Nanoshells as a high-pressure gauge

Nick Van den Broeck[†], Katrijn Putteneers[†], Jacques Tempere[†,‡] & Isaac F. Silvera[‡]

[†]Theory of Quantum and Complex systems, Universiteit Antwerpen, Universiteitsplein 1, 2610 Wilrijk, Belgium

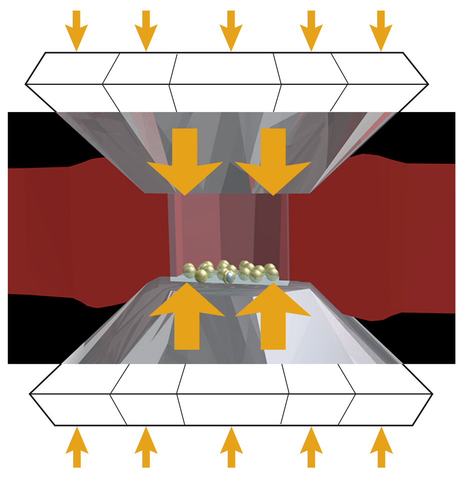
[‡]Lyman Laboratory, Harvard University, 14 Oxford street, Cambridge MA02138, USA

Introduction

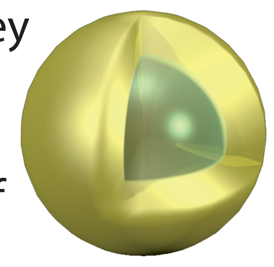
We introduce a new method for measuring the pressures in high-pressure Diamond Anvil Cell experiments. Using metallic nanoparticles as a gauge, our calculations predict a higher sensitivity in combination with more flexibility.

The Diamond Anvil Cell (DAC) is able to generate pressures up to 350 GPa by pressing two diamonds against each other. This setup is used to measure material properties under extreme static pressures.

Currently, the pressures inside such a cell are measured by tracing the fluoresence lines of ruby crystals. However, this method fails at about 150 GPa due to masking of the spectral lines by the diamonds and uncertainties in the calibration.



Our pressure gauge consists of nanoshells, nanoparticles with a silicon core and metallic shell. Their optical response can be engineered to be situated in a part of the spectrum where no other effects occure. Also, nanoshells give a stronger signal since they rely on extinction and not fluorescence. Furthermore, due to their smaller size compared to the rubies they provide the posibility of generating a pressure map of the entire cell.



Method

Combining Mie-theory with pressure dependencies.

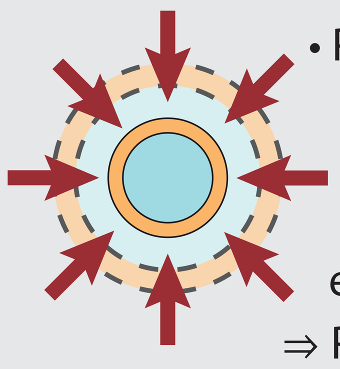
The optical properties of nanoshells can be calculated using Mie-theory. In Mie-theory the four Maxwell equations are solved in spherical coordinates using boundary conditions on the electric and magnetic field to implement the geometry of the physical problem (in this case the nanoshell).

Material parameters

- The radii of the particle.
- The permittivity of the dielectrics (e.g. $\varepsilon_{SiO_2}(P_{atm}) = 2.04$).
- The permittivity of metals: with the Drude Model $\varepsilon_s(\omega) = \varepsilon_b - \frac{\omega_{pl}^2}{\omega^2}$

Pressure influence

Under pressure changes will occur:



- Particle is compressed ⇒ radii decrease
- Density of conduction electrons increases ⇒ Plasma frequency increases
- The permittivity of dielectrics changes.

For the different materials, the volume change under pressure was calculated using the Vinet equation of state[1]:

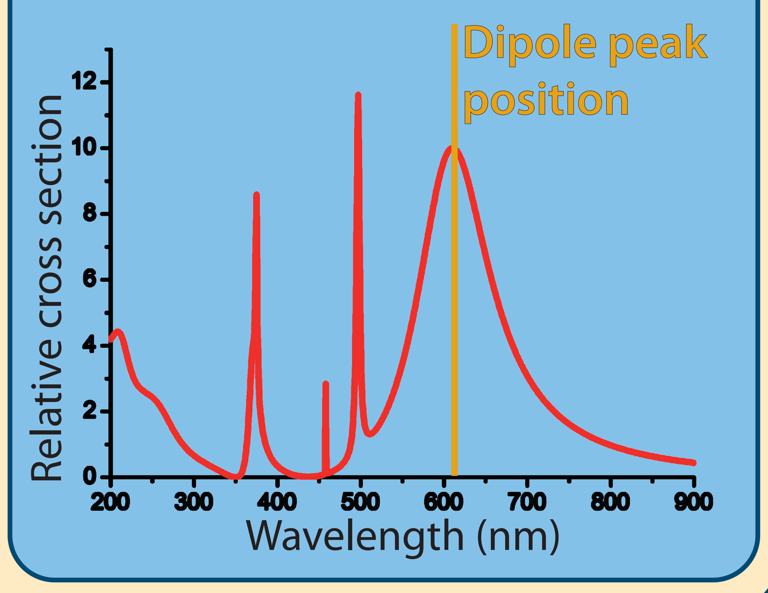
$$P = 3K_0 \frac{1-\left(\frac{V}{V_0}\right)^{1/3}}{\left(\frac{V}{V_0}\right)^{2/3}} \exp\left\{\frac{3}{2}(K_1-1)\left[1-\left(\frac{V}{V_0}\right)^{1/3}\right]\right\}$$

The change of permittivity of the dielectrics was derived from the Clausius-Mosotti relation[2]:

$$\frac{\varepsilon(\omega,P)-1}{\varepsilon(\omega,P)+2} = \frac{4\pi}{3} n(P)\,\alpha$$

Mie-theory

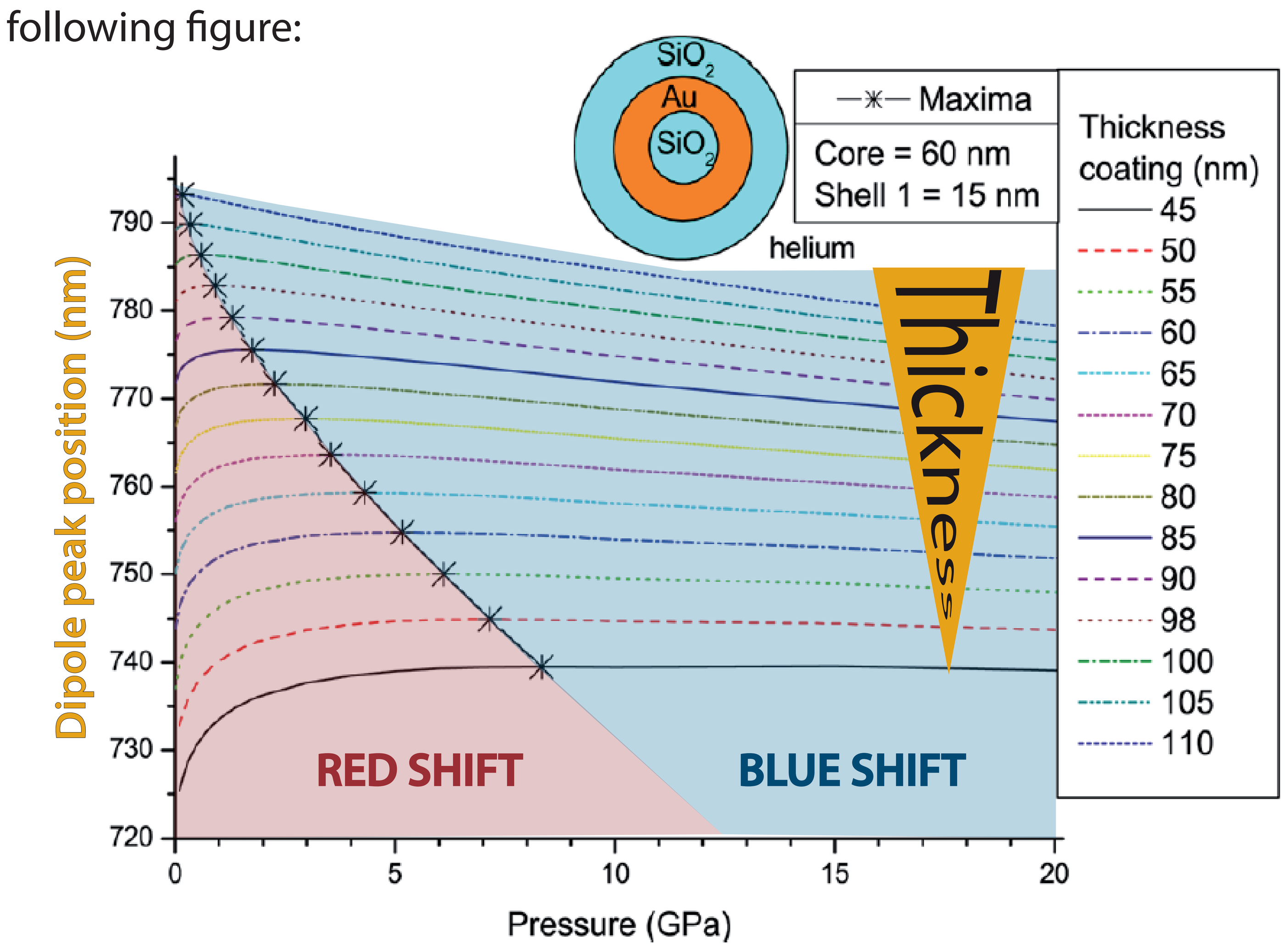
Maxwell equations → Boundary: Geometry → Solution: E & B-field → Cross section:



Results

The resonance wavelength of coated nanoshells under pressure

Using the method described in the left hand pane, we calculated the position of the resonances for a coated nanoshell in an helium environment. Tracing such a resonance peak as a function of the pressure results in the following figure:



As indicated by the red and blue background, we can see two regions with a different behaviour.

Red shift at low pressures:

- Due to change in permittivity of the surrounding medium
- Shift decreases for thicker silicon coatings ⇒silicon coating shields the nanoshell from its environment

Blue shift at high pressures:

- Due to compression of the nanoparticle
- Analogous to behaviour of a nanoshell in vacuum

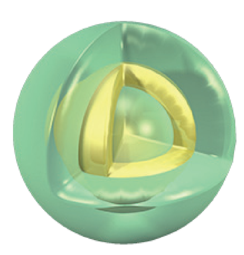
The resolution r = average wavelength shift corresponding to 1 GPa of pressure difference.

• Coated nanoshells:	r = 0.90 nm/GPa	P∈ [0, 20] GPa
• Rubies:	r = 0.36 nm/GPa	

Conclusion

Our theoretical calculations show that coated nanoshells can be used as pressure gauges in high pressure experiments with a higher resolution than the current ruby method and the advantage of their tunability and small size.

Using the blue shift of the resonance peak in the extinction spectrum under pressure we proved theoretically the usefulness of coated nanoshells as pressure gauge. By engineering the nanoshell with an extra coating we steer clear of negative effects.



Advantages of nanoshells over rubies:

- Tunability of resonance peak in the red and near-infrared region
- Smaller size makes pressure map possible
- Potentially useful as heating element

1) Vinet P. *et. al.* Geophys Res. 92 B2 9319-9325 (1987).
2) Kittel C., *Introduction to Solid State Physics*, 5th ed. (John Wiley & Sons, New York, 1976).

Further information:
Nanoshells as high-pressure gauge analyzed to 200 GPa, JAP **110**, 114318 (2011)
nick.vandenbroeck@ua.ac.be

Theory of Quantum and Complex systems

Universiteit Antwerpen