



**University of Dundee**

## **An Antipolar-driven Ferroelectric**

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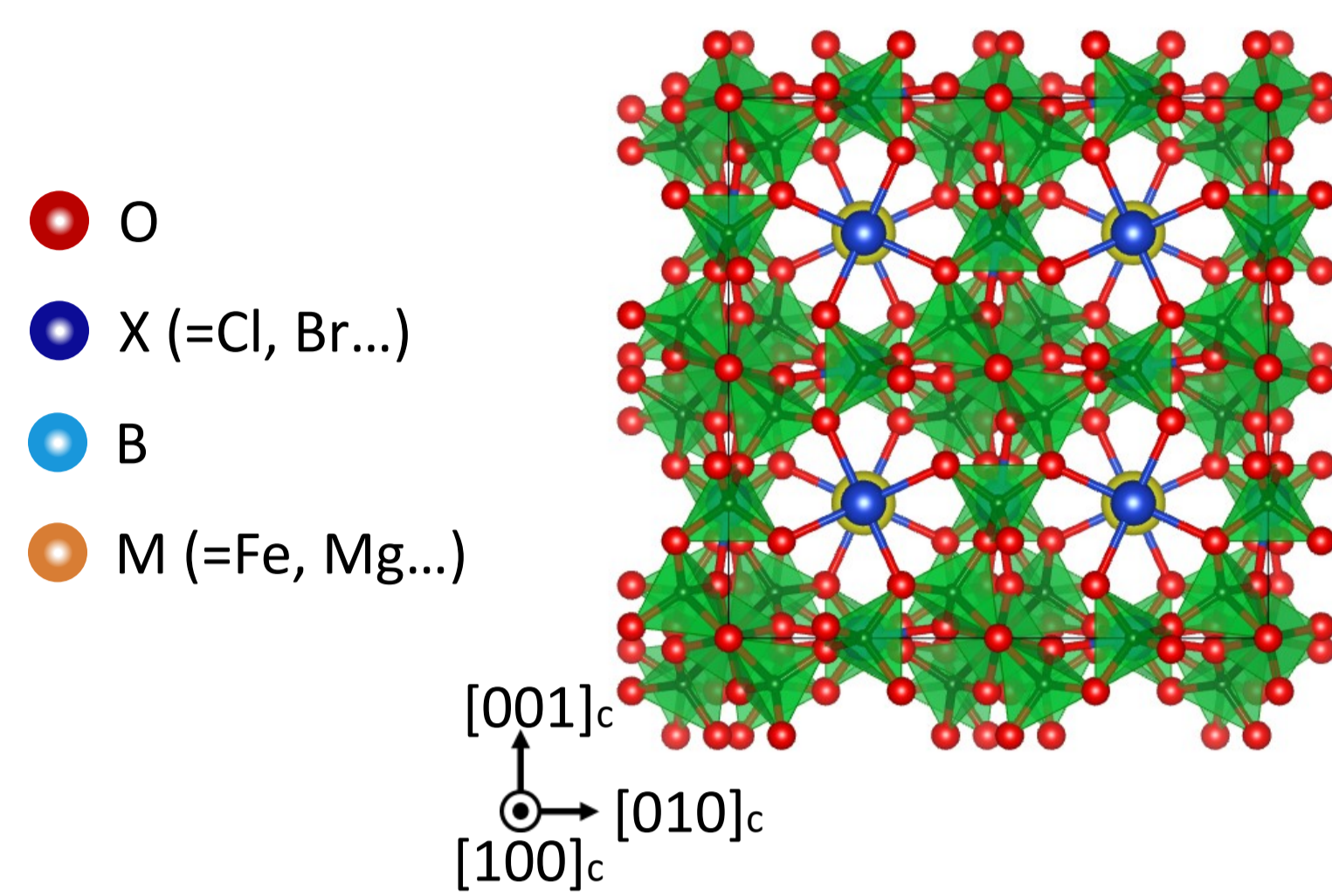
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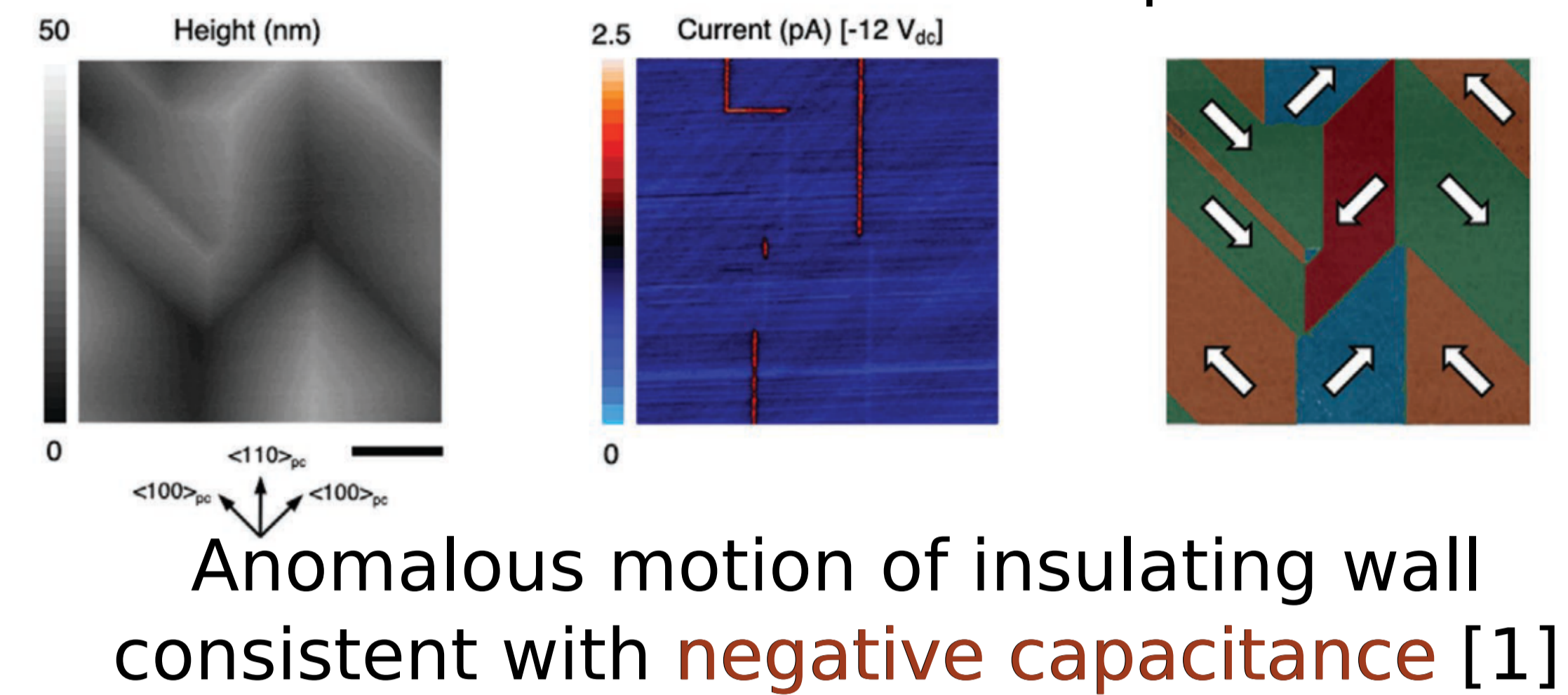
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## Boracite



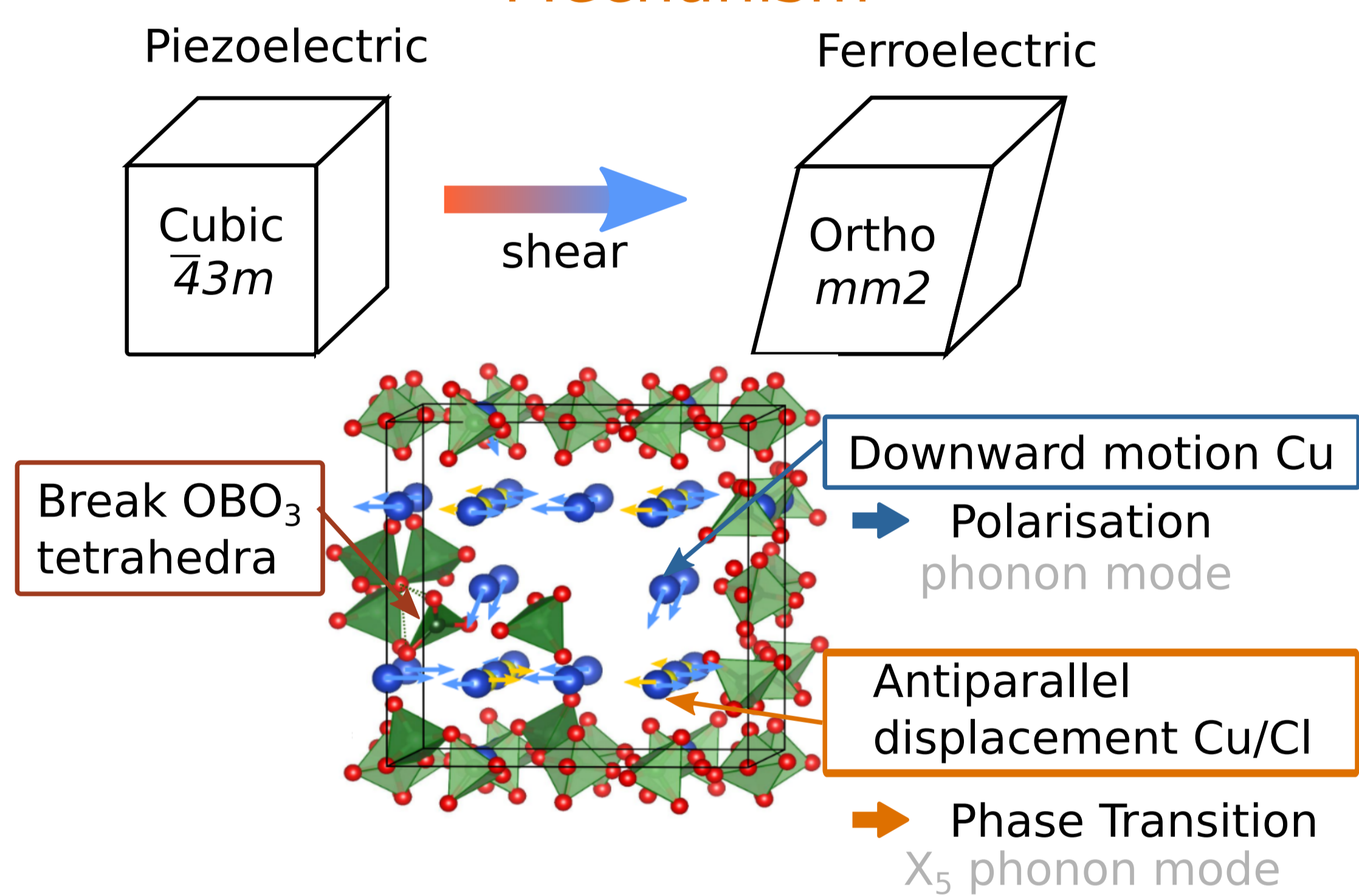
- Discovered in the XVIII century: "Lünenburger Diamanten"
- Dispute about its polarity for a long time
- Revival as class I multiferroic
- Strong potential for pyroelectricity

## Unusual Domain Wall Properties



## Phase transition

### Mechanism



### Landau expansion

Phase transition  $\bar{4}3m \rightarrow mm2$

$$G = \frac{1}{2}a(T - T_c)q^2 + \frac{1}{4}bq^4 + \frac{1}{6}cq^6$$

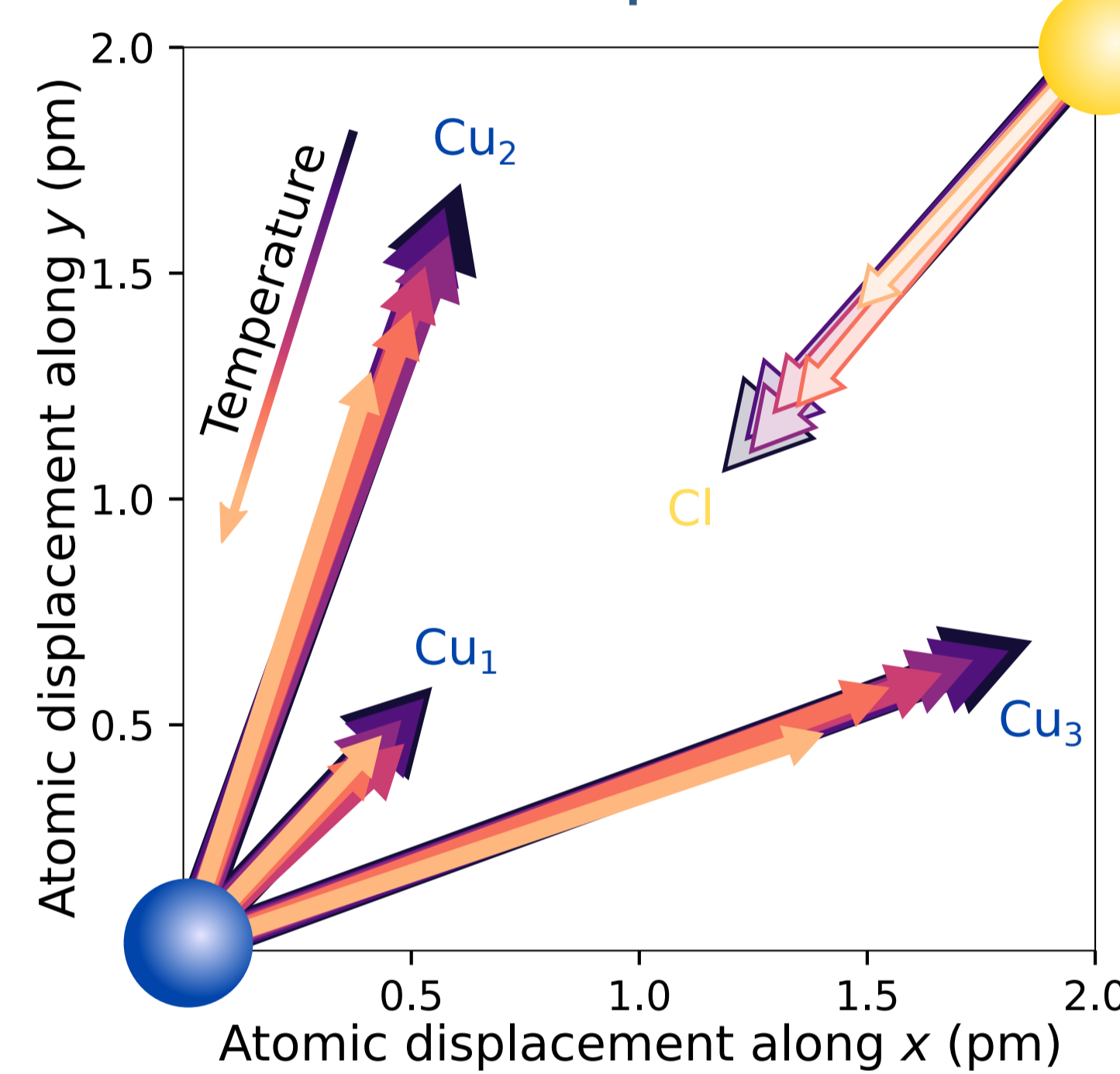
$$+ \lambda_1 e_v q^2 + \lambda_2 e_t q^2 + \lambda_3 e_6 q^2 + \lambda_4 e_6^2 q^2 + \lambda_5 (e_4^2 + e_5^2) q^2 + \lambda_6 e_4 e_5 q^2$$

$$+ \lambda_7 e_6 P + \lambda_8 e_v P^2 + \lambda_9 e_t P^2 + \lambda_{10} e_4 e_5 P + \lambda_{11} e_0 P^2 + \lambda_{12} q^2 P$$

$$+ \frac{1}{4}(C_{11}^0 - C_{12}^0)(e_0^2 + e_t^2) + \frac{1}{6}(C_{11}^0 - 2C_{12}^0)e_6^2 + \frac{1}{2}C_{44}^0(e_4^2 + e_5^2 + e_6^2) - EP$$

## Towards probing directly the order parameter

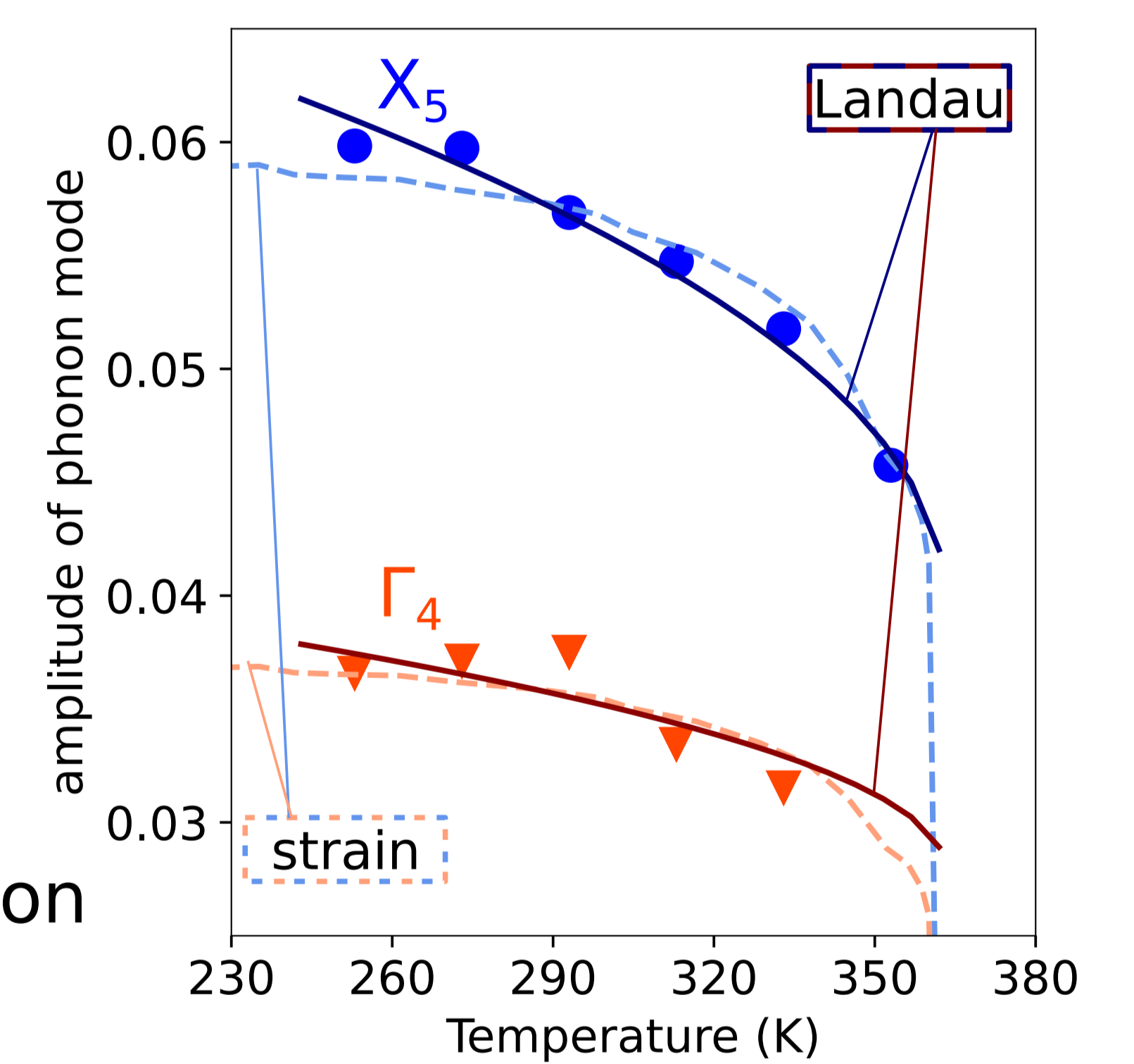
### Atomic displacement



Not full agreement between strain and phonon amplitude

Suggest **displacive** phase transition

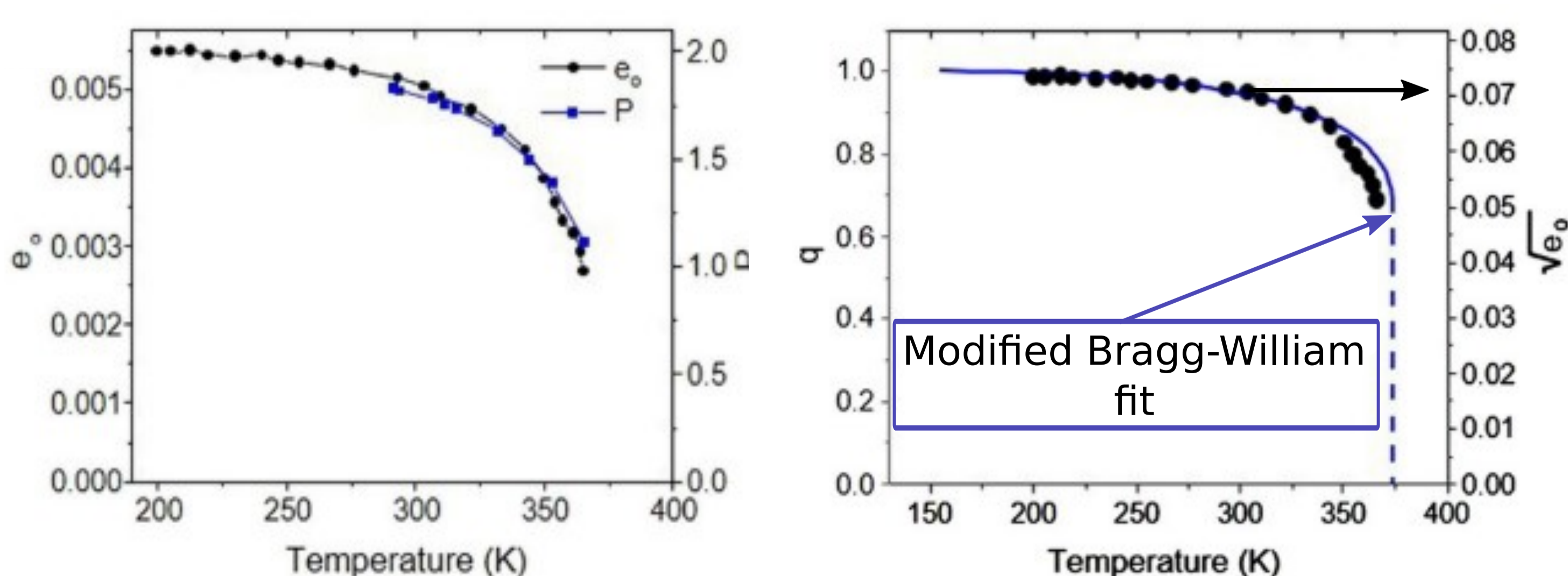
Separate the contribution of each phonon



## Phase transition- Macroscopic quantities

### Strain

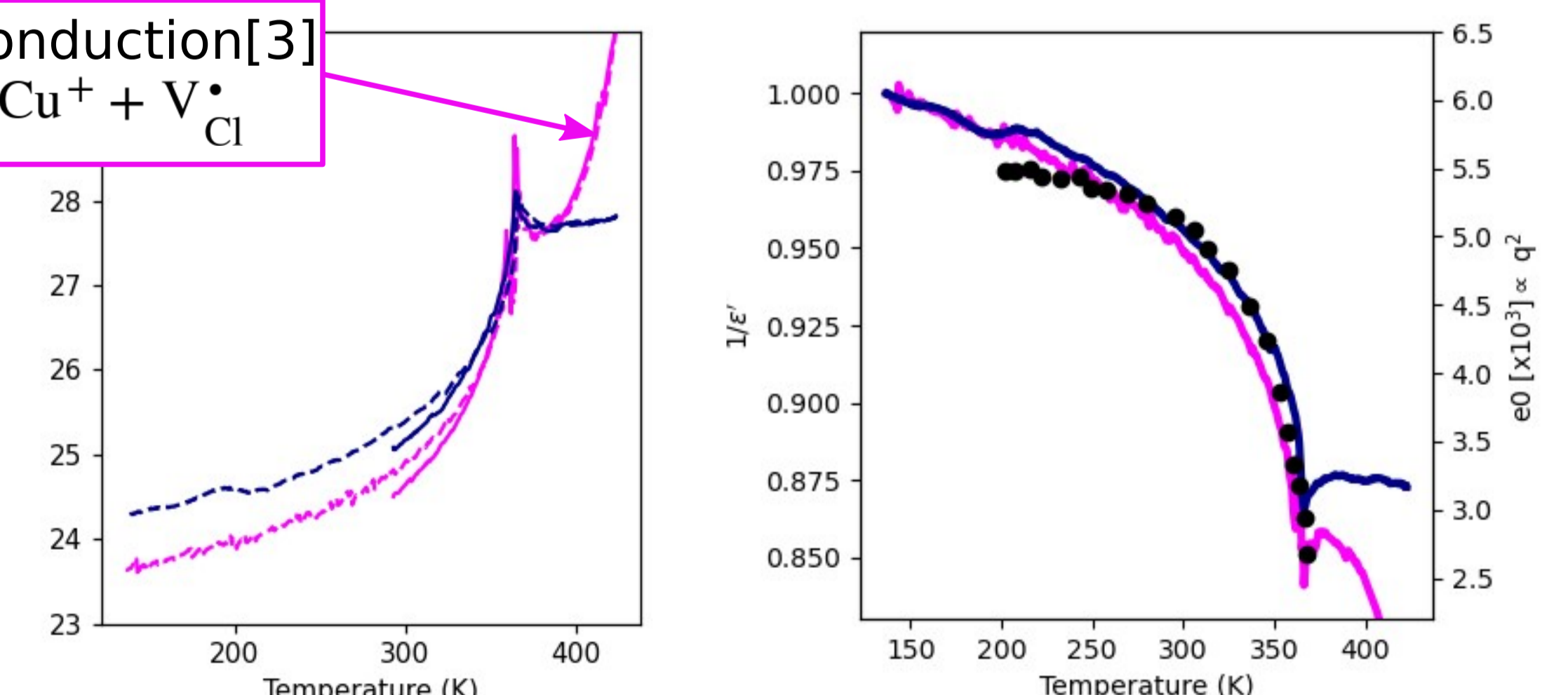
Good agreement between order-parameter and strain [2]



### Dielectric permittivity

Unusual temperature dependence  $\rightarrow$  Curie-Weiss

Relaxation+conduction [3]  
 $Cu^{2+} + O \rightarrow Cu^+ + V_{Cl}^{\bullet}$



Suggest **order-disorder** phase transition

## Conclusion

Ferroelectric phase transition driven by **antipolar** phonon modes

Attempt to **directly** probe the thermal evolution of the **order parameter**

## References

- [1] Guy, J. G. M. et al. Adv. Mater. 33, 2008068 (2021).
- [2] Fernandez-Posada, et al. J. Phys. Condens. Matter 33, 095402 (2021).
- [3] Cochard, C. et al. Appl. Phys. Lett. 119, 202904 (2021).

## Acknowledgment

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