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First Principles Nano-engineering of Organic-Electro Materials and Devices

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Goal: Tb/s Data Handing Capability With Milliwatt Power Requirements



APPROACH

Nano-engineering at all levels— Materials to Devices

Nano-structured Electro-Optic Materials



Hybrid Organic EO/Silicon Nano-Photonic Devices

 $r_{33} = \beta(\varepsilon, \omega) N < \cos^3 \theta >$



Quantum Mechanics: TD-DFT calculations to calculate molecular linear & nonlinear optical properties and charge distributions Statistical Mechanics: Pseudo-atomistic Monte Carlo/Molecular Dynamic Calculations to compute chromophore order and reaction fields



A Transformative Improvement



Getting Dielectric and Dispersion Effects Right





Solvent	3	λ_{max}/nm	μβ _ω /10 ⁻⁶⁹ SI (exp.)	$\mu\beta_0/10^{-44}$ esu(exp.)	$\frac{\mu\beta_0/10^{-44}}{\text{esu(theory)}}$
Dioxane	2.21	622	9291	3.41	4.9
Chloroform	4.81	675	27280	8.52	8.9

Pseudo-Atomistic Monte Carlo Calculations



Binary Chromophore Organic Glasses



The Role of Lattice Symmetry



Laser-Assisted Poling: Proof of Guest-Host Influence on $<\cos^3\theta >$





Simple Paradigm for Improved Linear & Nonlinear Optical Properties



SILICON SLOTTED-MICRORING RESONATORS



Drive Voltage-Bandwidth Parameters for Resonant Devices

Analog Signals

$$\begin{aligned} (V_{\pi \text{ equiv}} / \Delta f_{3dBe}) &= 4\pi d\lambda / [(3\sqrt{3})(n_{eff})2r_{33}c] \\ \Delta f_{3dBe} &= c/\lambda Q \end{aligned}$$

if n = 1.6, r_{33} = 300 pm/V, d = 6 $\mu m,$ and λ = 1.3 mm, then (V_{\pi} equiv/ Δf_{3dBe}) = 0.08 V/GHz

 \Rightarrow Have achieved 0.05 V/GHz or 20 GHz/V (smaller electrode spacing)

Digital Signals

$$V_{10dB} = 3d\lambda B/((n_{eff})2r_{33}c)$$

if B = 10 Gb/s, n = 1.6, r_{33} = 300 pm/V, d = 6 μ m, λ = 1.3 mm, Q = 5 x 10^3, then V_{10dB} = 1 V

Electro-optic Polymer Tuned Si Modulators 4x4x4 ROADM Constructed at Boeing

Summary of Results

- Demonstrated 20 *GHz/V* tuning in E-O polymer filled slotted ring resonators.
- These are the *lowest power E-O converters* operating at high frequencies, and are predicted to work at 100GHz/V tunability and well over 40Gb/sec.
- 20 Gb/sec modulators with 0.2 V driving voltage and 50 micron diameters using E-O polymer filled slotted waveguide modulators
- We have used these waveguides to detect light by optical rectification – predicted to function at very high frequencies

Wavelength Selective Cross-Connect Architectures



• Silicon is used both for waveguide and as transparent electrical contact –enabling very high electrostatic fields across the 100nm waveguide slot without absorption losses.

• The slot geometry provides massive optical and electrostatic field enhancement. So far, Q values of 23k and modulation at 10 GHz have been measured in our slot resonators – limited by measurement electronics

All-Optical Modulation > 5 THz

M. Hochberg et al., "All-Optical Modulator in Si with THz Bandwdith," *Nature Materials*, <u>5</u>, 703-709 (2006). Two other papers in press.

- ► Optical pump power < 1 mW (3 x 10⁶ V/m)
- ►1/3 power in organic NLO cladding
- ► $\chi^{(3)}$ = 6-7 x 10⁻²¹ (m/V)²
- Modulation to 10 THz



