OPTICAL TECHNOLOGY DIVISION NIST

Intrinsic Birefringence in Cubic Crystalline Optical Materials

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1901-2001
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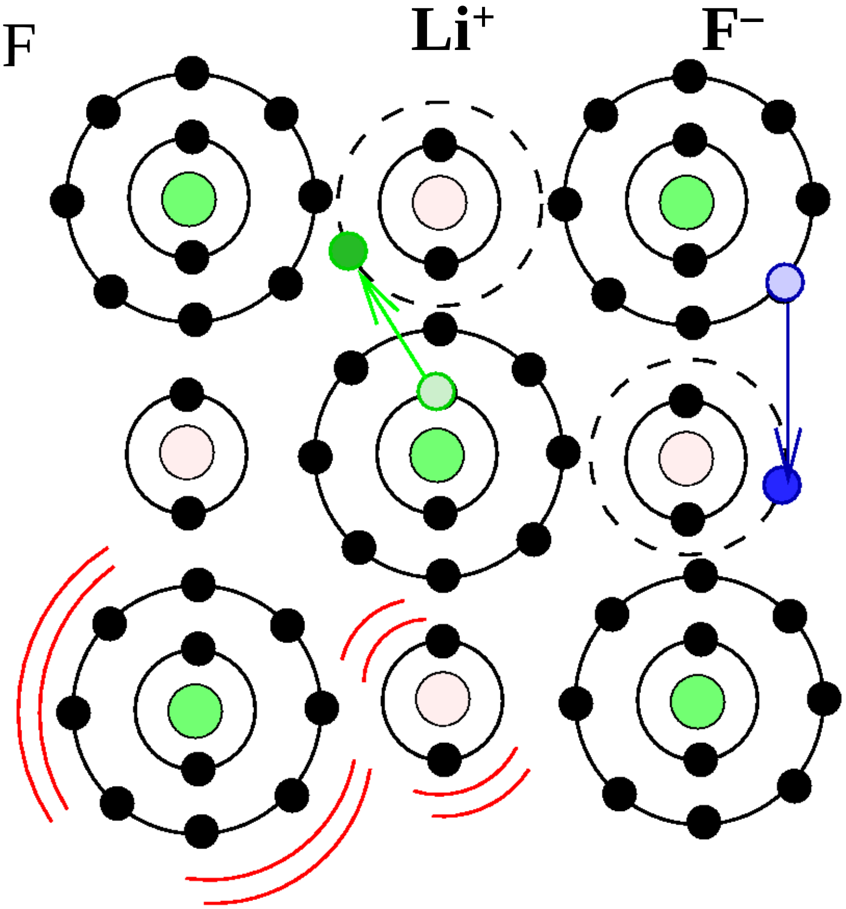
Conceptual view of a solid

Vibrational, valence electron & core electron degrees of freedom

Example: LiF

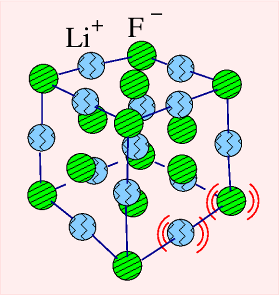


EXCITATIONS

Phonon excitations

Valence excitations

Core excitations



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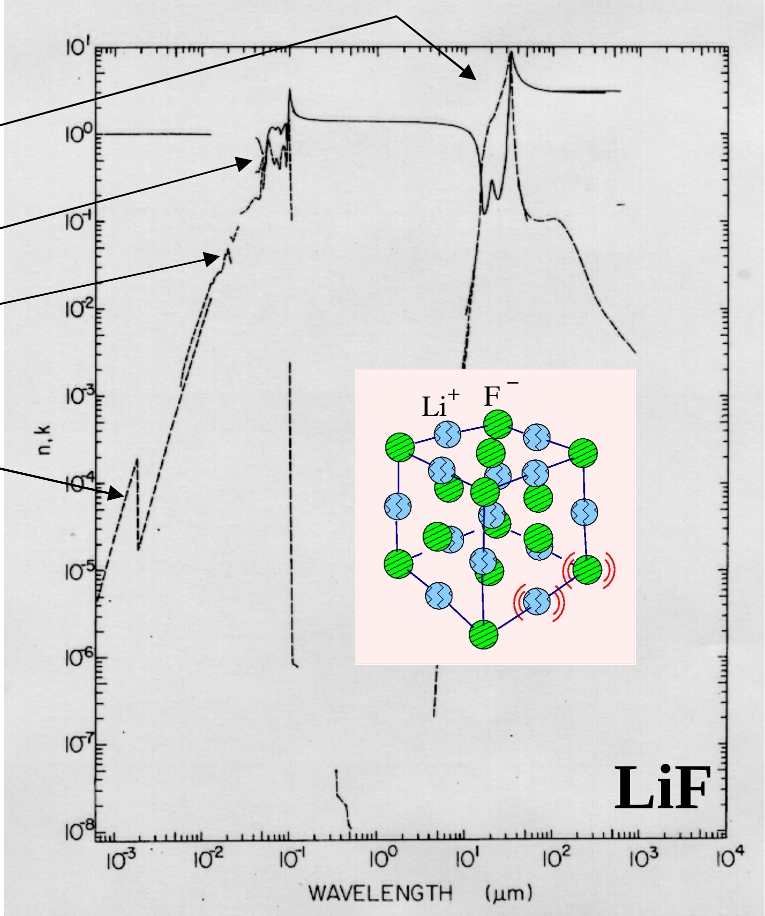
Optical properties throughout the spectrum

- * infrared absorption by phonons
- * absorption by inter-band transitions
- * absorption at x-ray edges



Plot taken from Palik.

Optical Constants:

n = index of refraction
k = index of absorption

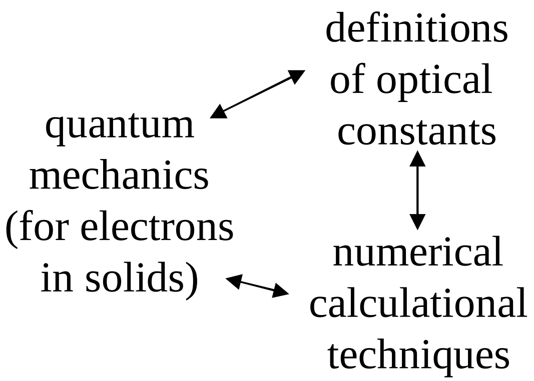
Properties can be approached with theory. Theory is helpful when it is predictive or complementary to experiment.

Goal: develop approach for unified (*n*,*k*)-curve from far-IR to x-ray region.

Outline

A winding, sparsely
detailed trajectory
circling between

- Introduction to optical excitations
- Model used to describe excitations & excitation spectra



definitions
of optical
constants

quantum
mechanics
(for electrons
in solids)

numerical
calculational
techniques

  - developed in collab. with L.X. Benedict (LLNL), R.B. Bohn (ITL), and J.A. Soininen (U. Helsinki)

- Sample ultraviolet (UV) & x-ray absorption spectra
- Intrinsic birefringence in cubic solids

Photon interaction with electrons: coupling electron **p** to photon **A**

Electron Schrödinger equation:

self-energy (accounts for many-body electron-electron interaction effects)

$$\left[\frac{\mathbf{p}^2}{2m}+V_{\text{ext}}+V_H\right]\psi_{n\mathbf{k}}(\mathbf{r})+\int d^3\mathbf{r}'\,\underline{\Sigma(\mathbf{r},\mathbf{r}';E_{n\mathbf{k}})}\,\psi_{n\mathbf{k}}(\mathbf{r}')=E_{n\mathbf{k}}\,\psi_{n\mathbf{k}}(\mathbf{r})$$

electron wave function (n=band/core level, k=crystal momentum

electron level energy

Light interacts with electrons (approximately) via the replacement,

$$-\frac{\hbar^2}{2m}\nabla^2$$

$$\frac{\mathbf{p}^2}{2m}\rightarrow\frac{(\mathbf{p}+e\mathbf{A}/c)^2}{2m}=\frac{\mathbf{p}^2}{2m}+\frac{e}{mc}\mathbf{p}\cdot\mathbf{A}+\left(\frac{e^2}{2mc^2}\right)\mathbf{A}\cdot\mathbf{A}$$

The first term is the ordinary electron kinetic-energy operator.

The second term couples electric fields to electron currents.

-- absorption, emission

electron momentum **p** ↔ electron current

vector potential **A** ↔ electric field **E** ↔force on electrons

The third term couples to electron density.

--scattering

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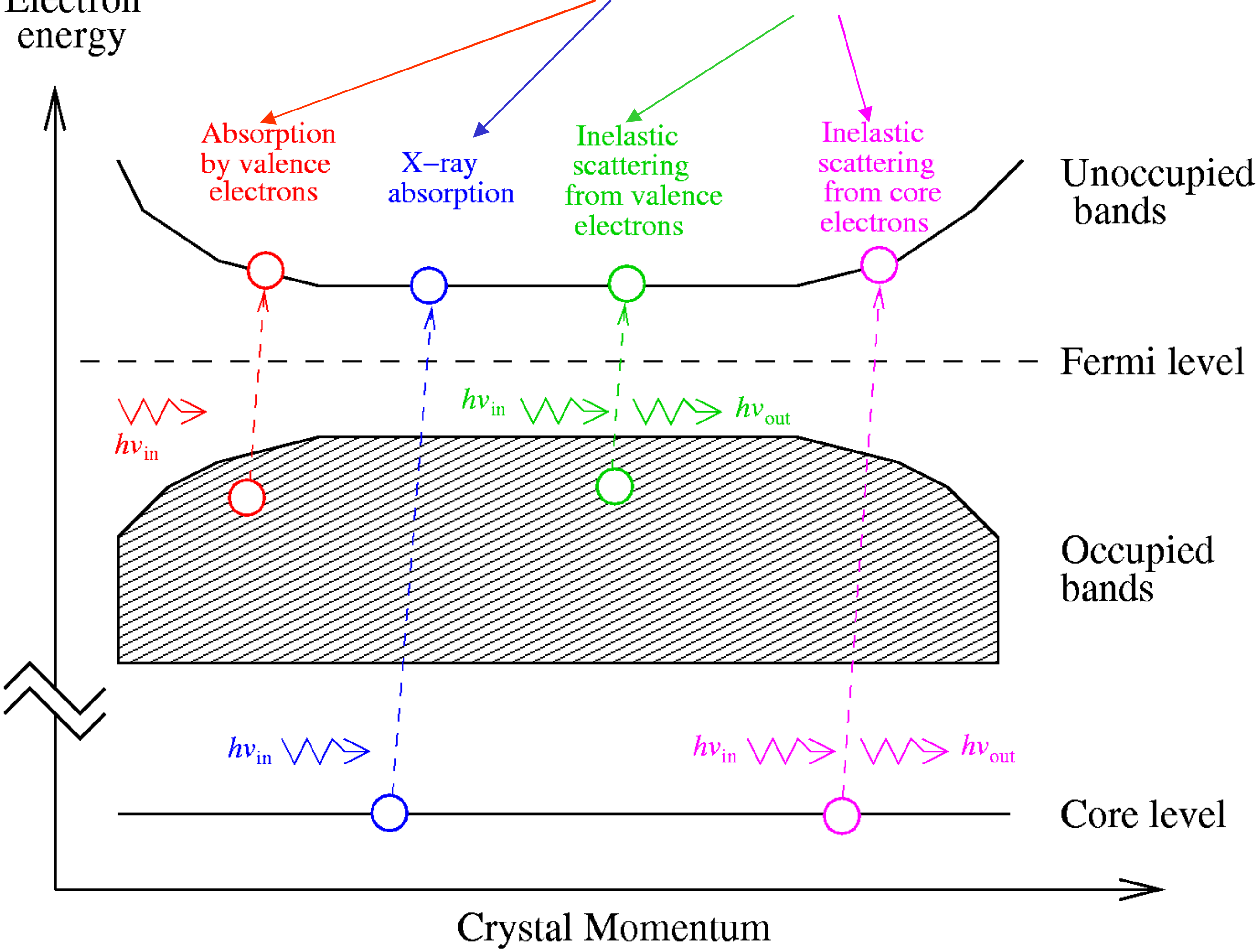
Light coupling to electronic degrees of freedom

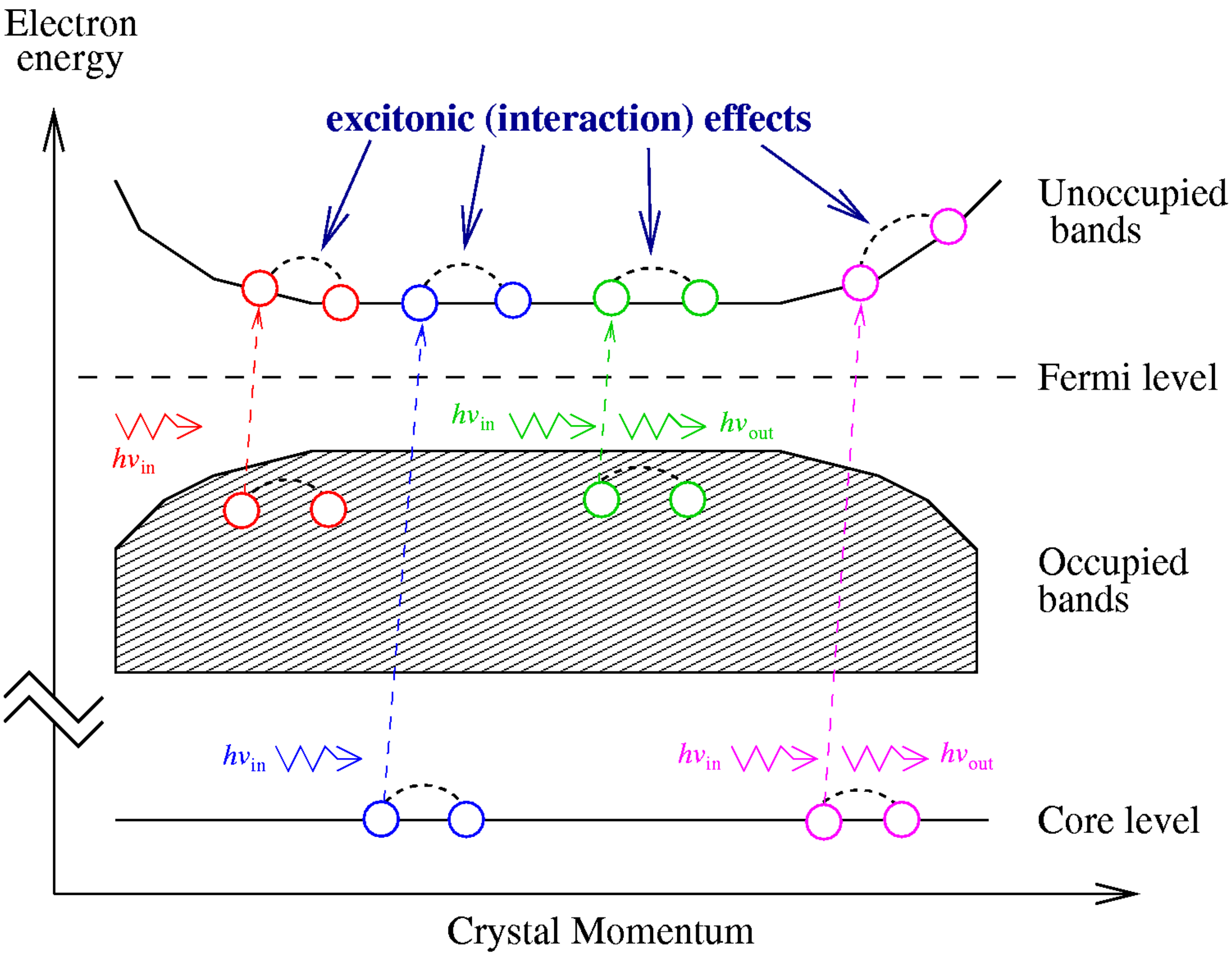
Optical electronic excitation mechanisms

$$\frac{\mathbf{p}^2}{2m} \rightarrow \frac{(\mathbf{p}+e\mathbf{A}/c)^2}{2m} = \frac{\mathbf{p}^2}{2m} + \frac{e}{mc}\mathbf{p}\cdot\mathbf{A} + \left(\frac{e^2}{2mc^2}\right)\mathbf{A}\cdot\mathbf{A}$$



Why are electronic excitations so hard to model?

Electron-hole interaction or excitonic effects in excited state



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Connection between optical excitations and optical constants, which depend on wave-vector **q** and angular frequency ω:

dielectric constant

$$\varepsilon = \varepsilon_1 + \mathrm{i}\varepsilon_2 = (n + \mathrm{i}k)^2$$

$$\varepsilon_1 = n^2 - k^2$$

$$\varepsilon_2 = 2nk$$

index of refraction

index of absorption

$$\mathbf{D} = \varepsilon \cdot \mathbf{E} = \mathbf{E} + 4\pi\mathbf{P} \text{ (atomic units)}$$

E = *total* electric field
D = electric displacement
P = polarization of material

$$\mathbf{P} = \mathbf{P}_{\mathrm{ion}} + \mathbf{P}_{\mathrm{val}} + \mathbf{P}_{\mathrm{core}}$$

$\mathbf{P}_{\mathrm{val}}$, $\mathbf{P}_{\mathrm{core}}$ = polarization because of val./core el.

$$\mathbf{P}_{\mathrm{ion}} = \sum_{i=\mathrm{ion}} \mathbf{Z}_i^* \cdot \delta\mathbf{R}_i$$

(Born effective charge tensor **Z***
times displacement $\delta\mathbf{R}$)

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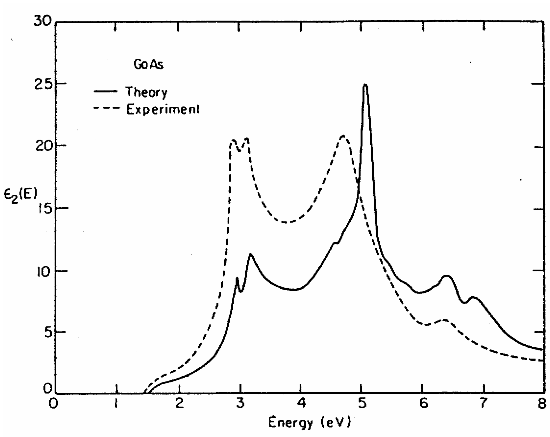
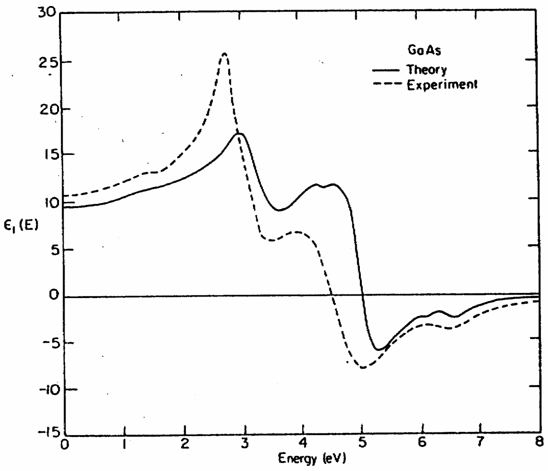
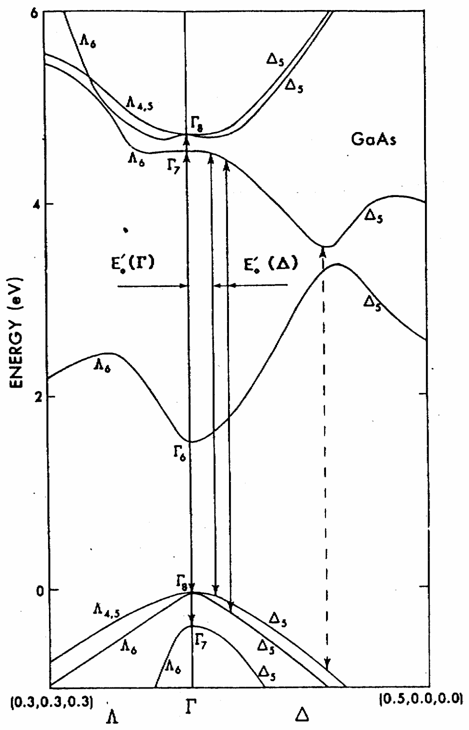
Example: empirical pseudopotential method

- * Non-interacting model
- * Optical absorption by electron inter-band transitions
- * Atomic pseudopotentials adjusted to match observed spectral features

Samples of work by Marvin Cohen group (UCBerkeley):







Modeling excitation spectra

(Standard time-dependent perturbation theory)

H = Normal Hamiltonian

$\hat{O}$ = perturbation

ω = excitation frequency

$|I\rangle, E_I$ = initial state

$|F\rangle, E_F$ = final state

A = prefactor

Fermi's Golden Rule:

For

$$H' = H + \hat{O}\exp(-\mathrm{i}\omega t) + \text{h.c.},$$

have

$$S(\omega) = A\sum_F \left|\langle F|\hat{O}|I\rangle\right|^2 \delta(E_I + \omega - E_F)$$

$$= -\frac{A}{\pi}\mathrm{Im}\left\{\langle I|\hat{O}^+ \frac{1}{E_I + \omega - H + \mathrm{i}\eta}\hat{O}|I\rangle\right\}$$

We use the Haydock recursion method,
which expresses final **expectation value**
as a continued fraction that depends on ω.

Haydock recursion method (a.k.a. Lánczos method):

Introduce normalized vector,

$$|v_0\rangle = (\langle I|\hat{O}^{+}\hat{O}|I\rangle)^{-1/2}\hat{O}|I\rangle \quad \rightarrow \quad \langle v_0|v_0\rangle = 1$$

Establish seq. of vectors, $\{|v_i\rangle\}$ in which $H=H^{\dagger}$ is tri-diagonal,

$$\begin{array}{lclclclcl}
H|v_0\rangle & = & a_0|v_0\rangle & + & b_1|v_1\rangle & & & & \\
H|v_1\rangle & = & b_1|v_0\rangle & + & a_1|v_1\rangle & + & b_2|v_2\rangle & & \\
H|v_2\rangle & = & & & b_2|v_1\rangle & + & a_2|v_2\rangle & + & b_3|v_3\rangle \\
 & \vdots & & & & & & &
\end{array}$$

NOTE:

Don’t need to **solve** *H*. Just need to **act** with *H*. Use structure of *H* to speed this up.

And deduce spectrum **(quickly!)** from linear algebra...

$$\begin{aligned}
S(\omega) &= -\pi^{-1} A\,\mathrm{Im}\langle I|\hat{O}^{+}(E_I+\omega-H+\mathrm{i}\eta)^{-1}\hat{O}|I\rangle \\
&= -\pi^{-1} A\langle I|\hat{O}^{+}\hat{O}|I\rangle\,\mathrm{Im}\langle v_0|(E_I+\omega-H+\mathrm{i}\eta)^{-1}|v_0\rangle \\
&= -\pi^{-1} A\langle I|\hat{O}^{+}\hat{O}|I\rangle\,\mathrm{Im}\underbrace{\{E_I+\omega-a_0+\mathrm{i}\eta-b_1^2/[E_I+\omega-a_1+\mathrm{i}\eta-b_2^2/(\ldots)]\}^{-1}}_{\text{continued fraction}}
\end{aligned}$$

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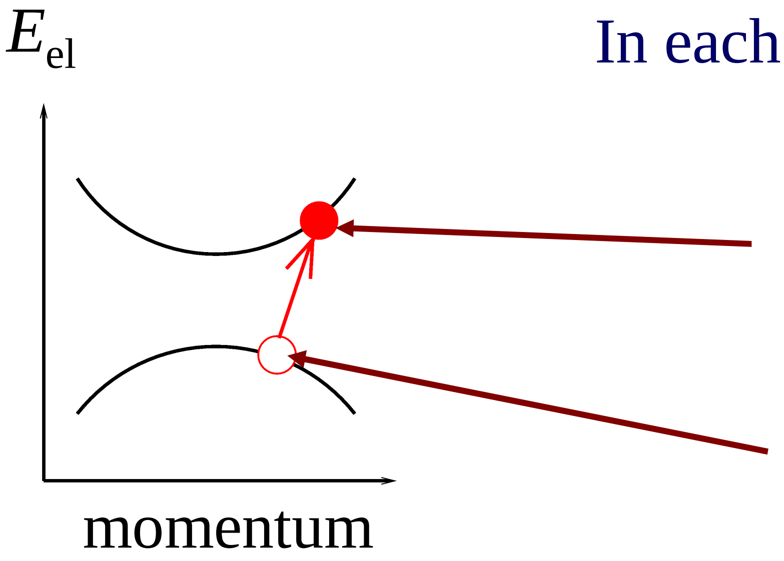
Incorporation of electron-hole interaction:

Excited state = linear superposition of all states produced by a single electron excitation.

In each such electron-hole pair state,



electron in band n',
with crystal momentum $\mathbf{k}+\mathbf{q}$.

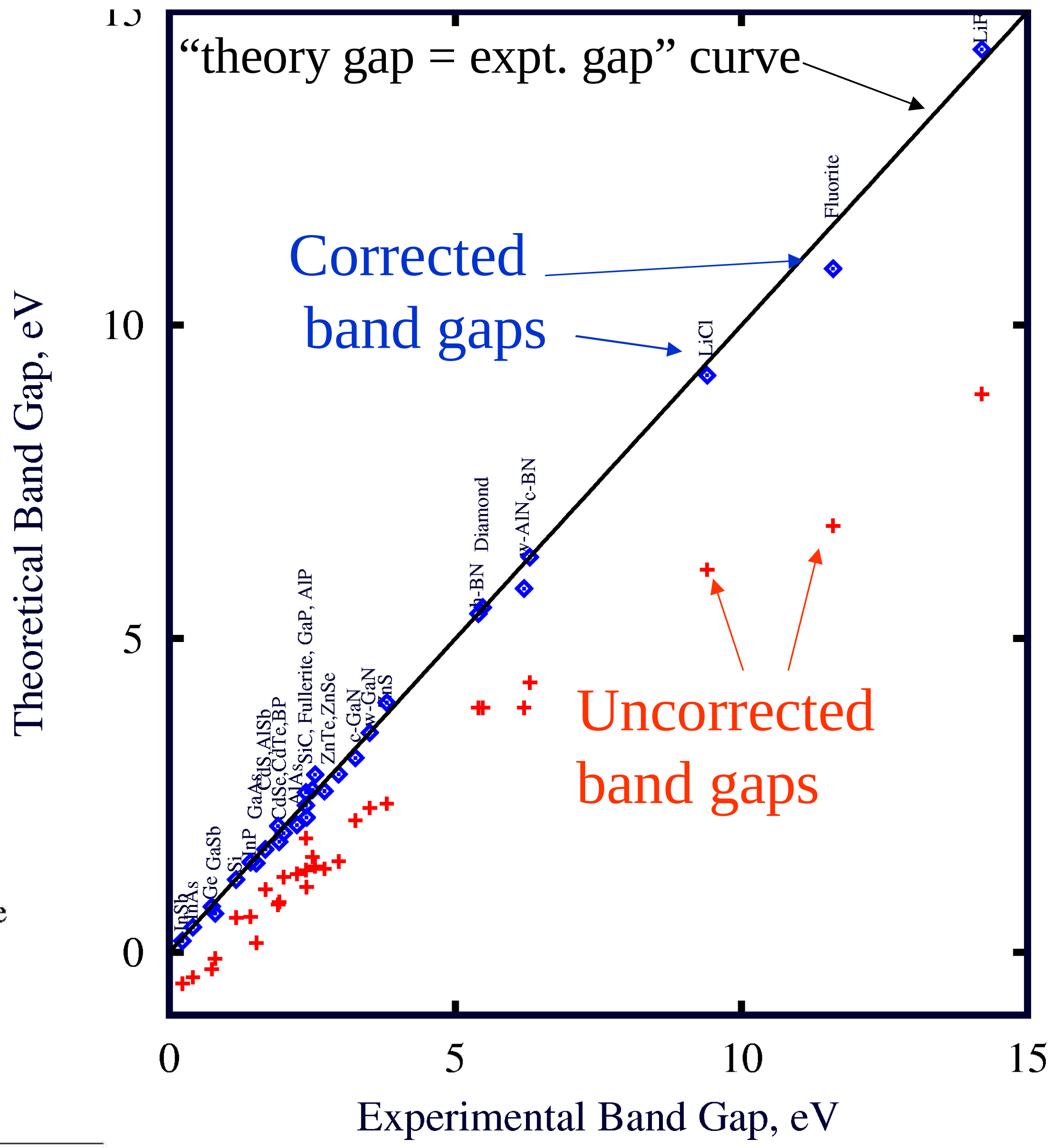
hole in [band/core-level] n,
with crystal momentum $\mathbf{k}$,

Call such a state $|n\ n'\ \mathbf{k}(\mathbf{q})\rangle$, total crystal momentum $\mathbf{q}$.

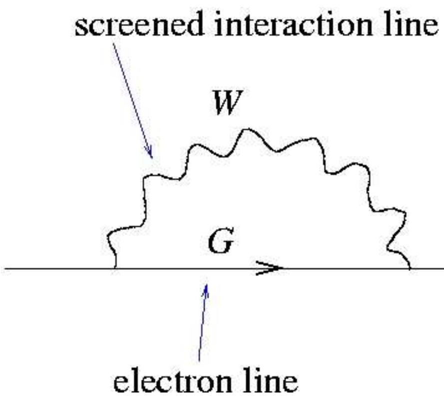
Predictive electron band theory:

Needs:

- * accurate band structure methods (Schrödinger equation in solids)
- * many-body corrections to band energies



GW self-energy of Hedin:



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Bethe-Salpeter equation, motivation:

In a non-interacting picture, one has

$$H\,|n\,n'\,\mathbf{k}(\mathbf{q})\rangle = [\,E_{\mathrm{el}}(\,n',\,\mathbf{k}+\mathbf{q}) - E_{\mathrm{el}}\,(\,n,\,\mathbf{k})\,]\,|n\,n'\,\mathbf{k}(\mathbf{q})\rangle.$$

Thus, the states $\{|n\,n'\,\mathbf{k}(\mathbf{q})\rangle\}$ diagonalize the Hamiltonian, H.

In an interacting picture, one has

$$H\,|n\,n'\,\mathbf{k}(\mathbf{q})\rangle = [\,E_{\mathrm{el}}(\,n',\,\mathbf{k}+\mathbf{q}) - E_{\mathrm{el}}\,(\,n,\,\mathbf{k})\,]\,|n\,n'\,\mathbf{k}(\mathbf{q})\rangle + \Sigma_{\,n''n'''\mathbf{k}'}\,V(n''n'''\mathbf{k}',\,nn'\mathbf{k})\,|n''n'''\,\mathbf{k}'(\mathbf{q})\rangle,$$

and the different states are coupled. Stationary states that diagonalize H are linear combinations of many electron-hole pair states.

Resulting *coupled, electron-hole-pair Schrödinger equation* (“Bethe-Salpeter” equation): difficult to solve, especially within a realistic treatment of a solid.

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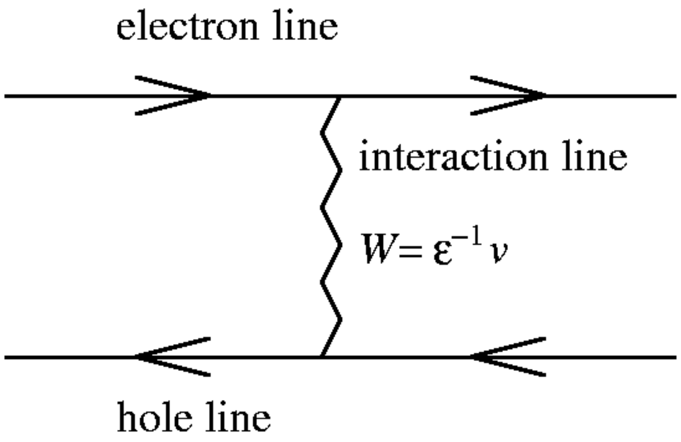
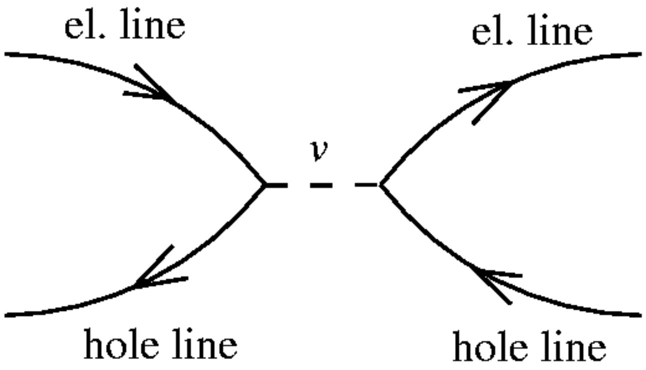
Interaction effects:

Electron-hole interaction matrix-element:





Attractive "direct part" of interaction: screened Coulomb attraction. Gives excitons, shifts spectral weight.

Repulsive "exchange part" of interaction: leads to plasmons.

Not included in a realistic framework until 1998.

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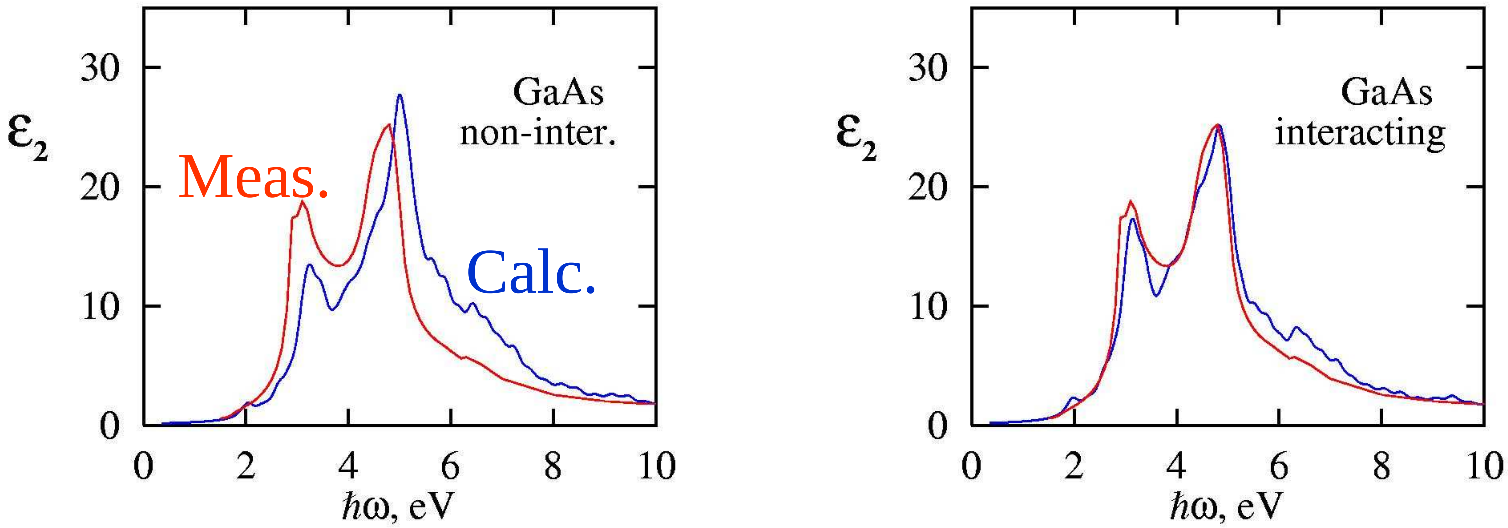
Improved results:

Incorporating effects of the electron-hole interaction in realistic calculations was made feasible and efficient through use of a wide variety of numerical & computational innovations.

The outcome (e.g., GaAs):



Besides affecting absorption spectra, index dispersion is greatly improved, especially in wide-gap materials.

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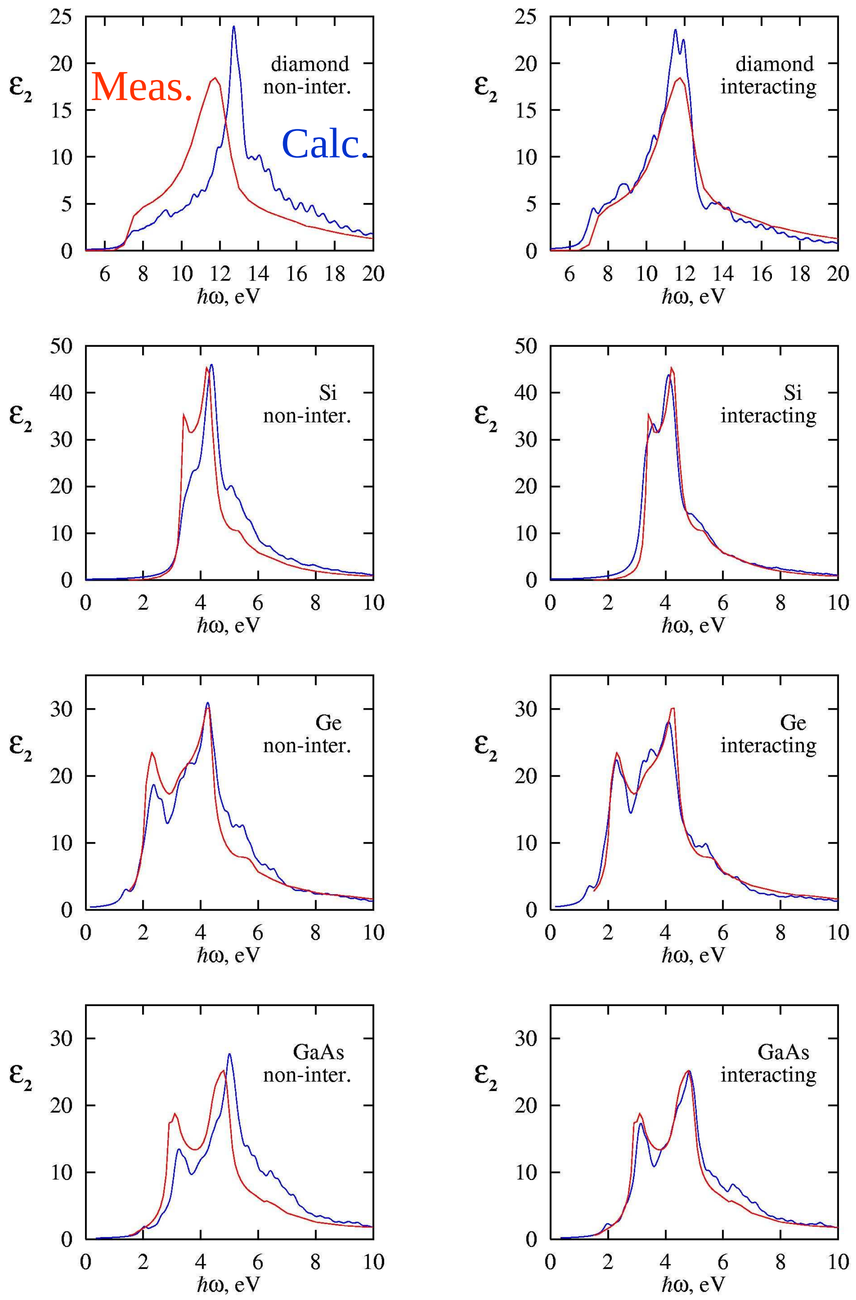
Consistently better results results when incorporating electron-hole interaction effects.



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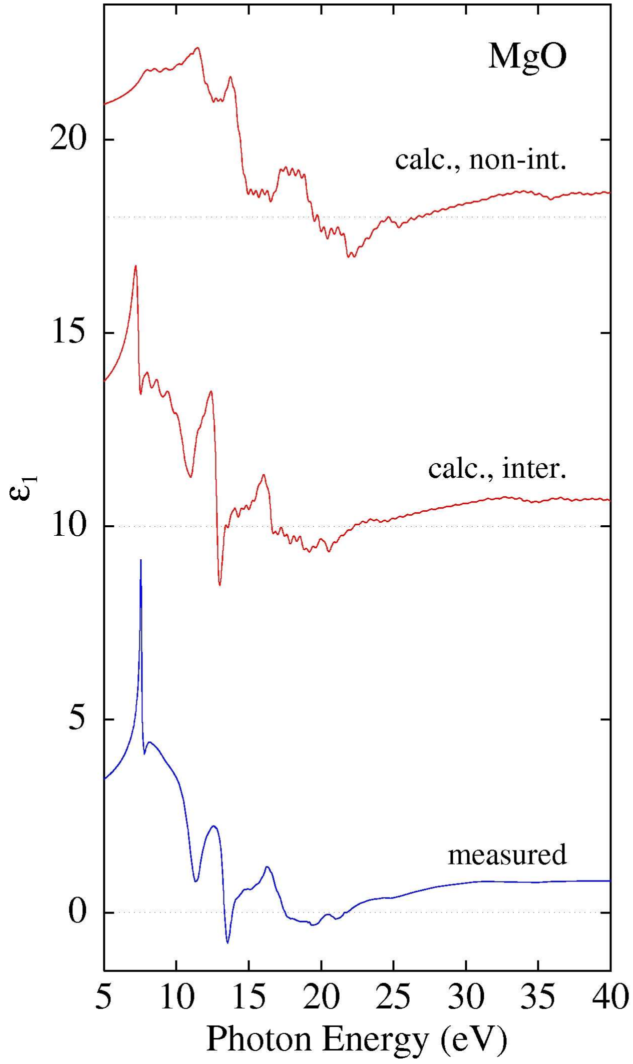
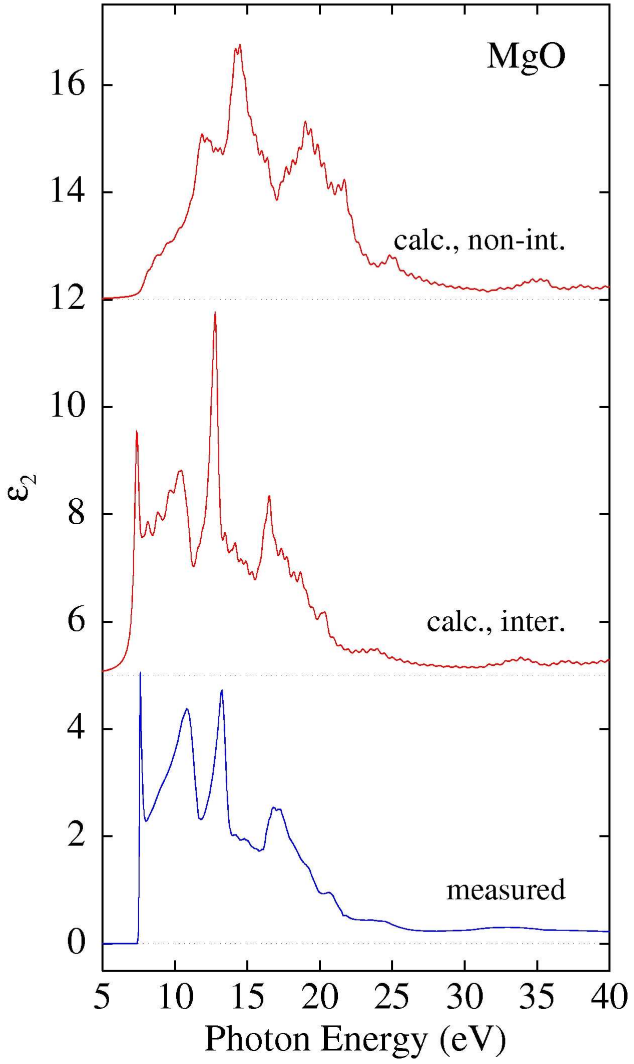
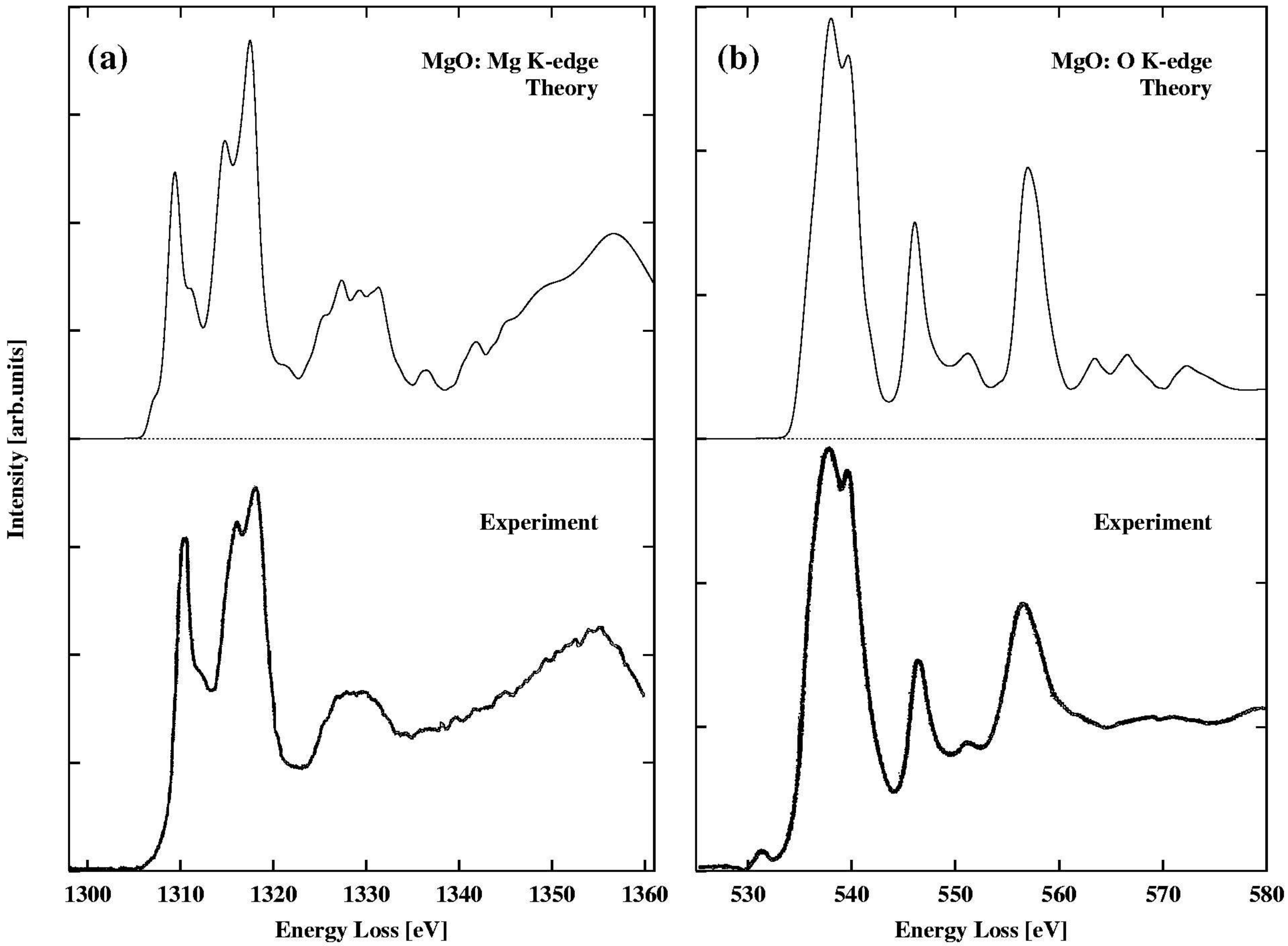
MgO optical constants:





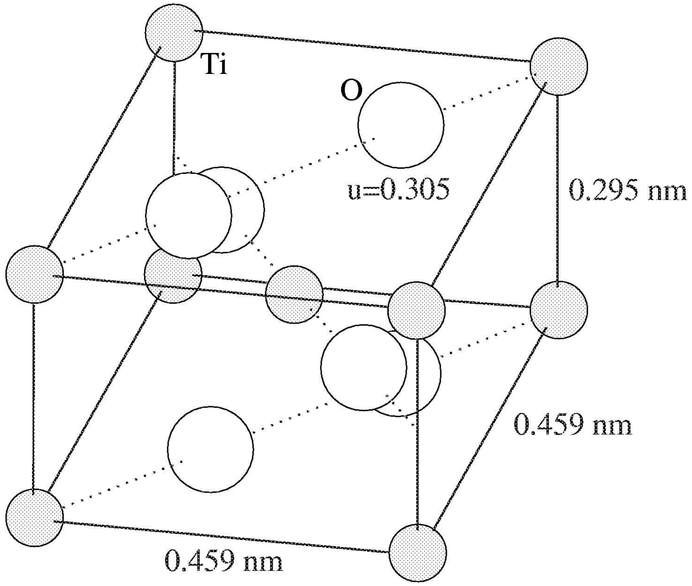
Core excitations in MgO

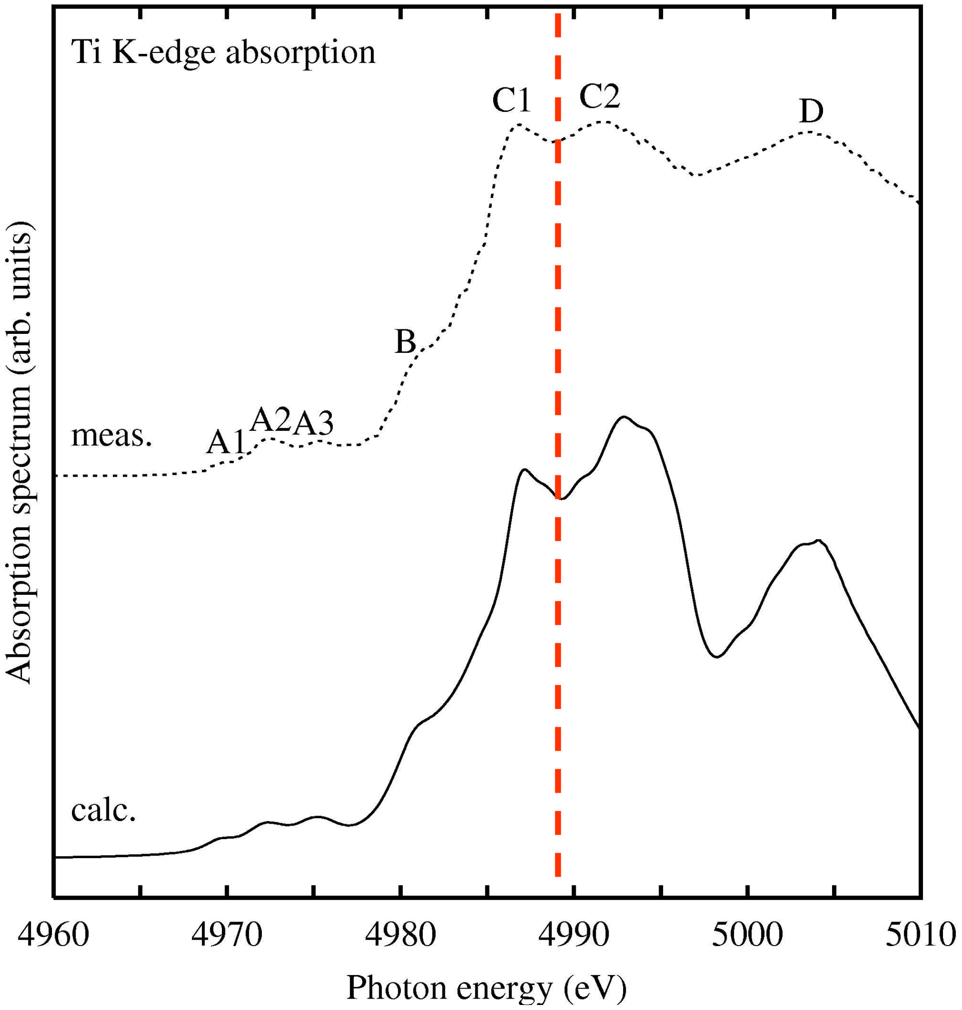
Excitation of magnesium & oxygen 1s electrons



Expt data from Lindner et al., 1986

Quadrupole (and dipole) core-excitation spectra:
Pre-edge and near-edge excitations in rutile TiO_2





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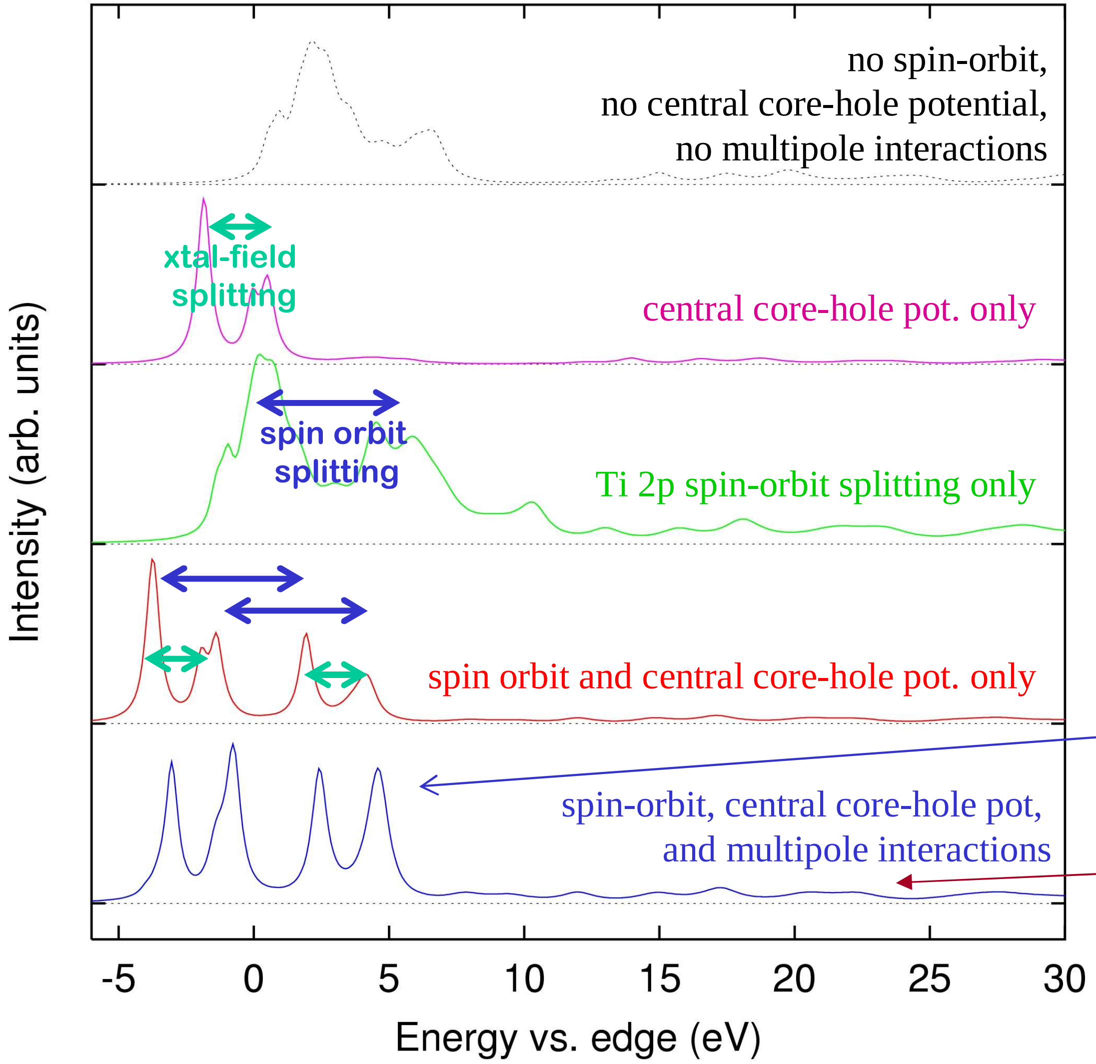
Multiplet effects in 3d $L_{2,3}$ oxide spectra: Ti $L_{2,3}$ in SrTiO$_3$

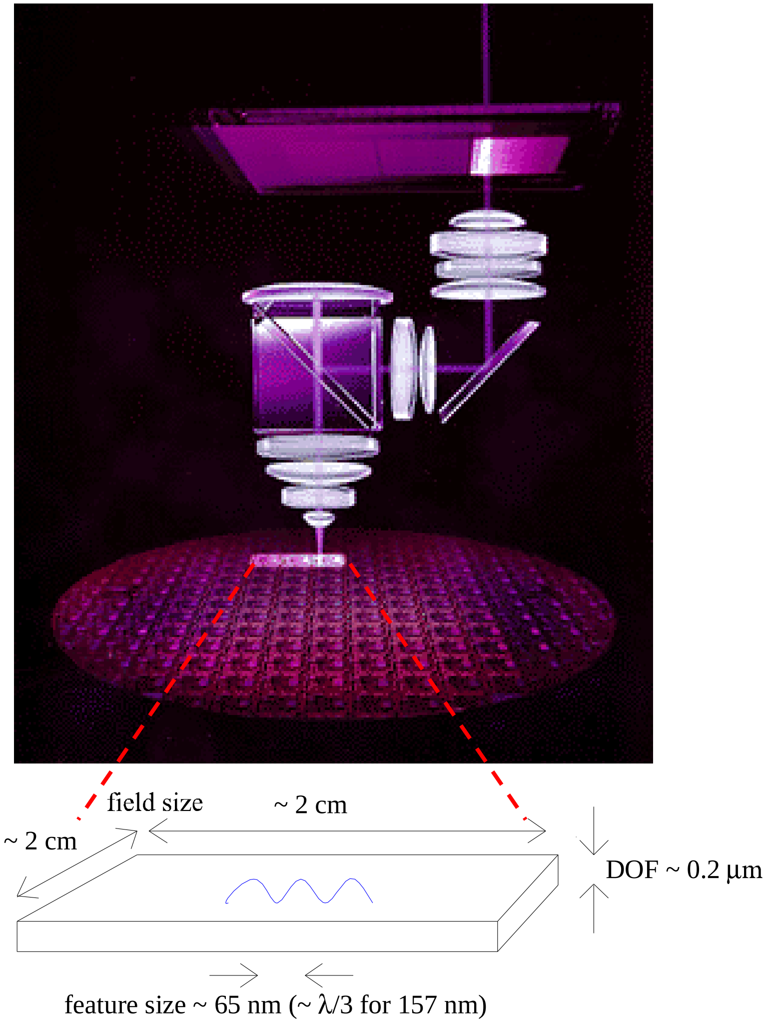
Bethe-Salpeter result:



banding-induced width included naturally

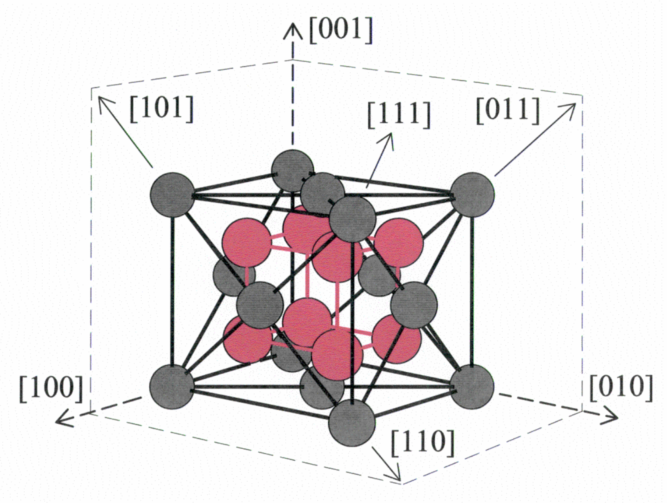
higher-lying spectral features

157 nm Lithography Index Specifications



To obtain resolution ~ 65nm (~ λ/3):
phase retardance for all rays d λ/8
⇒ index variation ~ 1×10^{-7}

CaF_2 cubic crystal
(fluorite crystal structure)



⇒ isotropic optical properties?

Material problems extrinsic

- **index inhomogeneity**
- **stress-induced birefringence**

May 2001 announced an intrinsic birefringence and index anisotropy
~11×10^{-7} over $10 \times$ specs.
Cannot be reduced!

Spatial-Dispersion-Induced Birefringence

Origin of effect:

Finite wave vector of light, **q**, breaks symmetry of light-matter interaction.

History:

H.A Lorentz (Lorentz contraction) considered this small symmetry-breaking effect in "regular crystals" in 1879,

PRIOR to verified existence crystal lattices! (Laue 1912, Bragg 1913)

Worked out simple theory by 1921 - measured in NaCl?

H.A. Lorentz, "Double Refraction by Regular Crystals," *Proc. Acad. Amsterdam.* **24**, 333 (1921).

First convincingly demonstrated by Pastrnak and Vedam in Si (1971).

J. Pastrnak and K. Vedam, "Optical Anisotropy of Silicon Single Crystals," Phys. Rev. B **3**, 2567 (1971).

Confirmed, extended by others, esp. Cardona & colleagues – academic curiosity

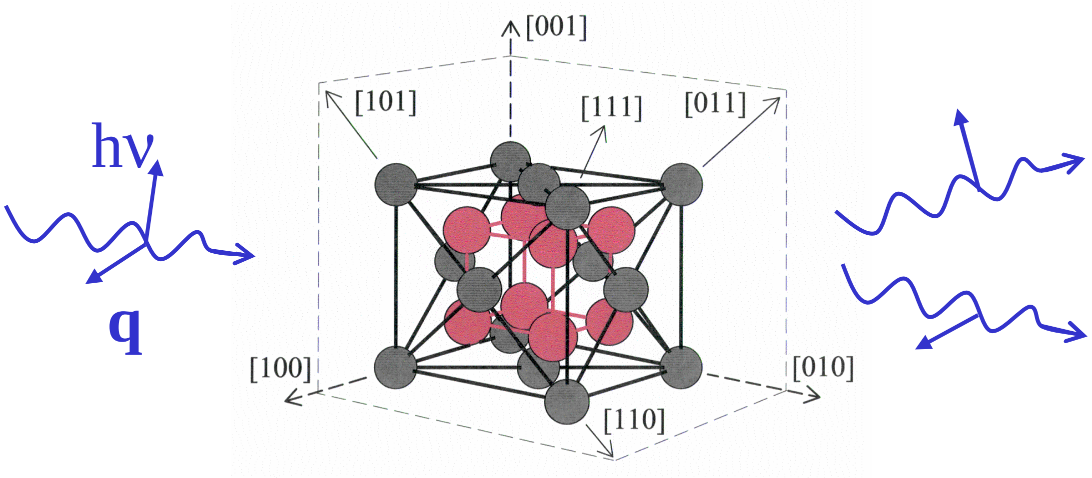
Values "too" small to have implications for optics – Optics industry oblivious!

We measured in CaF_2, material for precision UV optics for 193 nm and 157 nm lithography, and worked out the implications for optics - alerted industry.

J.H. Burnett, Z.H. Levine, E.L. Shirley, "Intrinsic birefringence in calcium fluoride and barium fluoride," Phys. Rev. B **64**, 241102 (2001).

Wave Vector Dependence of the Index in Cubic Crystals

spatial-dispersion-induced birefringence



Symmetry arguments “prove” natural birefringence forbidden in cubic crystals

Isotropy “~~proof~~” assumes **D** linearly related to **E** by 2nd-rank tensor indept. of **q**

$E_i = \Sigma_j \varepsilon^{-1}{}_{ij} D_j$ ($\varepsilon^{-1}{}_{ij}$ inverse dielectric constant) - but assumes λ large!

Actually $\mathbf{D} = \mathbf{D}_0 e^{\,i\mathbf{q}\cdot\mathbf{r}} = \mathbf{D}_0(1 + i\mathbf{q}\cdot\mathbf{r} - (\mathbf{q}\cdot\mathbf{r})^2/2 + \cdots)$ $(q = 2\pi n/\lambda)$

Cannot neglect $(\mathbf{q}\cdot\mathbf{r})$ terms if $(a_{\text{unit cell}}/\lambda) \sim 1$ or equivalently $(q/K_{\text{reciprocal lattice}}) \sim 1$

Perturbation due to $(\mathbf{q}\cdot\mathbf{r})$ terms: azimuthal symmetry about **q**

For crystal axes w/ 3-fold or 4-fold symmetry $(\mathbf{q}\cdot\mathbf{r})$ reduces isotropic to uniaxial

⇒ NO birefringence for **q** || <111> or **q** || <001>

Theory of Intrinsic Birefringence

$$\varepsilon^{-1}{}_{ij}(\mathbf{q},\omega)=\varepsilon^{-1}(0,\omega)\delta_{ij}+\cancelto{0}{\sum\nolimits_k\gamma_{ijk}(\omega)q_k}+\sum\nolimits_{kl}\alpha_{ijkl}(\omega)q_kq_l \quad (\quad \alpha_{ijkl}\ \text{respects cubic symmetry})$$

Cubic crystals (classes $\bar{4}3m, 432, m3m$) symmetry ⇒ α_{ijkl} has 3 indep. comp. $\alpha_{11},\alpha_{12},\alpha_{44}$

$$\alpha_{ij}=\begin{pmatrix}\alpha_{11}&\alpha_{12}&\alpha_{12}&0&0&0\\ \alpha_{12}&\alpha_{11}&\alpha_{12}&0&0&0\\ \alpha_{12}&\alpha_{12}&\alpha_{11}&0&0&0\\ 0&0&0&\alpha_{44}&0&0\\ 0&0&0&0&\alpha_{44}&0\\ 0&0&0&0&0&\alpha_{44}\end{pmatrix}$$

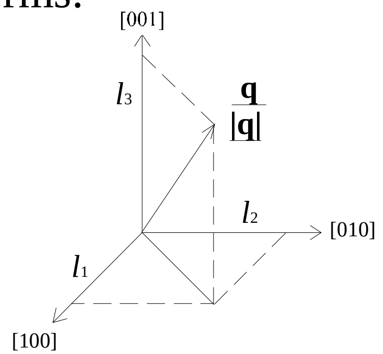
(same form as for piezo-optic tensor)

Using the 2 independent scalar invariants of a 4th rank tensor to separate terms:

$$\varepsilon^{-1}{}_{ij}(\mathbf{q},\omega)=\left[\varepsilon^{-1}(0,\omega)+\alpha_{12}q^2\right]\delta_{ij}+\alpha_{44}2q^2l_il_j+\left(\alpha_{11}-\alpha_{12}-2\alpha_{44}\right)5q^2\delta_{ij}l_i{}^2$$

$$\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}\qquad\begin{bmatrix}l_1^2&l_1l_2&l_1l_3\\ l_2l_1&l_2^2&l_2l_3\\ l_3l_1&l_3l_2&l_3^2\end{bmatrix}\qquad\begin{bmatrix}l_1^2&0&0\\0&l_2^2&0\\0&0&l_3^2\end{bmatrix}$$

isotropic longitudinal anisotropic



isotropic index shift **isotropic** L-T splitting

- induces dir. dep. birefringence
- induces dir. dep. index variation

⇒ anisotropy governed by one parameter $(\alpha_{11}-\alpha_{12}-2\alpha_{44})$

⇒ angular dependence determined by ONE measurement: **q** along <110>, meas. $n_{<110>}$- $n_{<001>}$

J.H. Burnett, Z.H. Levine, E.L. Shirley, and J.H. Bruning, "Symmetry of Intrinsic Birefringence and its Implications for CaF_2 UV Optics," J. Microlith., Microfab., Microsyst., **1**, 213 (2002).

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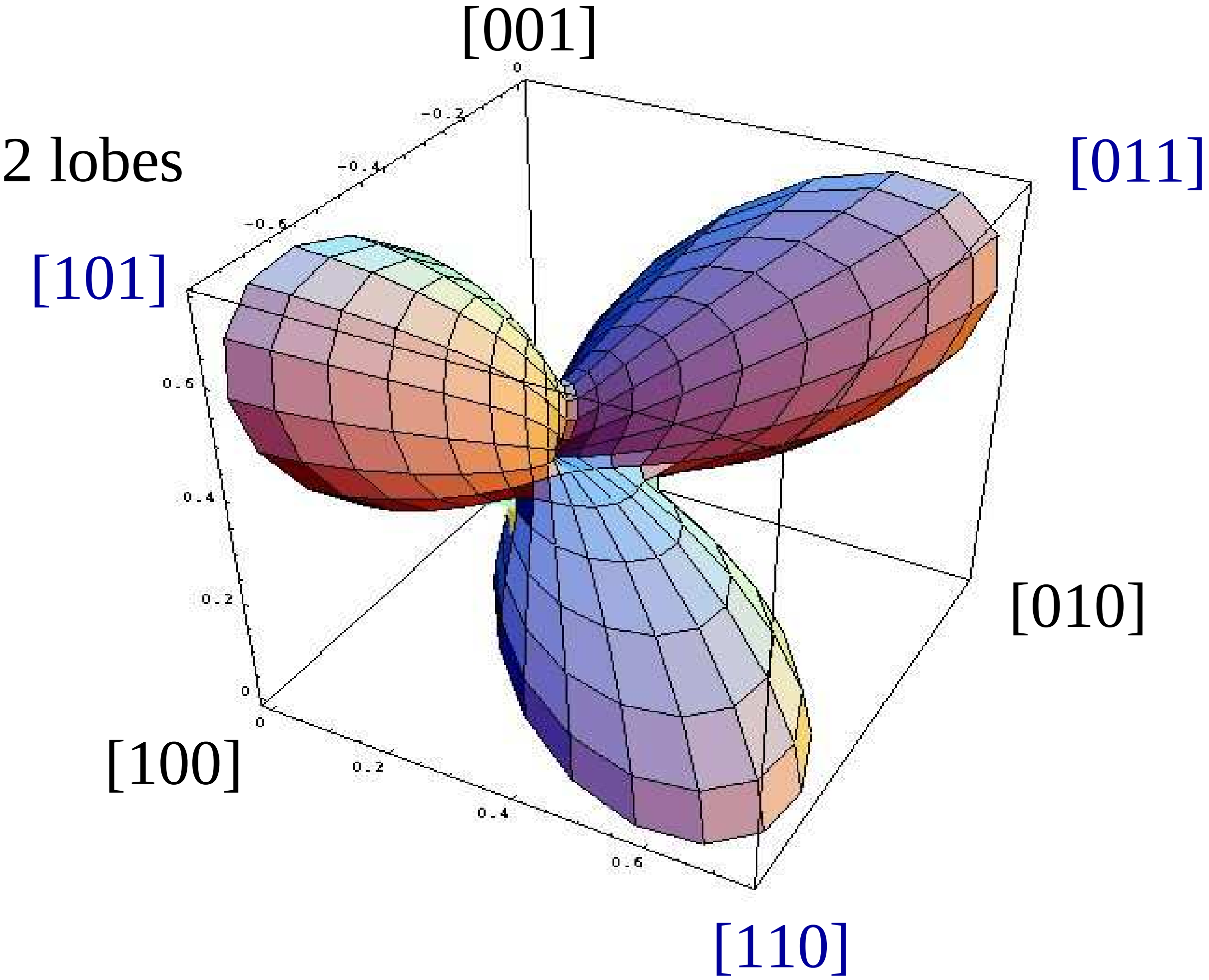
Angular Dependence of Intrinsic Birefringence

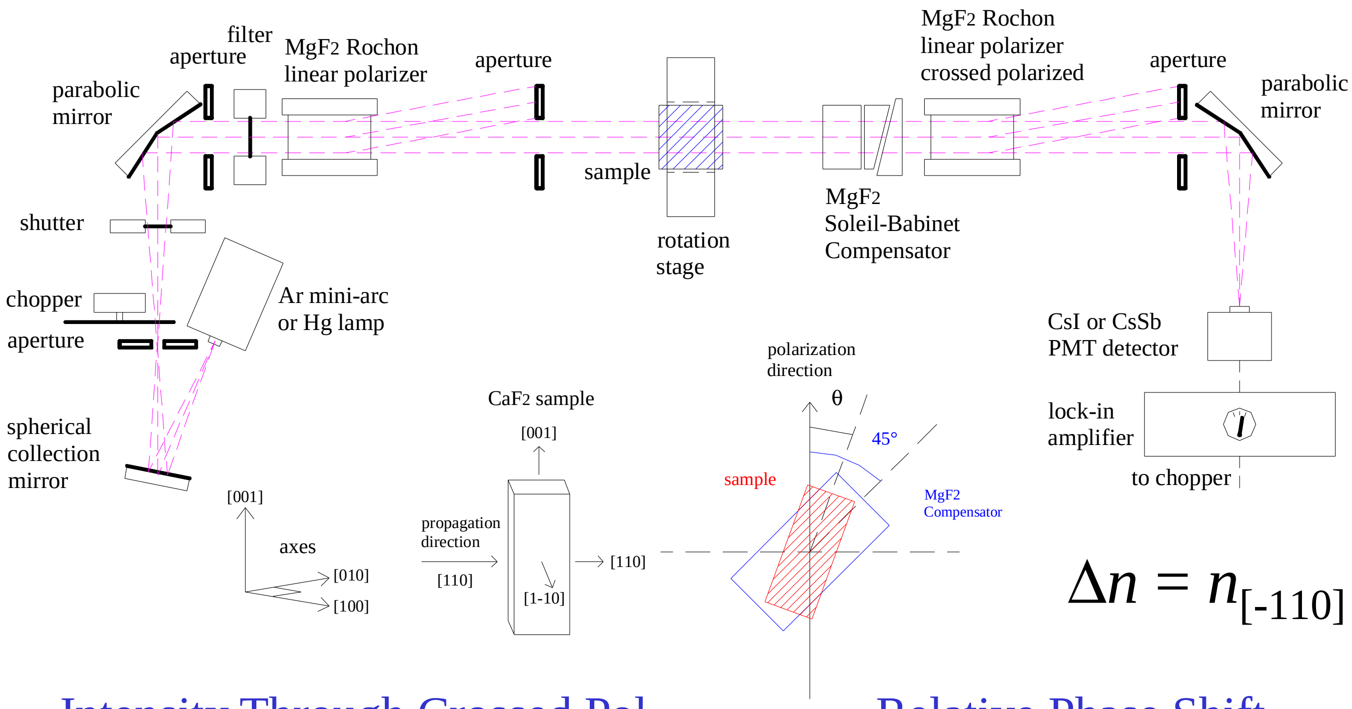
$$n(l_1,l_2,l_3)=\left[(5/2)(1-S_4)\right]\pm\left[-(5/2)\left(4S_4-4S_6+S_4{}^2-1\right)^{1/2}\right], \qquad S_n=l_1{}^n+l_2{}^n+l_3{}^n$$

One octant - scaled according to $\Delta n_{max} = 1$, for **q** || [110]

Has 12 lobes

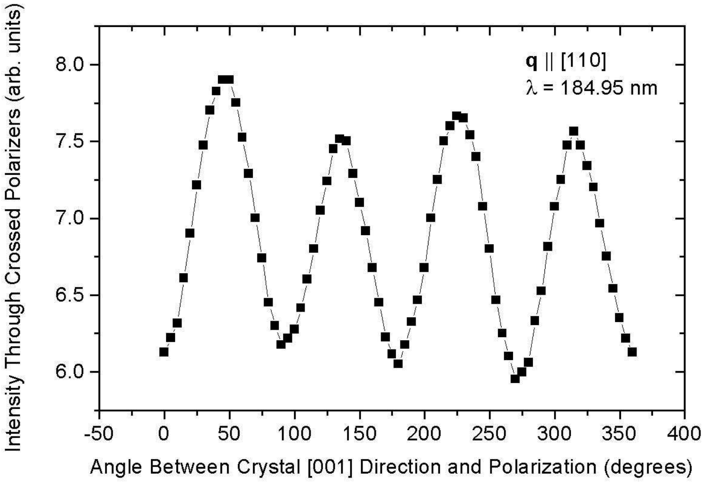


Birefringence Measurement



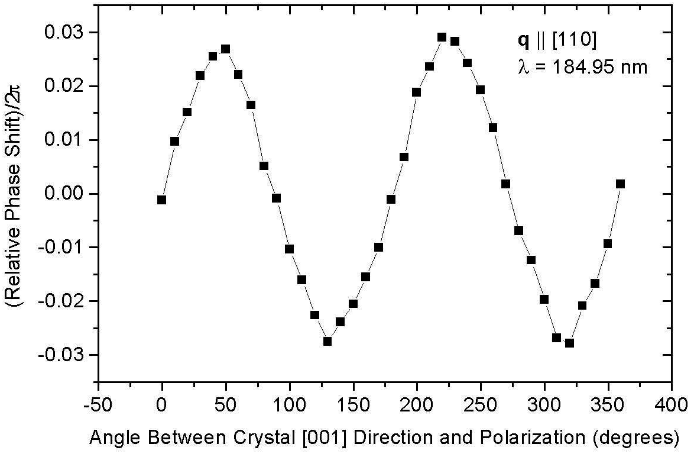
$$\Delta n = n_{[-110]} - n_{[001]}$$

Intensity Through Crossed Pol



$$I/I_0=\sin^2(\pi d\Delta n/\lambda)\sin^2(2\theta)$$

Relative Phase Shift



$$\Delta n = (\lambda/d)(\mathrm{RPS}/2\pi)$$

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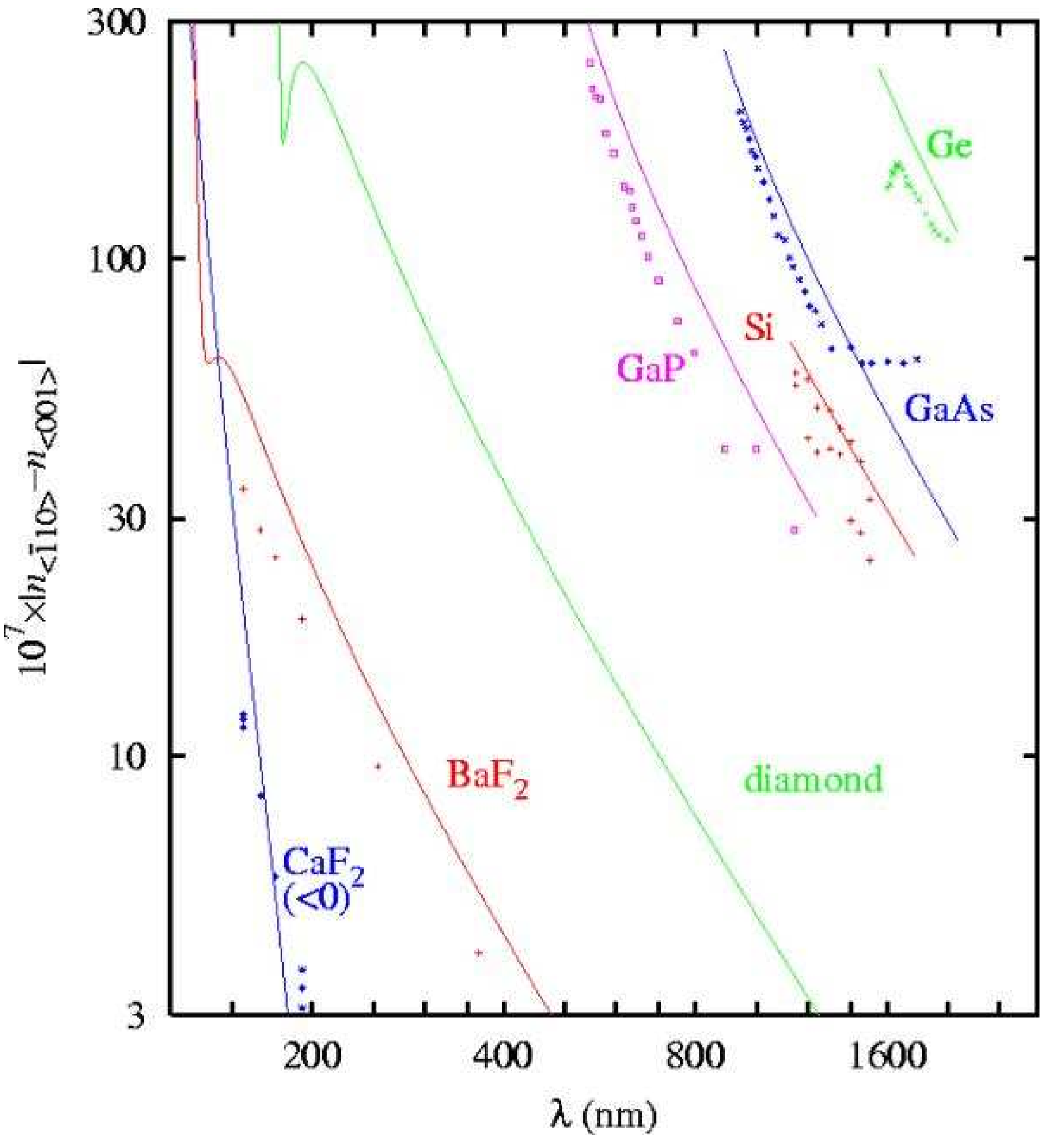
Intrinsic birefringence in CaF_2, BaF_2, diamond, and four semiconductors.

CaF_2 and BaF_2 meas. results by J.H. Burnett (NIST); semiconductor measurements found in literature as cited by Burnett *et al*.



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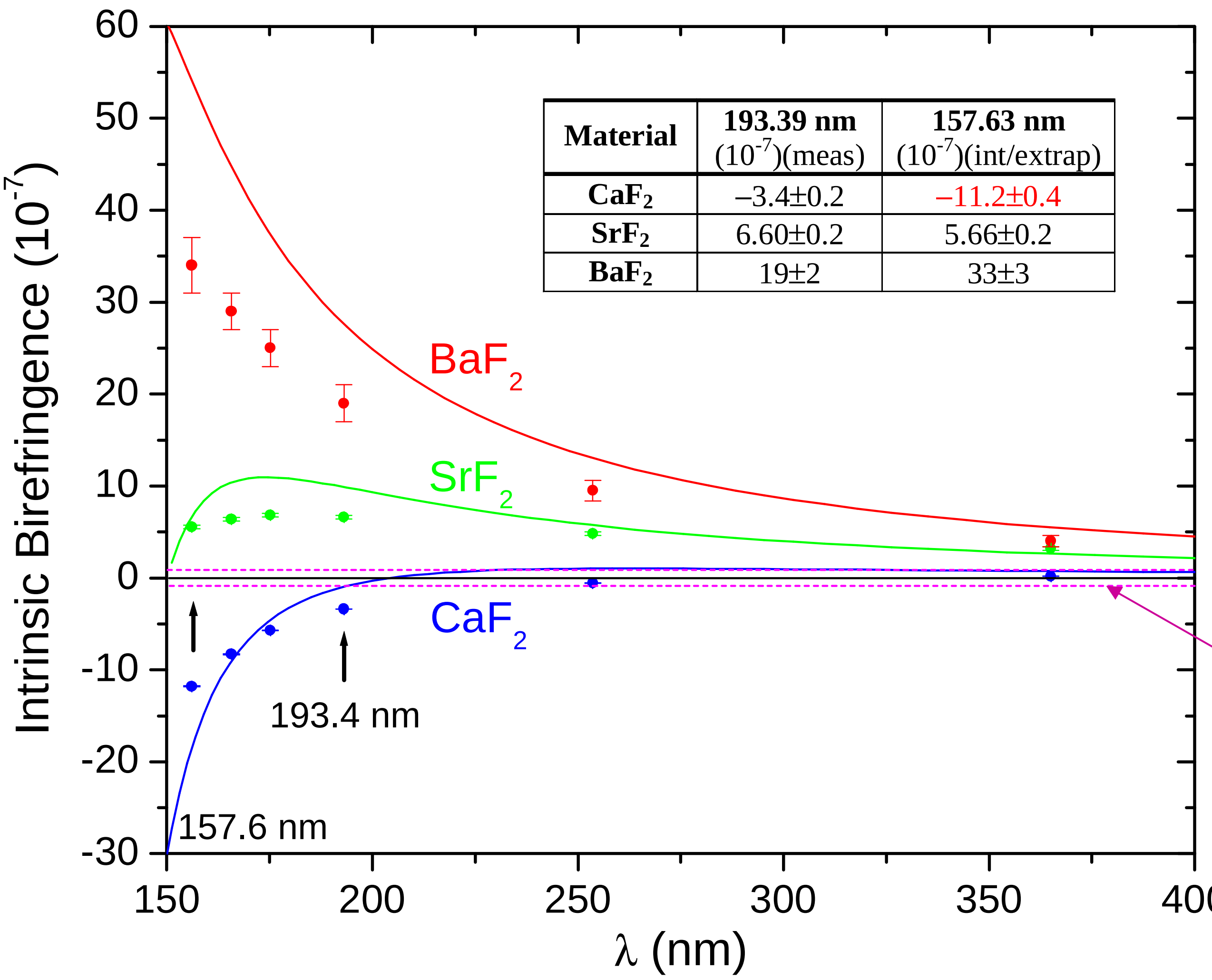
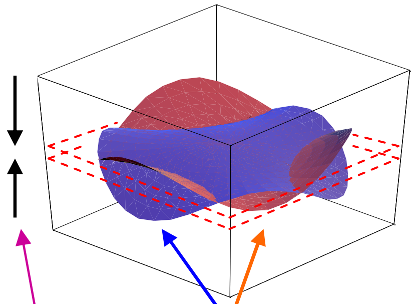
Intrinsic Birefringence of CaF_2, SrF_2, and BaF_2



Material	**193.39 nm** (10^{-7})(meas)	**157.63 nm** (10^{-7})(int/extrap)
CaF_2	–3.4±0.2	–11.2±0.4
SrF_2	6.60±0.2	5.66±0.2
BaF_2	19±2	33±3

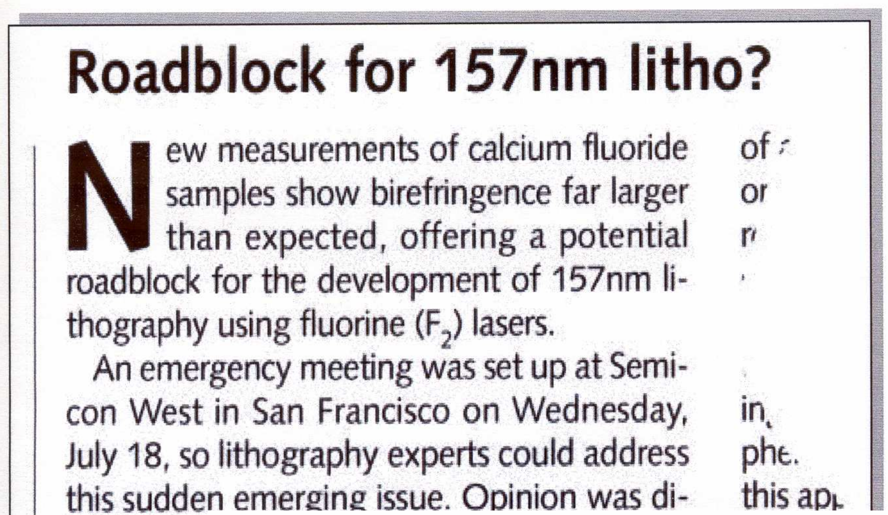


polarized
phase fronts

SEMATECH
157nm target:
1×10^{-7}=1 nm/cm

Industry Concern

WaferfabNews, July 2001



Roadblock for 157nm litho?

New measurements of calcium fluoride samples show birefringence far larger than expected, offering a potential roadblock for the development of 157nm lithography using fluorine (F_2) lasers.

An emergency meeting was set up at Semicon West in San Francisco on Wednesday, July 18, so lithography experts could address this sudden emerging issue. Opinion was divided on v

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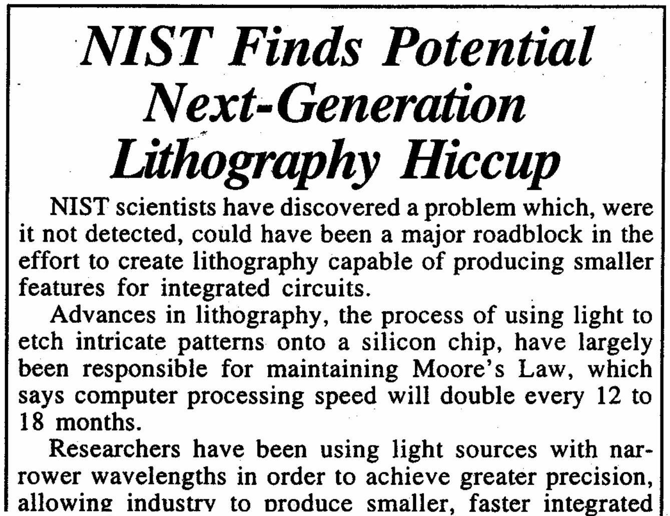
New Technology Week, July 16, 2001



NIST Finds Potential Next-Generation Lithography Hiccup

NIST scientists have discovered a problem which, were it not detected, could have been a major roadblock in the effort to create lithography capable of producing smaller features for integrated circuits.

Advances in lithography, the process of using light to etch intricate patterns onto a silicon chip, have largely been responsible for maintaining Moore's Law, which says computer processing speed will double every 12 to 18 months.

Researchers have been using light sources with narrower wavelengths in order to achieve greater precision, allowing industry to produce smaller, faster integrated

uing lithography us-
ich should result in
n the next few years.
is for lithography to
features as small as

litional glass lenses,
n wafer, start to lose
to avoid this, scien-
from cubic calcium

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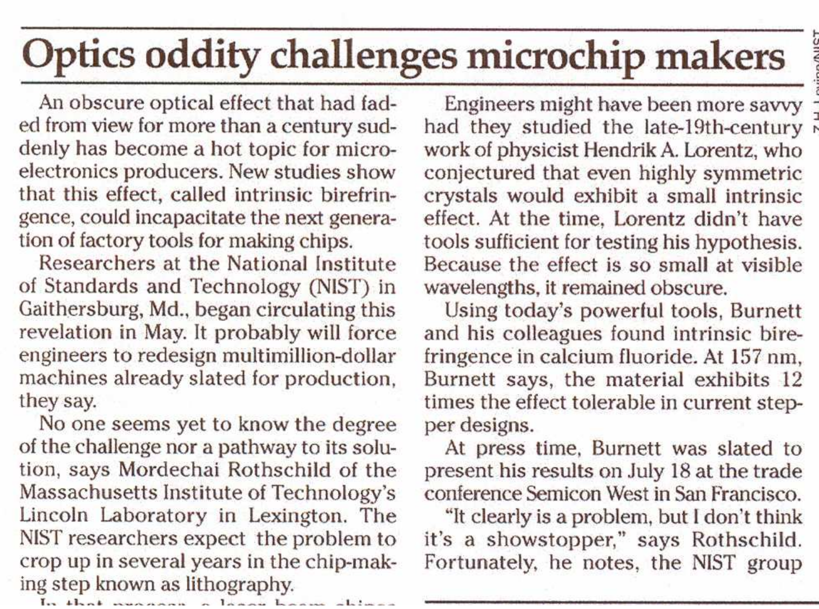


Optics oddity challenges microchip makers

An obscure optical effect that had faded from view for more than a century suddenly has become a hot topic for microelectronics producers. New studies show that this effect, called intrinsic birefringence, could incapacitate the next generation of factory tools for making chips.

Researchers at the National Institute of Standards and Technology (NIST) in Gaithersburg, Md., began circulating this revelation in May. It probably will force engineers to redesign multimillion-dollar machines already slated for production, they say.

No one seems yet to know the degree of the challenge nor a pathway to its solution, says Mordechai Rothschild of the Massachusetts Institute of Technology's Lincoln Laboratory in Lexington. The NIST researchers expect the problem to crop up in several years in the chip-making step known as lithography.

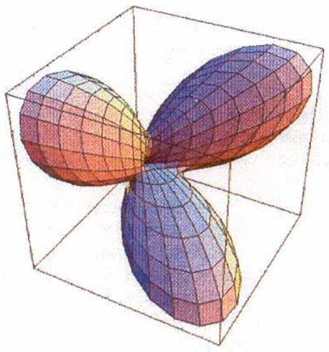
Engineers might have been more savvy had they studied the late-19th-century work of physicist Hendrik A. Lorentz, who conjectured that even highly symmetric crystals would exhibit a small intrinsic effect. At the time, Lorentz didn't have tools sufficient for testing his hypothesis. Because the effect is so small at visible wavelengths, it remained obscure.

Using today's powerful tools, Burnett and his colleagues found intrinsic birefringence in calcium fluoride. At 157 nm, Burnett says, the material exhibits 12 times the effect tolerable in current stepper designs.

At press time, Burnett was slated to present his results on July 18 at the trade conference Semicon West in San Francisco.

"It clearly is a problem, but I don't think it's a showstopper," says Rothschild. Fortunately, he notes, the NIST group found the difficulty before manufacturers actually started making and shipping the 157-nm machines.

—P. Weiss



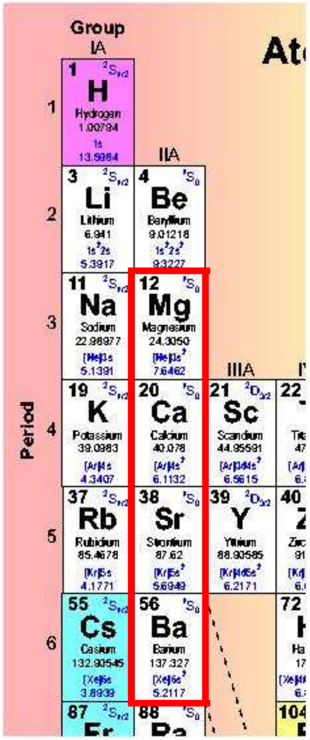
Z.H. Levine/NIST

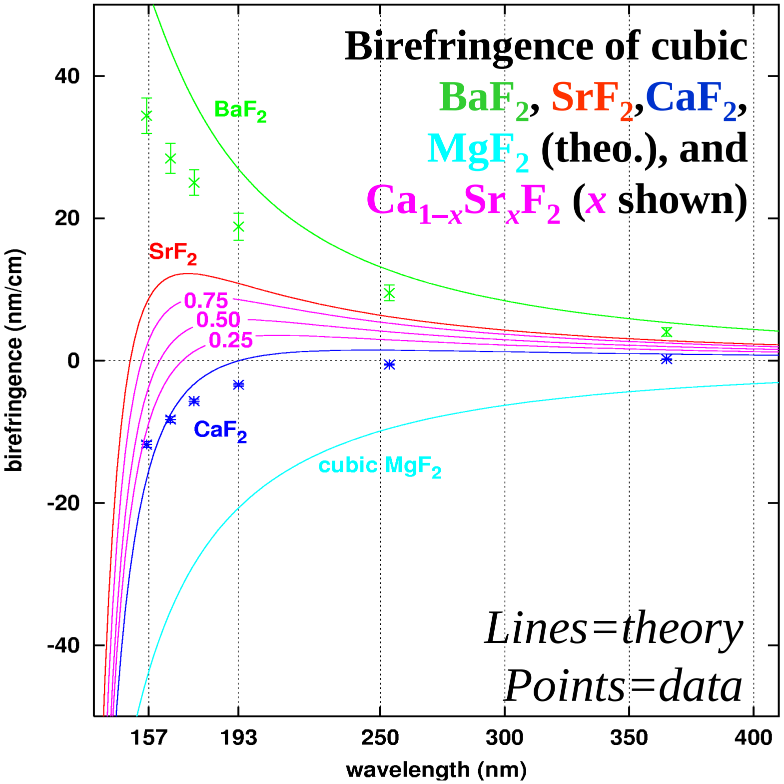
In directions of greater bulging (colored lobes), a calcium-fluoride cube more strongly exhibits a nonuniform optical effect. A crystal contains many such cubes.

Science News, July 21, 2001

Possible Alternative Solution: Mixed Crystals

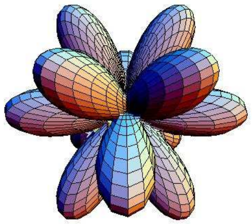
- CaF_2, SrF_2, and BaF_2 all have same fluorite crystal structure.
- Mixed crystals that retain the cubic symmetry can be made: $Ca_{1-x}Sr_xF_2$ (all x), $Sr_{1-x}Ba_xF_2$ (all x), $Ca_{1-x}Ba_xF_2$ (some x), $Sr_{1-x}Mg_xF_2$ (some x)
- SrF_2 and BaF_2 have birefringence of opposite sign compared to CaF_2 ⇒ $x \approx |\Delta n(CaF_2)/[\Delta n(CaF_2)] - \Delta n(YF_2)]|$, Y = Ba,Sr nulls birefringence
- $Ca_{0.3}Sr_{0.7}F_2$ nulls IBR at 157.9 nm, $Ca_{0.7}Sr_{0.3}F_2$ nulls IBR at 193.4 nm
- Have made $Ca_{1-x}Sr_xF_2$ for x=0.1-0.9 – characterizing now!

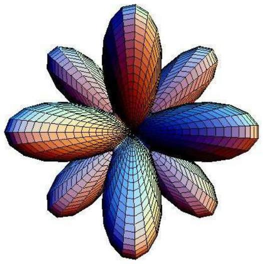


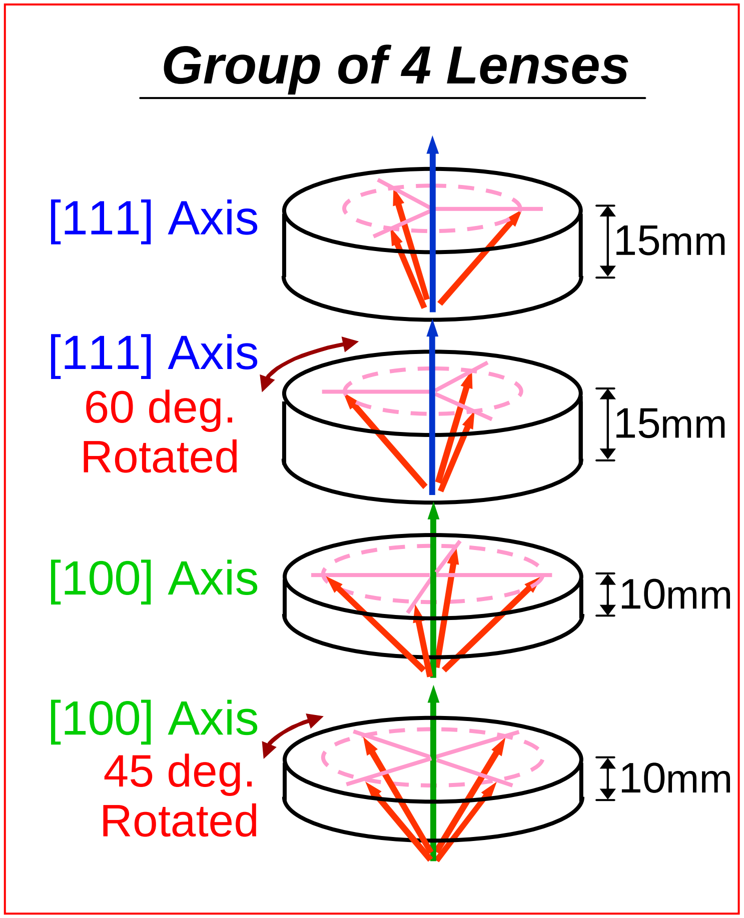


Combination of [111] Pair and [100] Pair

Simulated 2D-Distribution of Intrinsic Birefringence – Nikon Corporation







Group of 4 Lenses

[111] Axis

15mm

[111] Axis
60 deg.
Rotated

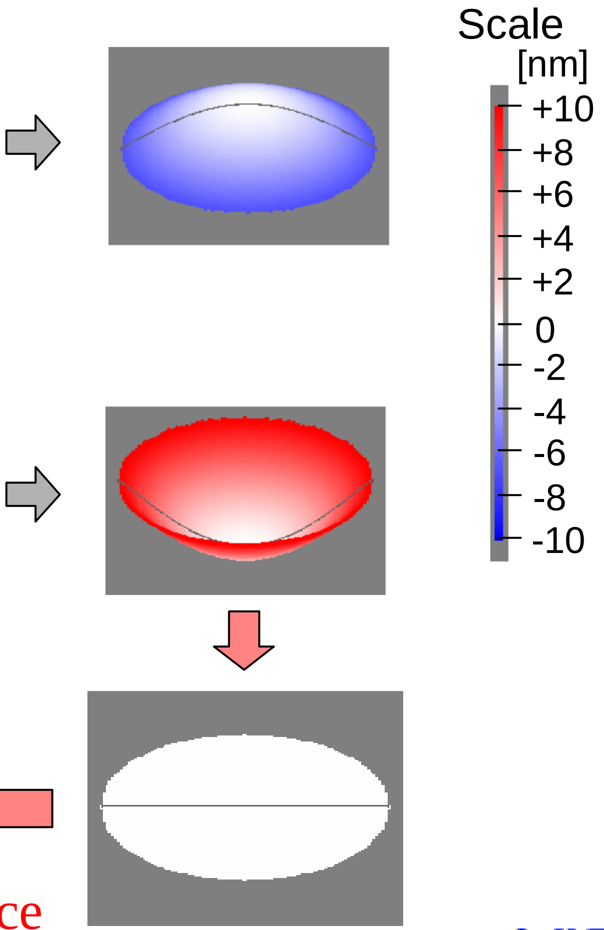
15mm

[100] Axis

10mm

[100] Axis
45 deg.
Rotated

10mm



Wave aberration is perfectly corrected.

However, must then give up “clocking” to reduce figure errors! ⇒ higher figure specs.

New Crystal Optics

conventional optics classification

isotropic

1 principal ε
cubic

uniaxial

2 principal ε's
hexagonal
tetragonal
trigonal

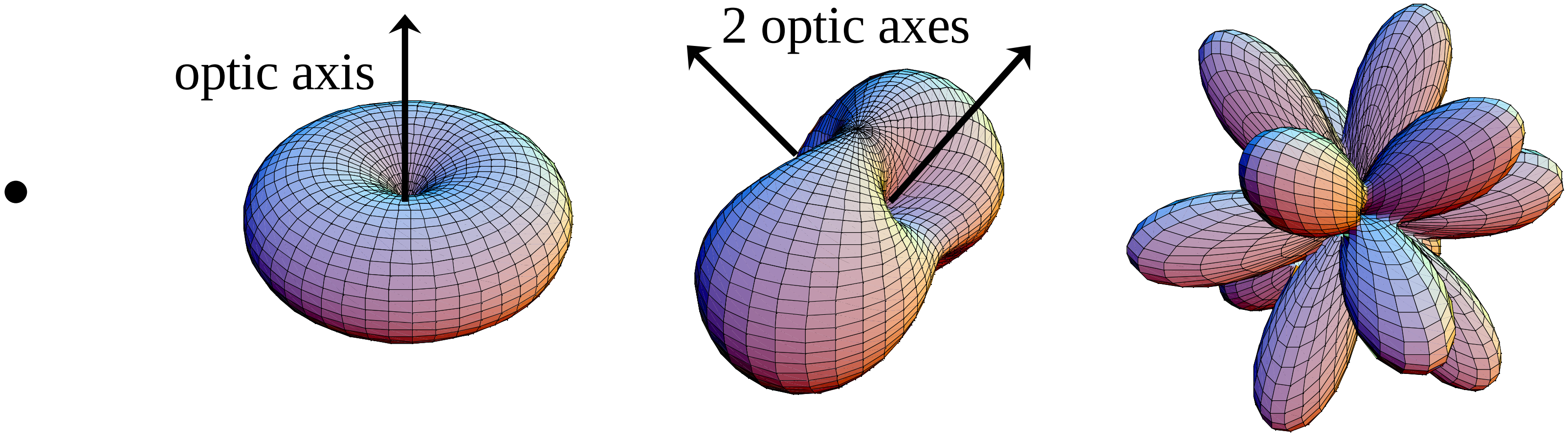
biaxial

3 principal ε's
orthorhombic
monoclinic
triclinic

with spatial dispersion

(e.g, cubic fluorite structure)

heptaxial



all prop. dir's
non-birefringent

1 prop. dir.
non-birefringent

2 prop. dir's
non-birefringent

7 prop. dir's
non-birefringent

Sensitivity of birefringence to interaction (exciton) effects:

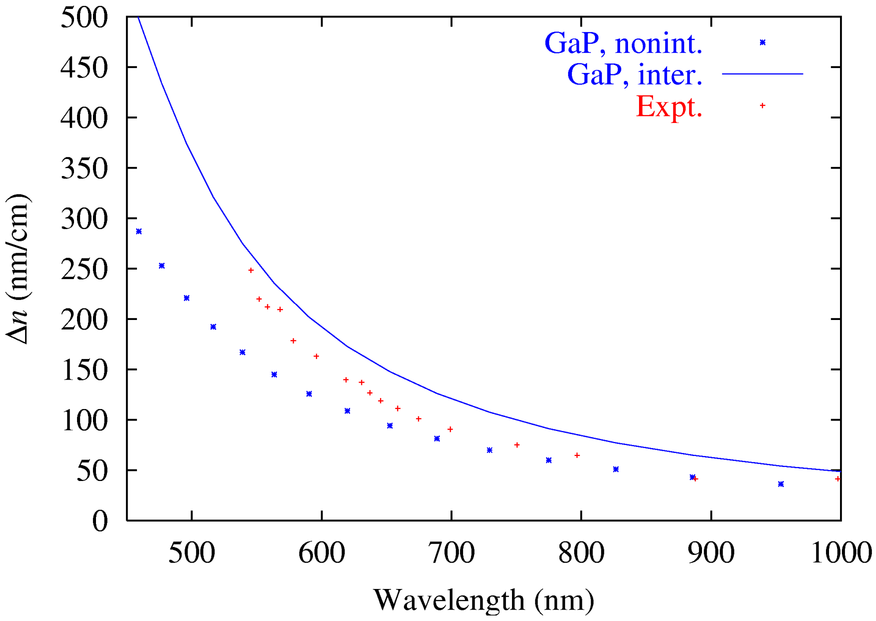
Behavior: $\Delta n(\omega) \sim A\omega^2 + B\,/\,(\omega^2 - \omega_0^2) + C\,/\,(\omega^2 - \omega_0^2)^2$

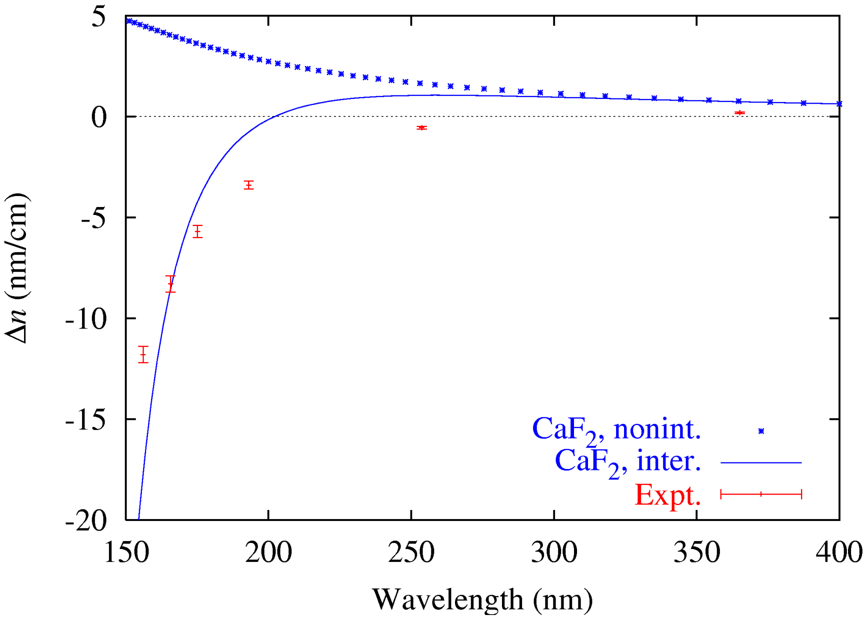
“Interband” contribution

Contribution from exciton peak because of anisotropy in exciton oscillator strengths

Contribution from exciton peak because of splitting of exciton energies

Each effect can dominate!





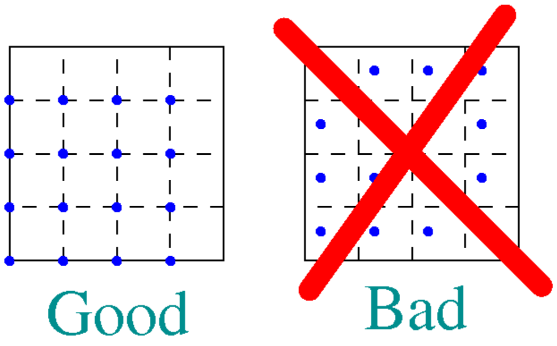
Spurious symmetry breaking culprits:

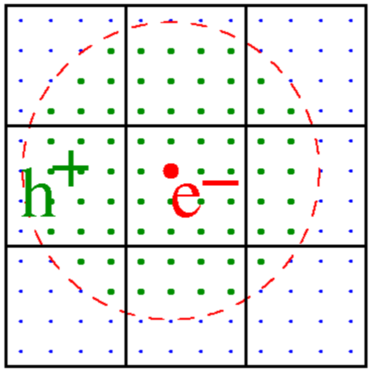
$H=H_e+H_h+H_{eh,\mathrm{D}}+H_{eh,\mathrm{X}}$, plus matrix elements!

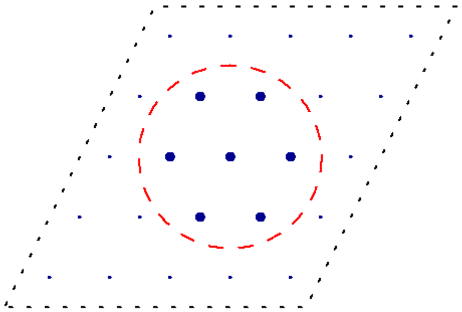
H_e, H_h: for faster convergence, **k**-point meshes can be displaced from having complete symmetry. DON’T SHIFT! (Or shift & average birefringences obtained for certain “equivalent” directions.)

$H_{eh,\mathrm{D}}$: for convenience, might cut off e-h interaction in real-space in non-symmetric way, e.g., related to supercell implied by **k**-point mesh spacing. USE LENGTH!

$H_{eh,\mathrm{X}}$: for convenience, might have **G**-vectors for treating off-diagonal dielectric screening organized in a parallelepiped. USE LENGTH!







Basis-set can convey bias from non-symmetric **k**-point & band sampling (PRB **54**, 16464, 1996). <u>Form basis set symmetrically, In regards to **k**-points and degenerate band partners!</u>

Basis set for $u_{n\mathbf{k}}(\mathbf{r})$, for $\psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{r}}$.

Summary

- Theoretical investigation relating
  - optical constants
  - quantum mechanics of electrons in solids
  - numerical modeling of physical systems

- Method results shown for
  - semiconductors
  - wide-gap insulators
  - core excitations

- Intrinsic birefringence in cubic crystalline materials

Acknowledgements:

JB: Office of microelectronic programs, SEMATECH International

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