SIMULATIONS OF NANOSCALE DYNAMICS FOR HIGH-REPETITION RATE LCLS EXPERIMENTS:

Superconducting YBCO films

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INTRODUCTION

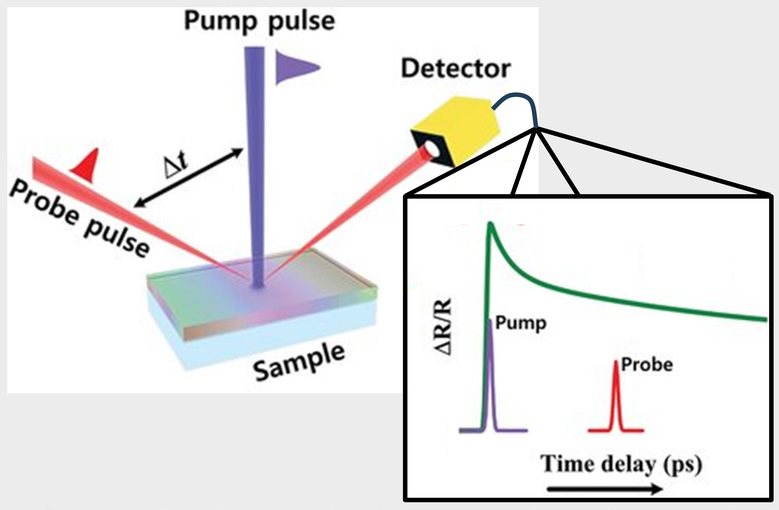
Motivation

The development of high-repetition rate capabilities at LCLS II have unlocked the possibilities for new measurements to observe, in detail, the photoinduced electron dynamics in quantum materials such as superconductors.

This understanding is important for:

- **Fundamental and applied sciences** to inform an approach towards room-temperature superconductivity.
- Furthering the development of **quantum electronics**.

Pump-probe



Pump-probe schematic showing the experimental setup and example of data acquisition. [1]

- Transient effects can be mapped by taking multiple measurements using short laser pulses and precisely changing the delay between pump/probe.

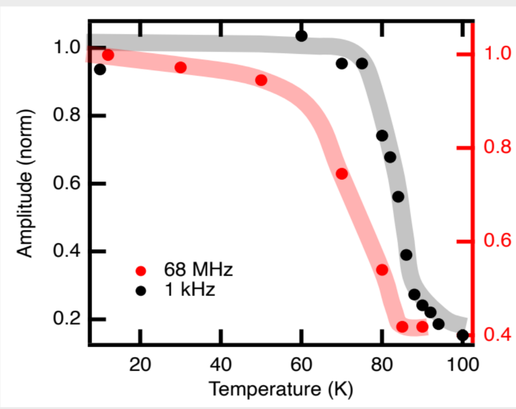
High-repetition rate

Advantages:

- More sensitive measurements with **higher signal to noise ratio.**
- Accelerated data taking throughput.

Challenges:

- **Thermal heating effect** (especially problematic for measuring superconducting effects at low temperatures).
- X-ray/laser penetration depth mismatch, when comparing on- and off-resonance responses.

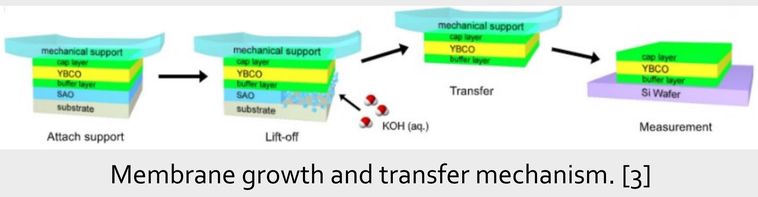


Temperature dependence of normalized ΔR/R in optimally doped YBCO single crystal with two different laser repetition rates. [2]

Approach

To address these challenges:

- Use thin and transferrable membrane on high thermal conductivity substrate.



Membrane growth and transfer mechanism. [3]

- Use **simulations to quantify and validate the improvements** in thermal dissipation using the new membrane method.
- Determine limitations and potential improvements.

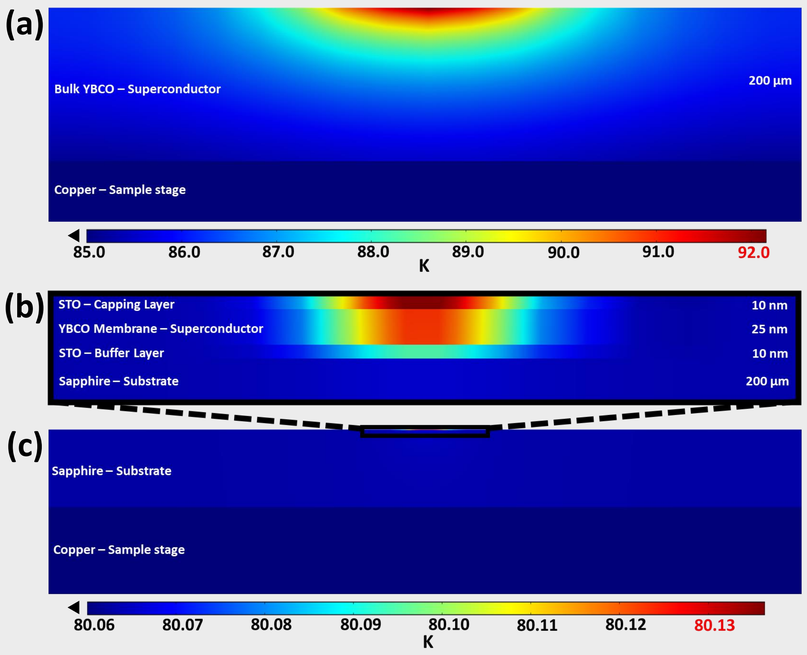
RESULTS

Thermal simulations

Bulk and membrane YBCO on sapphire were simulated in COMSOL under pumped beam power.

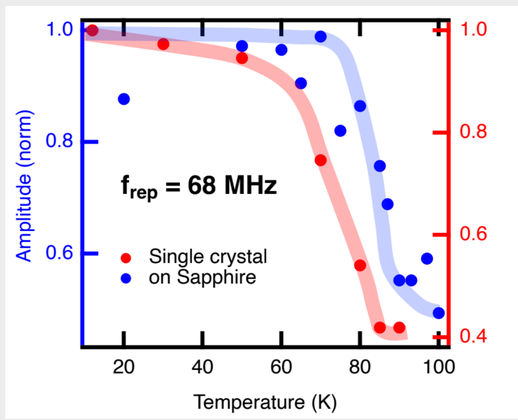
Simulation Parameters:

- Material parameters such as $C_p(T)$ and $\kappa(T)$ taken from literature values. [4]
- Heat in-flow from 800 nm wavelength pump beam at 15 mW with 0.1 mm radius gaussian footprint.
- Heat out-flow from fixed temperature on copper face.
- Thermal contact boundary condition (BC) between membrane layers, thin layer BC between samples and cold finger.



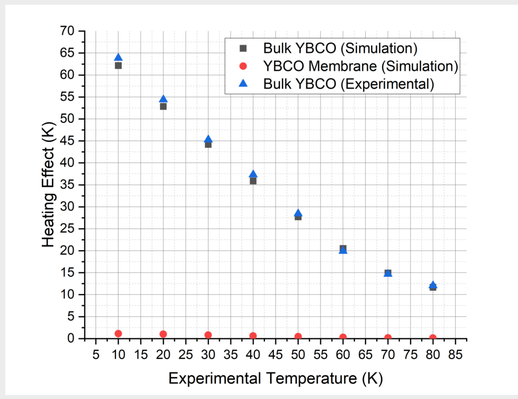
Thermal simulation results: (a) Cross-section of Bulk YBCO; (b) Cross-section of YBCO membrane on sapphire; (c) Zoomed-out cross-section of (b). **Note color scale difference.**

Experimental Data



Normalized amplitude in optimally doped YBCO single crystal and membrane on Sapphire as a function of temperature. [2]

Data Comparison



Plot of simulation versus experimentally measured the heating effect. (Note: Experimental YBCO membrane data near zero)

Data Analysis

The **simulations and experimental data match**. The simulation yields the insight that:

- The thermal boundary conductance between layers in the membrane is extremely high.
- The silver paint used to mount samples to the stage is the limiting factor for thermal transfer.
- Sapphire substrate distributes thermal load over a much larger surface area.
- Future improvements can be made by increasing sample-stage thermal transfer efficiency.

OTHER

Order-parameter simulations

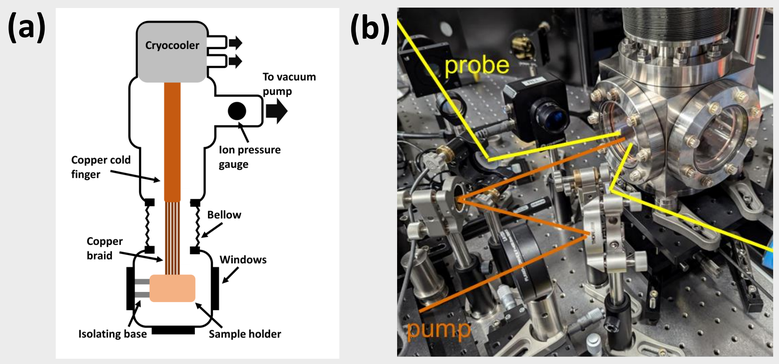
Working on simulating non-equilibrium perturbations of the order-parameter in finite-gap superconductors using TDGL theory.

Progress:

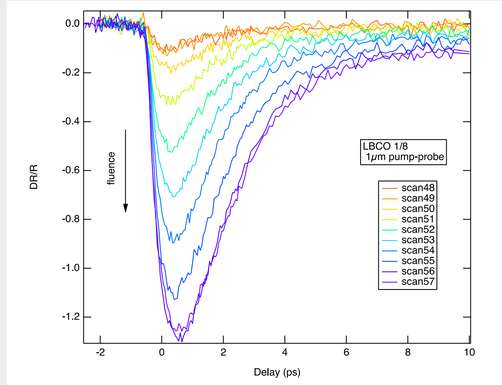
- Successfully simulated zero-gap superconductors.
- Completed modification of differential equations for finite-gap superconductors.
- Solving convergence problems with current solver.

Vibration isolated cryostat

Helped construct and take measurements of LCO, LBCO, V2O3 qRIXS early science samples with our cryostat.



(a) Schematic of in-house vibration isolated cryostat; (b) Photo of experimental setup including in-house cryostat.



Example of initial data: fluence dependance of 1 µm pump-probe response from bulk LBCO as 25K.

ONGOING AND FUTURE WORK

- High-repetition rate experiments of YBCO.
- Completing finite-gap order parameter simulations.
- Perform thermal simulations and analysis on V_2O_3.
- Complete data analysis of numerous measurements taken using the cryostat and 1 µm carbide laser.

CONCLUSIONS

- **Successfully produced thermal simulations** for bulk and membrane YBCO on sapphire samples.
- **Simulations agree with experimental data**.
- YBCO membranes on high thermal conductivity substrates **perform substantially better** than bulk YBCO.
- **Produced order-parameter simulation** for zero-gap superconductors using TDGL theory.
- **Vibration isolated cryostat was a great success** achieving < 5×10^{-9} hPa pressure under cryocooling and no visible vibration transfer.
- Cryostat enabled the **first testing of the qRIXS early science samples** at 1µm and high repetition rates.

ACKNOWLEDGEMENTS

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[3] Z. Chen *et al.*, Phys. Rev. Mater. 3, 060801(R) (2019)
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