Ab Initio Property Prediction with Density Functional Theory (DFT) Relevant to Coating Thermal Noise

Laser Interferometer Gravitational-Wave Observatory

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LIGO in Hanford, WA. The twin detector is located in Livingston, LA. When a spacetime wave is generated by black hole or neutron star inspiral, arm lengths change in opposition as it moves though the detector, and a signal results. ΔL(wave) ~ 1/1000 of a proton. Atomic motion in the mirrors is a noise source ΔL(noise)!

Fluctuation Dissipation Theorem:

Brownian motion of material ↔ mechanical loss φ

↕

Brownian motion of material ↔ arm length noise

Coating Thermal Noise:

- Limiting noise source for Advanced LIGO.
- Arm Cavity Mirror Coatings chief source.
- Mirrors are 1064 nm dielectric coatings.

Goal – Loss Angle Minimization in Coatings:

- ***L*** material is IBS SiO_2.
- ***H*** material is IBS Ta_2O_5.
- Seek lower φ_H or φ_L coating materials.
- Seek designs minimizing ***H*** volume.
- $\varphi_L(SiO_2) \sim 10^{-5}$ rad.
- $\varphi_H\ (Ta_2O_5) \sim 10^{-4}$ rad.
- TiO_2 doped into Ta_2O_5 lowers loss angle φ_H.
- ***Mechanism not well understood !***

Basic Noise Formulae:

$$\varphi_{phonon-phonon} = \frac{C_{V-at} T g^2}{\overline{M} v_{sound}^2} \frac{\omega \tau_{ph}}{1+(\omega \tau_{ph})^2}$$

$$\varphi_{therm-damp} = \frac{v_D^2 \alpha^2 \overline{M} T \omega \tau_{ph}}{27 C_{V-at}}$$

$S = (z_{low} + \gamma z_{high})$, Equations for thermal noise figure of merit S in a coating.

where,

$z_{high\ (low)}$ = total thickness of the high (low) index coating material in units full wave optical thickness at the reference wavelength.

$\gamma = abc/d$

$a = (\varphi_{high} / \varphi_{low})$

$b = (n_{low} / n_{high})$

$c = (Y_{high} / Y_{sub} + Y_{sub} / Y_{high})$

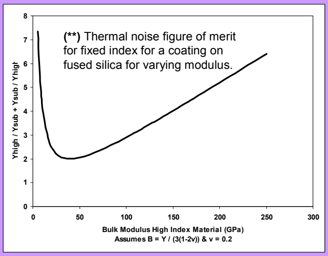
$d = (Y_{low} / Y_{sub} + Y_{sub} / Y_{low})$

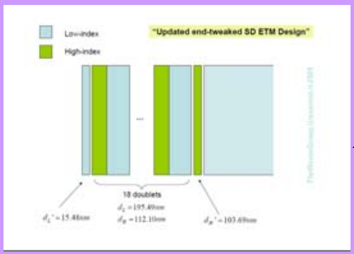
Noise Inputs Predictable with DFT:

- Specific atomic heat capacity C_{V-at}.
- Elastic Moduli B and Y.
- Gruneisen Parameter g.
- Thermal expansion $\alpha = gC_{V-at}/3B$.

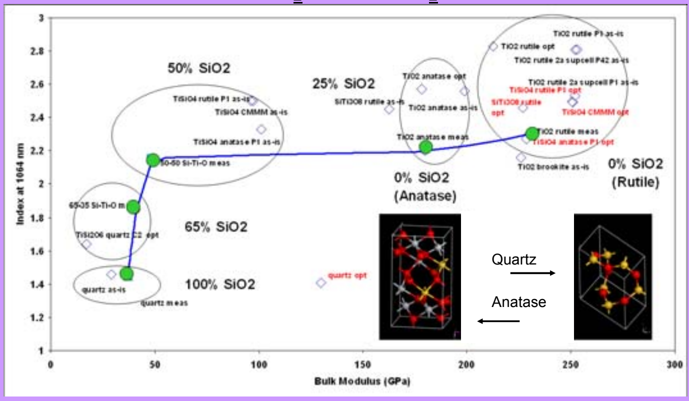
Other Things Predictable with DFT:

- Refractive index dispersion.
- Band structure and gap.
- UV optical properties.
- IR vibrations.





Ab Initio Example 1: SiO_2-doped-TiO_2:



CASTEP Density Functional Theory calculation showing that when TiO_2 rutile and anatase phases are doped with SiO_2, there is a plateau in the refractive index for a broad range of bulk moduli. Green points are experimental data, all else is a DFT prediction. Noting (**), coating thermal noise could be minimized in TiO_2 by SiO_2 doping.

Ta_2O_5 n ~ 2.09, φ ~ 3.8x10^{-4}, Y_H = 140 GPa → ***S = 38.13 (52.6% worse)***

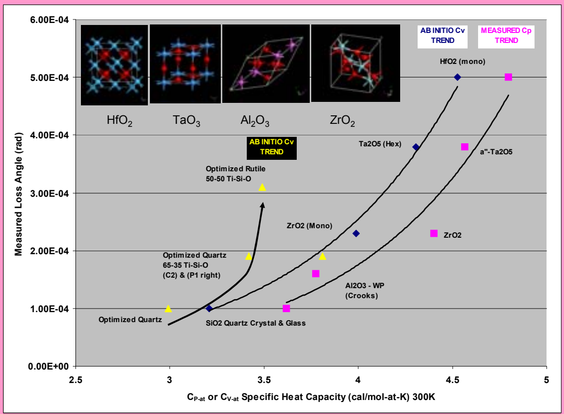
$Ti{:}Ta_2O_5$ n ~ 2.09, φ ~ 2.3x10^{-4}, Y_H = 140 GPa → ***S = 24.97 (baseline)***

$Si{:}TiO_2$ (50-50) n ~ 2.08 (same thicknesses), φ ~ 3.1x10^{-4}, Y_H = 87 GPa → ***S = 27.39 (9.7% worse)***

$Si{:}TiO_2$ (65-35) n ~ 1.85 (thickness ≈ doubles!), φ ~ 1.9x10^{-4}, Y_H = 73 GPa → ***S = 30.16 (20.7% worse)***

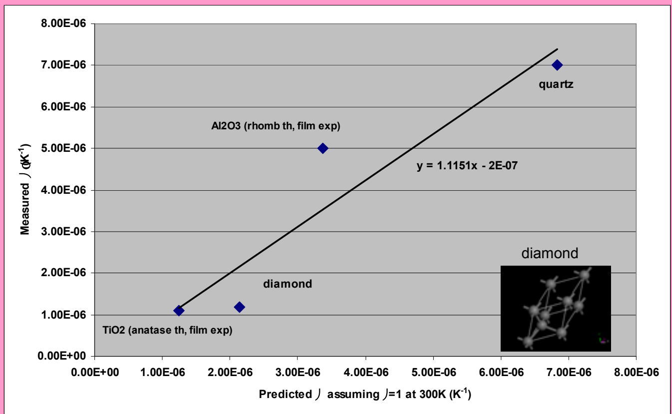
Modulus tuning in $Si{:}TiO_2$ almost effective as loss angle reduction in $Ti{:}Ta_2O_5$

Ab Initio Example 2: Heat Capacity – Loss Correlation



CASTEP Density Functional Theory calculation showing a trend with specific (atomic) heat capacity, with measured loss angle. The magenta data uses experimental values of the heat capacity C_p, demonstrating a reasonable prediction of that property as well, Comparing the predicted *ab initio* C_V (blue and yellow).

Ab Initio Example 3: Thermal Expansion Coefficient



CASTEP Density Functional Theory calculation of CTE using computed values of *C, B* and the expression *α = gC/3B* for Gruneisen parameter *g=1*.

Conclusions & Further Work:

- **DFT gives reasonable predictions of many properties for films, despite that the DFT input structures are crystalline, but films are amorphous.**
- **DFT cannot directly predict thermal noise, but relations between predictable parameters and thermal noise is suggested.**
- **Crown jewel of coating thermal noise $Ti{:}Ta_2O_5$ simulations will have to wait until more processors are available (all on 16 processors).**

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