Study of optical conductivity of highly disordered MoC films by spectroscopic ellipsometry

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Optical conductivity

- Drude model

$$\sigma(\omega) = \sigma'(\omega) + i\sigma''(\omega) = \frac{\sigma_0}{1 - i\omega/\Gamma}$$

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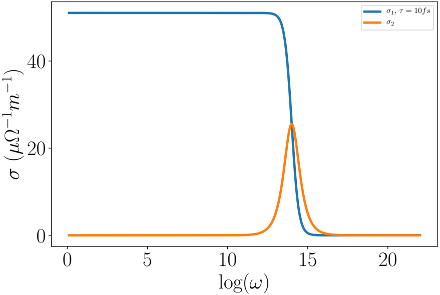

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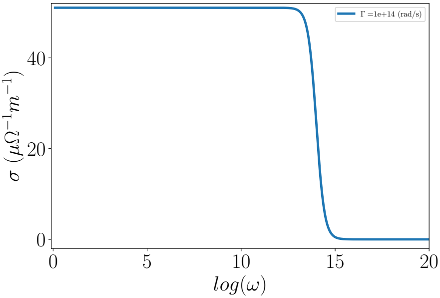

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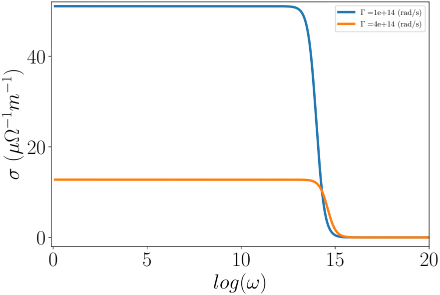

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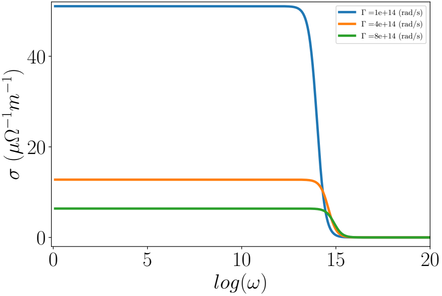

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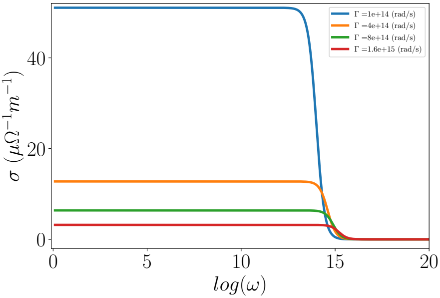

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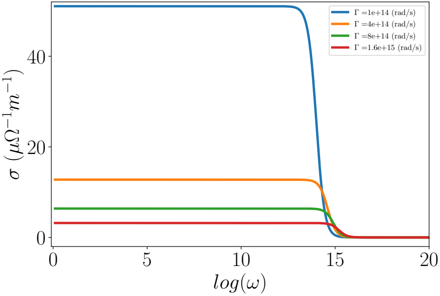

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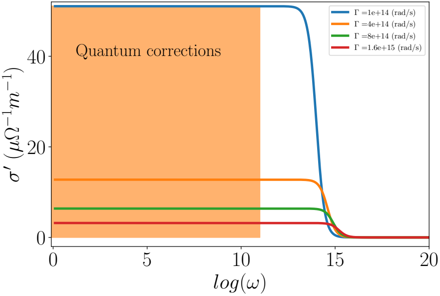

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Quantum correction to conductivity

- Weakly disordered metals

$$\sigma(\omega) = \sigma_{\text{reg}}(\omega) + \delta\sigma(\omega)$$

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- Quantum correction $\delta\sigma(\omega)$:
  - Weak-localization
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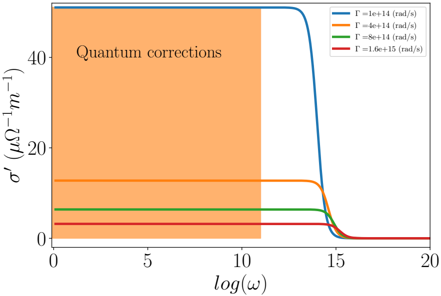

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  - 3D: $\delta\sigma(\omega) \sim \sqrt{\omega}$
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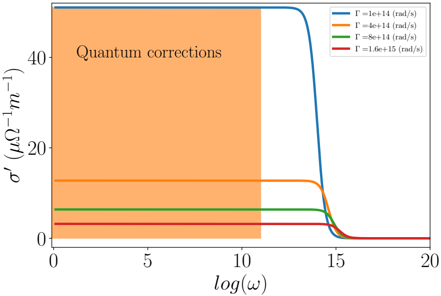

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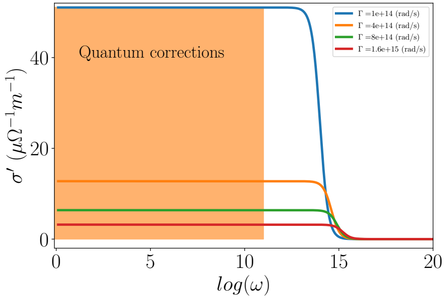

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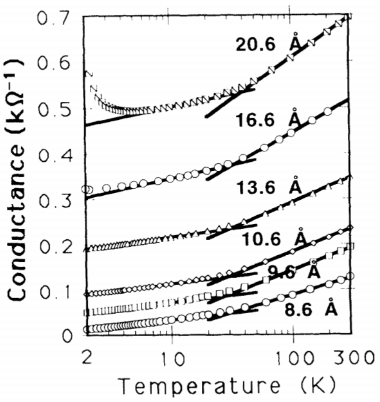
- Theoretically should be present up to $\omega^* \sim \Gamma$

Transport measurements of MoC at low temperatures

- MoC, thickness - tuned disorder
- 2D weak-localization and *e*-*e* interaction effects up to RT



S.

J. Lee et al., PRB **49**, 13882 (1994)

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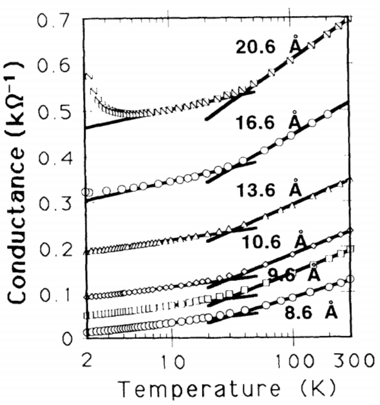

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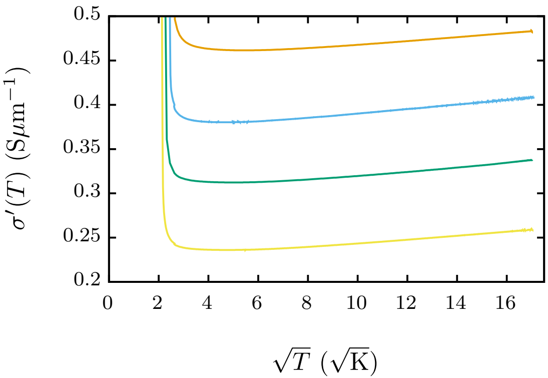
- *"... extending the weak localization idea up to room temperature to interpret our data may be controversial."*

MoC sample preparation

- Magnetron sputtered in argon-acetylene atmosphere
- Mo - target and sapphire substrates
- Sample characterisation - sheet resistance $R_{\square} = \rho/t$
- Mo_xC_{1-x}; stoichiometry tuned disorder - acetylene flow rate
- Two sets of 5 nm thin samples:
  - 1. set: $R_{\square}$ from 420 to 720 $\Omega/\square$
  - 2. set: $R_{\square}$ from 390 to 3900 $\Omega/\square$

Transport measurements

- 1. set: $R_\square$ = 420, 500, 590 a 720 $\Omega/\square$



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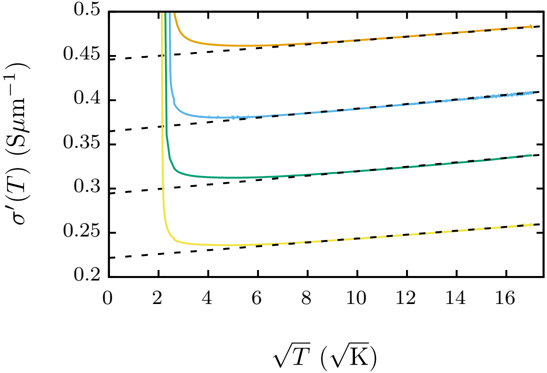

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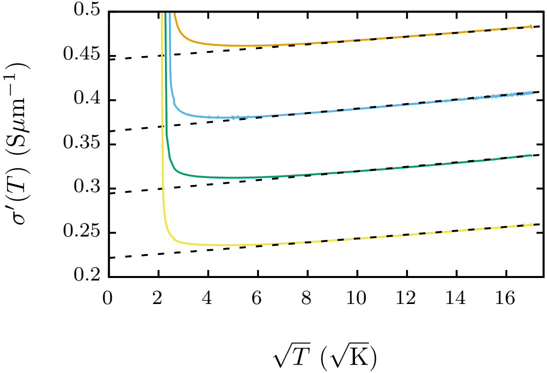

- $\sigma = \sigma_0 + b\sqrt{T}$; 3D quantum corrections up to T= 300K
- How far do they extend?

Optical measurements

- Ideal for study of thin films

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$$\mathcal{T}(\omega) \approx \frac{\mathcal{T}_s(\omega)^2}{[1 + g'(\omega)/(n_s + 1)]^2 + [g''(\omega)/(n_s + 1)]^2}$$

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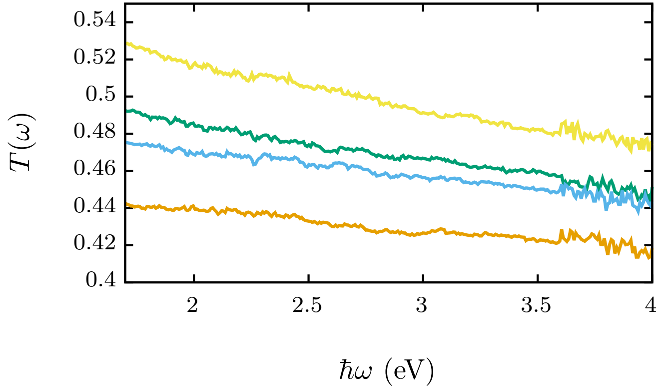
- **Spectroscopic ellipsometry**

- Reflection measurement, evaluation of σ_1 and σ_2
- Our experimental frequency range 300-810 THz

Optical transmission spectra

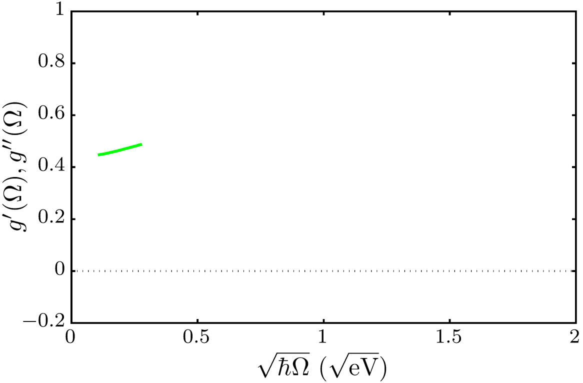
- 1. set of MoC: $R_\square$ = 420, 500, 590 a 720 $\Omega/\square$
- Smooth transmission spectra



- $T(\omega)$ decreases with frequency $\omega/2\pi$
- The opposite is expected from Drude model

Optical conductivity of MoC with R$_\square$=720$\Omega/\square$

- For interaction effects: $\Omega = \sqrt{\omega^2 + (\pi k_B T/\hbar)^2}$



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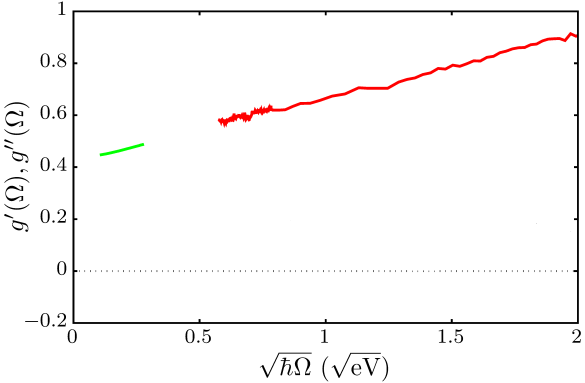

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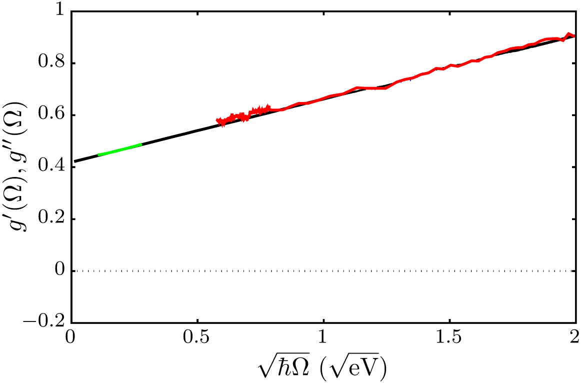

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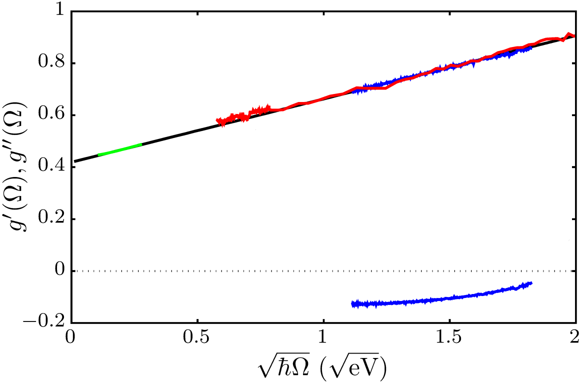


- Agreement between 3 data sets, $\hbar\Omega \approx 14$ meV up to 4 eV

Proposed model

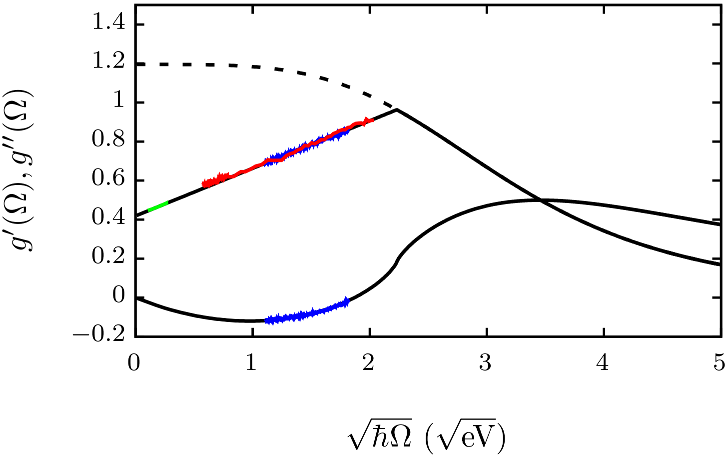
- Postulate for the σ:

$$\begin{aligned}\sigma'(\omega,T) &= \sigma_0\left[1-\mathcal{Q}^2+\mathcal{Q}^2\sqrt{\Omega/\Gamma}\right] \quad \text{if } \Omega<\omega^* \\ \sigma'(\omega,T) &= \frac{\sigma_0}{1+(\Omega/\Gamma)^2} \quad \text{if } \Omega\geq\omega^*\end{aligned}$$

- Imaginary part σ'' given by Kramers-Kronig relations
- 3 parameters:
  1. $\mathcal{Q}$ - "Quantumness"
  2. Γ - Scattering rate
  3. $\sigma_0 = ne^2/m\Gamma$, whereas $\sigma(0,0) = \sigma_0(1-\mathcal{Q}^2)$
- Fermi liquid theory, for interaction effects:

$$\Omega = \sqrt{\omega^2 + (\pi k_B T/\hbar)^2}$$

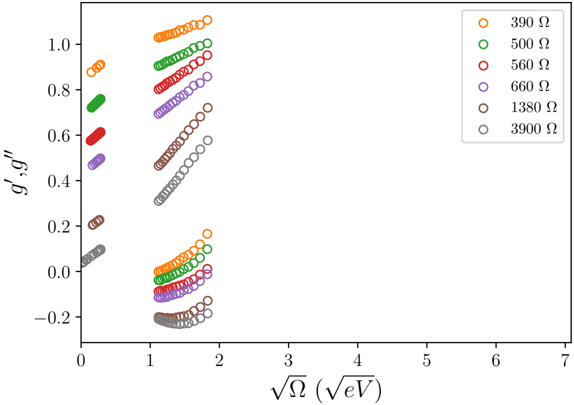
Conductivity $\sigma(\omega)$ fit



- Observation of quantum corrections to conductivity up to optical frequencies, Phys. Rev. B 100, 241106(R) (2019)

Conductivity $\sigma(\omega)$ of second set

- 2.set of MoC samples $R_\square$ from 390 to 3900 $\Omega/\square$



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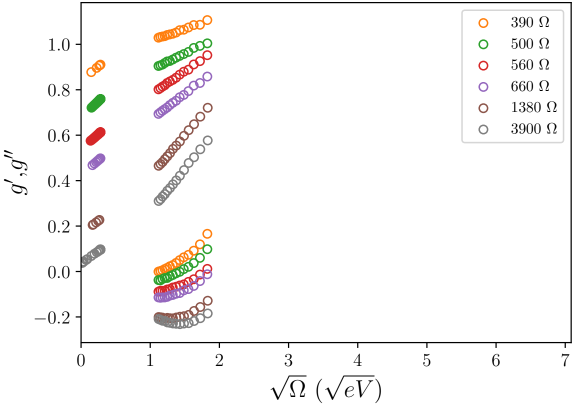

- Fit function:

$$g_1(\omega, T) = e^{-(\Omega/\Gamma)^2} + Q^2\left(\sqrt{\Omega/\Gamma} - 1\right) e^{(-\Lambda\Omega/\Gamma)^2}$$

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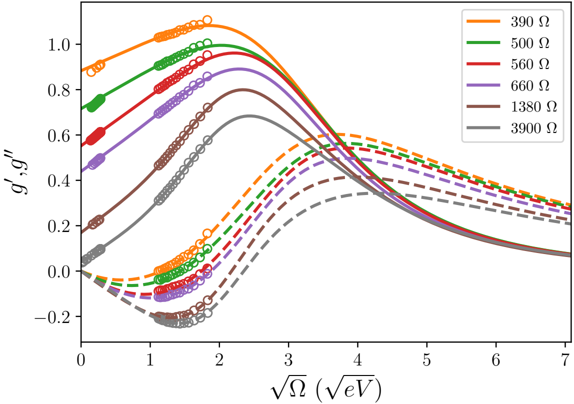

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Fit parameters

$\mathbf{R}_s[\Omega/\Box]$	$\mathbf{g}_0$	$\mathbf{Q}^2$	Γ[eV]	Λ
390	1.35	0.35	12.1	1.85
500	1.32	0.46	12.3	1.54
560	1.31	0.58	12.2	1.74
660	1.22	0.64	12.3	1.92
1380	1	0.83	13.4	3.08
2240	0.96	0.89	15.0	3.39
3900	0.83	0.95	15.2	3.66

- Increased disorder $\implies$ higher value of Q

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\- Metal - Insulator transition is approached

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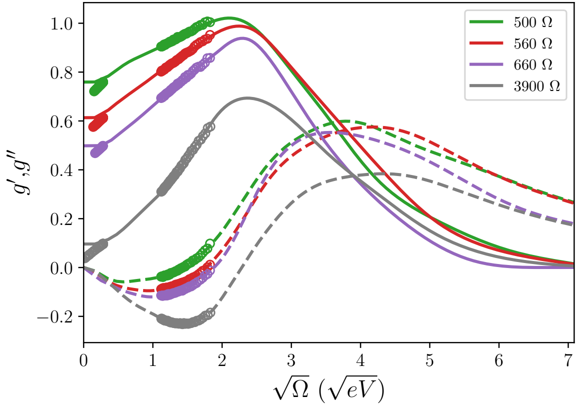
  - Randomly generated conductivity curves that obey the Kramers-Kronig relations and fit the experimental data to a chosen degree
  - Prolongation is given by the average of the selected curves
  - Reasonably smooth conductivity without rapid changes and oscillations - fulfilled in strongly disordered (MoC) films

Prolongation of optical conductivity

- Numerical extrapolation method for complex conductivity of disordered metals



- S. Kern et al., Phys. Rev. B 103, 134205 (2021)

Conclusion

- Optical conductivity of MoC films; $R_s \in \langle 390, 3900 \rangle \Omega/\Box$
- Transport and optical measurements
- Observed quantum corrections to conductivity up to optical frequencies
- Parameters σ_0, $\mathcal{Q}$ and Γ were extracted
- Appropriate for the study of Metal-Insulator transition
- Utilized a numerical extrapolation method for complex conductivity of disordered metals

Thank you for your attention

Neilinger et al., Physical Review B100, 241106 (R) (2019)
S. Kern et al., Phys. Rev. B 103, 134205 (2021)