Dielectric Function Approach to Room-Temperature Superconductivity in Nanomaterials

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Introduction

Our task is to apply the predictive power of theory of superconductivity formulated in terms of the dielectric function $\varepsilon(\mathbf{q},\omega)$, to nanostructures, such as the decorated nanotubes. Importance of the dielectric function $\varepsilon(\mathbf{q},\omega)$ became very clear after the BCS approach (see, *e.g.*, Ref. [1]). Kirzhnitz [2] explored the admissible negative sign of $\varepsilon(\mathbf{q},\omega=0)$ in 1976. Dolgov and Maksimov [3] demonstrated in 1979 that negative sign $\varepsilon(\mathbf{q},\omega=0)<0$ really takes place in superconductors, such as Sn, Al, but not in non-superconducting K. Using this approach it was obtained recently that using metamaterial nanoengineering triples the superconducting critical temperature of bulk aluminum [4].

For dielectric function $\varepsilon(\mathbf{q},\omega)$, our calculations make use of the Density Functional Theory (DFT) code ABINIT [5] and the add-on Time Dependent Density Functional Theory (TDDFT) code DP [6]. ABINIT was used to compute the electronic density and band structure. The computed data were then fed into DP to calculate the dielectric function. Graphical interface of QuantumWise commercial software was used for acceleration of relaxation studies.

We obtained data on ab-initio calculations of $\varepsilon(\mathbf{q},\omega)$ for GaAs, Si, Ge, Al, as well as for Ti-decorated nanotubes and the ropes of carbon nanotubes. Negative sign of dielectric function and its possible cause of very high-T_c superconductivity is under exploration in nanomaterials [7].

Predictive Power of Theory

BCS, 1957:

$$T_c \sim \omega_D \exp(-1/\lambda)$$

Bogolyubov et al., 1958; Eliashberg, 1960; MacMillan, 1968:

$$T_c \sim w_D \exp\{1.04[(1+\lambda)]/[\lambda-\mu^*(1+0.62\lambda)]\}$$

Little, Ginzburg, 1964: $T_c>300K$

Cohen, Anderson, 1972: $T_c<10K$

Importance of $\varepsilon(q,\omega)$

Kirzhnitz, 1976: $\varepsilon(\mathbf{q},\omega=0)<0$ is admissible!

Dolgov, Maximov 1979: $\varepsilon(\mathbf{q},\omega=0)$ is negative!!

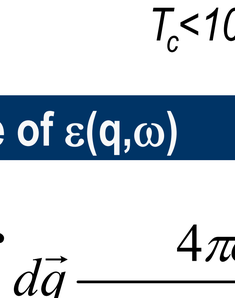
$$\int d\vec{q}\,\frac{4\pi e^2}{\varepsilon(q,\omega=0)q^2}=\mu-\lambda$$

Known $\varepsilon(\mathbf{q},\omega)$ means the dynamics of the system is determined:

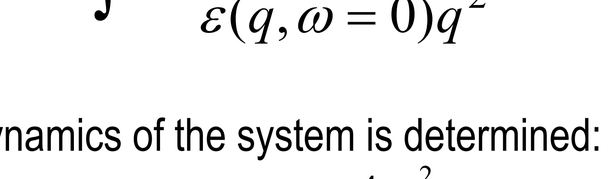
$$V(q,\omega)=V_{(Coulomb)}+V_{(el-ph)}=\frac{4\pi e^2}{\varepsilon(q,\omega)q^2}$$

$$\frac{1}{\varepsilon(q,\omega)}=\frac{q^2}{q^2+k_{TF}^2}\left[1+\frac{\omega_q^2}{\omega^2-\omega_q^2}\right]$$

Historic suggestions by **Little** and others

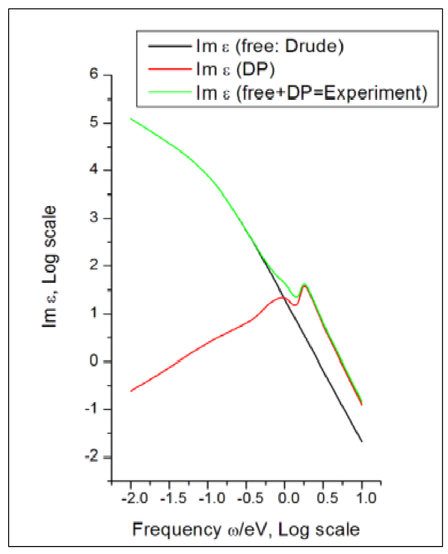


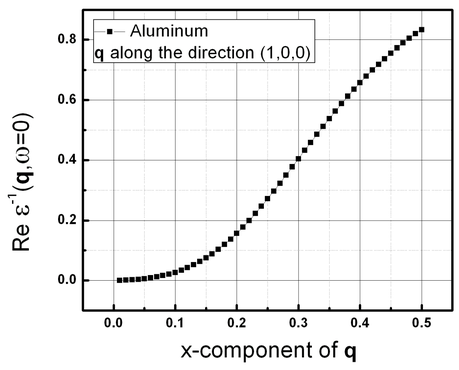
Nanostructures calculable *ab-initio* and achievable experimentally



Ab-Initio Calculations of $\varepsilon(q,\omega)$

First principle calculations for Aluminum

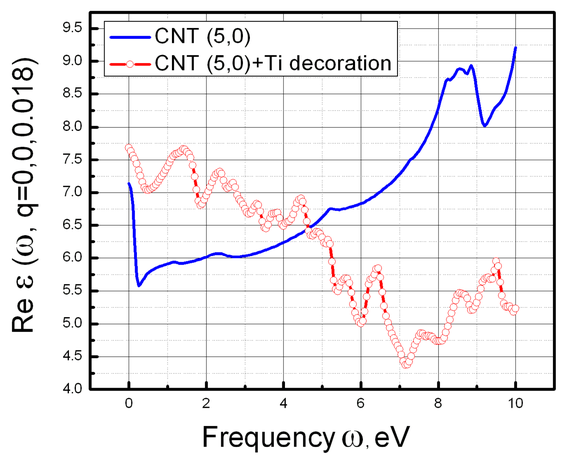


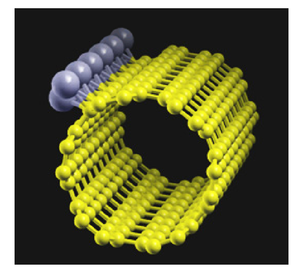


No negativity of Re $\varepsilon^{-1}(\mathbf{q},\omega=0)$ in the frozen lattice model.

Conclusion: phonons are important for SC in this material!

However, Ti-decorated nanotube delivers the desired tendency:

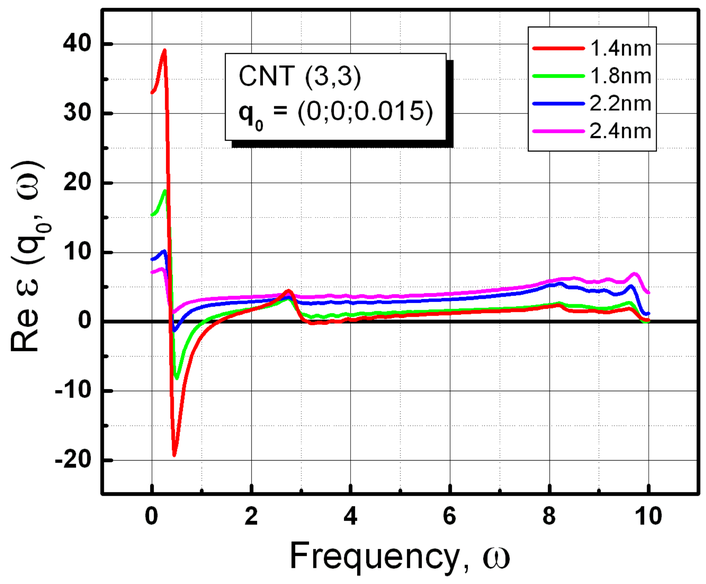




$$V(q,\omega)=\frac{4\pi e^2}{\varepsilon(q,\omega)q^2}$$

Purely electronic mechanism!

Moreover, for the ropes of CNTs: $\varepsilon(\mathbf{q}_0,\omega)<1$:



Negativity of $\varepsilon(\mathbf{q}_0,\omega)$ means we can expect SC!
Still requires more work which is ongoing…

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