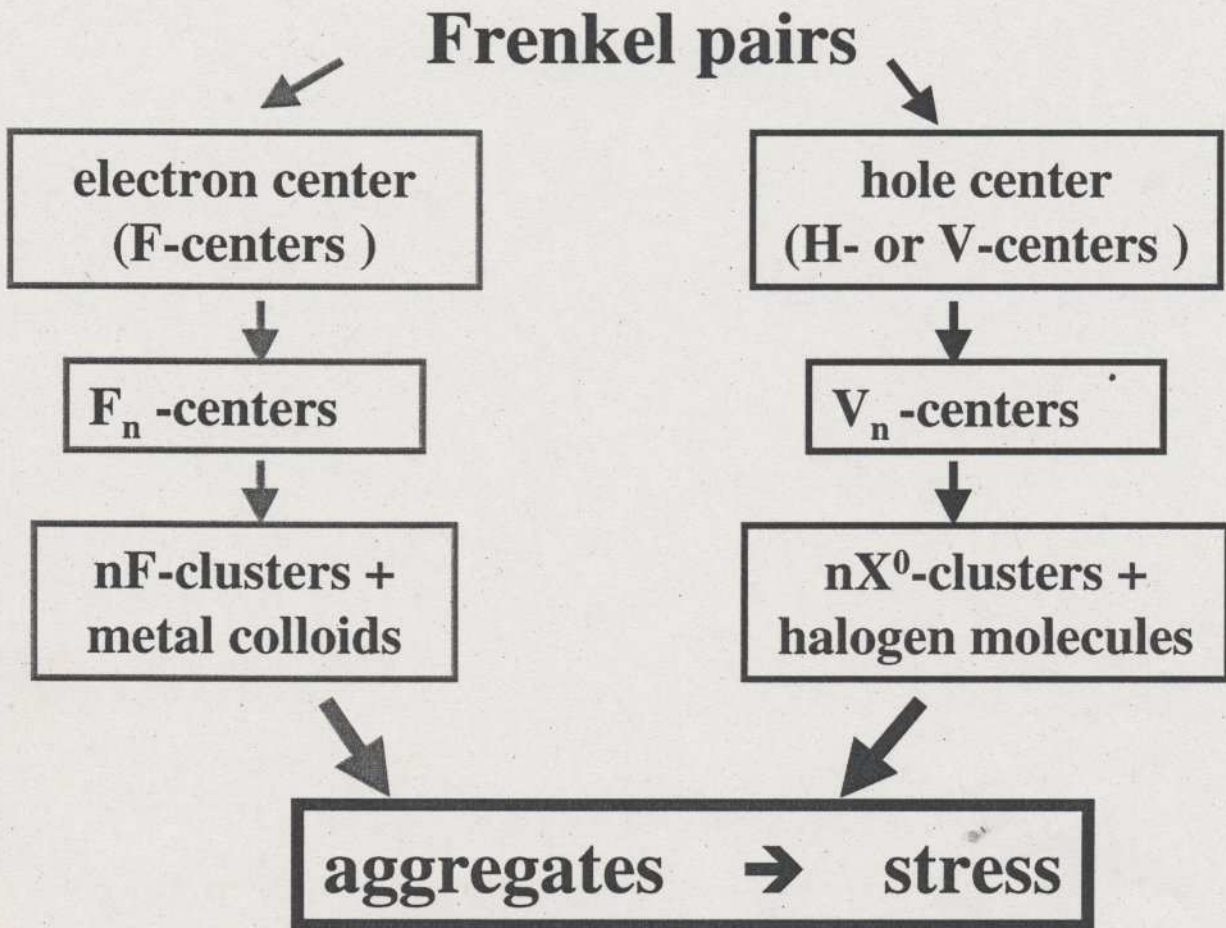
defects

luminescence

vibrations

$$\sum N_{\text{electr}} = \sum N_{\text{holes}}$$

Aggregation of single defects



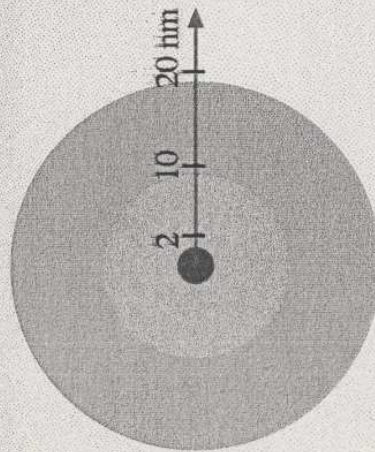
N. Itoh and A. M. Stonham
 "Materials Modification by Electronic
 Excitation", Cambridge University Press,
 Cambridge, 2001, p. 439



Self Trapping and Threshold Stopping Power for Track Registration

System	Threshold stopping power (keV/nm)	Self-trapped exciton?	Reference (stopping power)
<i>Continuous tracks</i>	1-10	Yes	
SiO ₂	2	Yes	Meftah <i>et al.</i> (1993)
Y ₃ Fe ₅ O ₁₂	4	Probably yes	Toulemonde <i>et al.</i> (1994)
Mica	5	Possibly yes	Toulemonde <i>et al.</i> (1994)
LiNbO ₃	7	Probably yes	Meftah <i>et al.</i> (1993)
LiF	≥10	Yes	Schwartz <i>et al.</i> (1998)
<i>Fragmentary tracks</i>	>20		
MgO	20		Canut <i>et al.</i> (1995)
Al ₂ O ₃	21		Canut <i>et al.</i> (1995)
Bi	31		Wang <i>et al.</i> (1996)
Si	>28		Dunlop <i>et al.</i> (1998)

Lithium Fluoride

- * complex damage structure
- * since amorphisation is not possible, swelling is probably linked to the formation of defect aggregates
- * SAXS radii in LiF are much smaller than any radii measured in amorphisable crystals



 F⁻-centers
 swelling
 SAXS

Oxides

- * swelling can be explained by a transition from the crystalline to the amorphous phase
- * the swelling radii and the threshold is about the same as observed by other techniques (TEM and RBS/C)

swelling

occurs at a lower threshold than track etching

	LiF	SiO ₂ quartz
swelling	4 keV/nm	2 keV/nm
etching	10 keV/nm	7 keV/nm



 RBS/C and TEM
 swelling

References

1. N. Itoh and A. M. Stoneham "Materials Modification by Electronic Excitation", Cambridge University Press, Cambridge 2001.
2. F. Agullo-Lopez, C. R. A. Catlow, P. D. Townsend "Point Defects in Materials", Academic Press, London 1988.
3. Ch. B. Lushchik "Creation of Frenkel Defect Pairs by Excitons in Alkali Halides" In: Physics of Radiation Effects in Crystals, North-Holland, Amsterdam – Oxford 1986, pp. 473 – 525.
4. F. W. Clinard, L. W. Hobbs "Radiation Effects in Non-Metals" In: Physics of Radiation Effects in Crystals, North-Holland, Amsterdam – Oxford 1986, pp. 387 – 471.
5. K. Schwartz "Fast Ion Induced Damage in Ionic Crystals", Phys. Sta. Sol. c 2 (2005) 355 – 361.
6. K. Schwartz, C. Trautmann, R. Neumann " Electronic Excitations and Heavy – Ion-Induced Processes in Ionic Crystals", Nucl. Instr. Meth. **B 209** (2003) 73 – 84..
7. N. Itoh "Subthreshold Radiation-Induced Processes in the Bulk and on Surfaces of Solids", Nucl. Instr. Meth. **B 135** (1998) 175 – 183.
8. N. Itoh "Bond Scission Induced by Electronic Excitation in Solids: A tool for Nanomanipulation", Nucl. Instr. Meth. **B 122** (1997) 405 – 409.
9. R. C. Alig, S. Böoom "Electron-Hole-Pair Creation Energies in Semiconductors", Phys. Rev. Lett. **35** (1975) 1522 – 1525.
10. W. A. Sibley "Radiation Damage Processes in Insulating Materials", Nucl. Instr. Meth. **B 1** (1984) 419 – 426.
11. B. Henderson "On the Nature, Characterisation and Applications of Point Defects in Insulators" Radiaton Effects **64** (1982) 35 – 47.
12. M. Kirm, A. Lushchik, Ch. Lushchik "Creation of Groups of Spatially Correlated Excitations in Wide-Gap Solids" Phys. Sta. Sol. **a 202** (2005) 213 – 220.