Nickelate Superconductors

Charge density waves in infinite-layer $NdNiO_2$ nickelates

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Overview

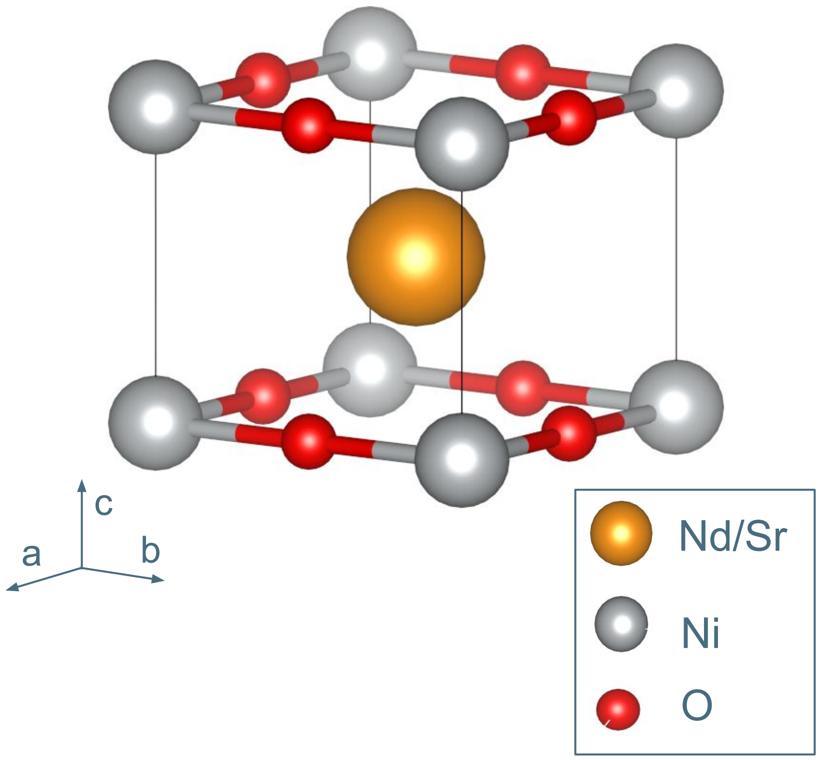
Infinite Layer Structure of $Nd_{0.8}Sr_{0.2}NiO_2$

Resonant Inelastic X-Ray Scattering

Methods and Key Findings

Infinite Layer Structure of $Nd_{0.8}Sr_{0.2}NiO_2$

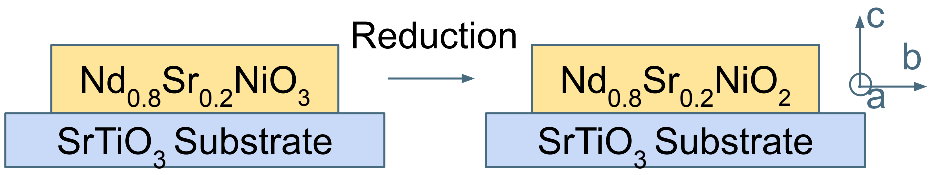
- Tetragonal unit cell†
  - a = b = 3.92Å
  - c = 3.36Å
- Neodymium/Strontium dopant in cell center
  - 80%/20% ratio
- “Layer” from cell repetition in a-b plane
  - “stacks” in c direction
- Macro material is a thin film
  - fewer c repetitions

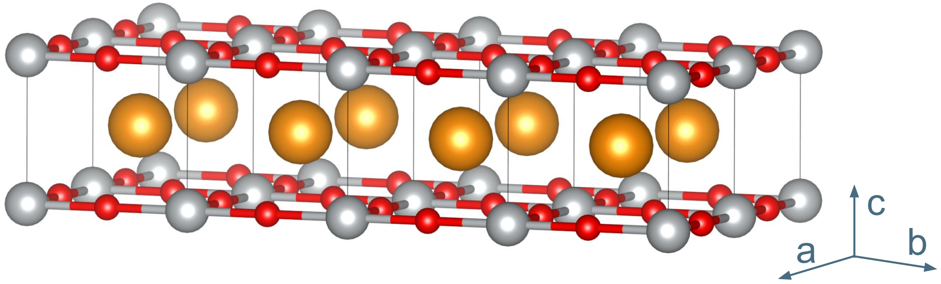


†Li, D., Lee, K., Wang, B.Y. et al.Nature 572, (2019). https://doi.org/10.1038/s41586-019-1496-5

Infinite Layer Structure of $Nd_{0.8}Sr_{0.2}NiO_2$

- **Thin Film** built with deposition and reduction process
- When not thin film, behaves as an insulator
  - Likely due to crystal defect, grain boundaries inhibiting conduction[†]
- Doping introduces holes enabling conductivity in the NiO_2 planes



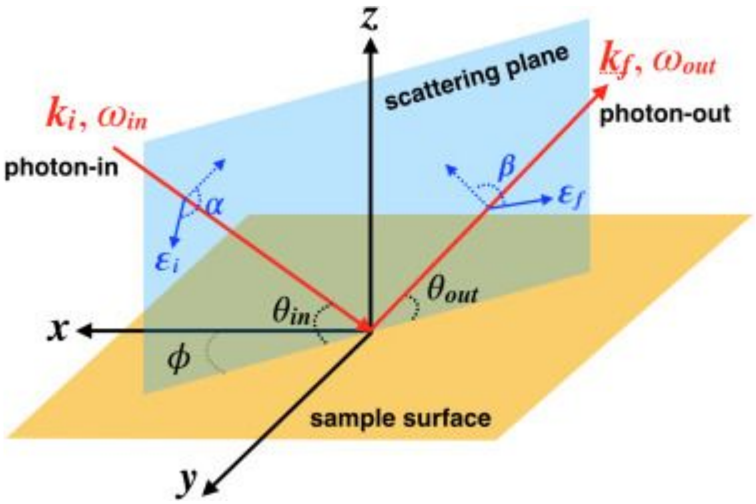


[†]Hu, K., Li, Q., et al. (2024). Nature communications, 5104 https://doi.org/10.1038/s41467-024-49533-1

Resonant Inelastic X-Ray Scattering (RIXS)

RIXS - Geometry

$$E_{loss} = \hbar\omega_{in} - \hbar\omega_{out}$$
$$\hbar\mathbf{q} = \hbar\mathbf{k}_i - \hbar\mathbf{k}_f$$
$$\theta = \pi - (\theta_{in} + \theta_{out})$$



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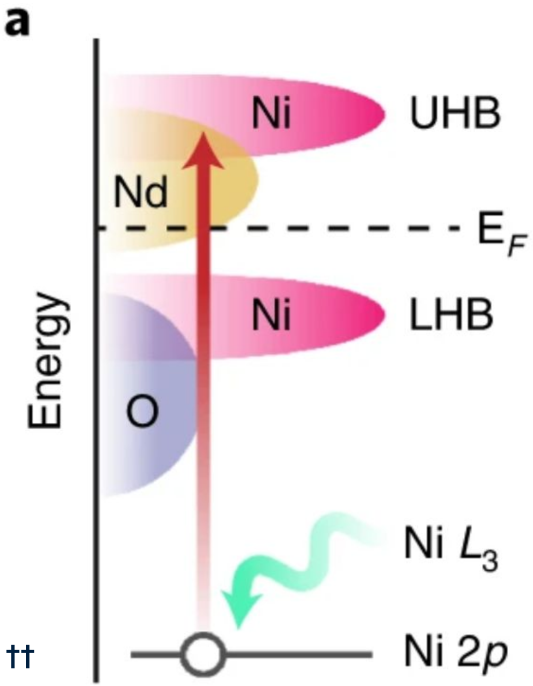
†Y.L. Wang, G. Fabbris, M.P.M. Dean, G. Kotliar. EDRIXS: An open source toolkit for simulating spectra of resonant inelastic x-ray scattering. *Computer Physics Communications*. 243, 151-165 (2019). https://doi.org/10.1016/j.cpc.2019.04.018.

RIXS - Resonance

X-Ray Energy is chosen to resonate with an absorption edge

Absorption Edge: An absorption edge corresponds to the minimum energy needed to excite a core electron into unoccupied states above the Fermi level.[†]



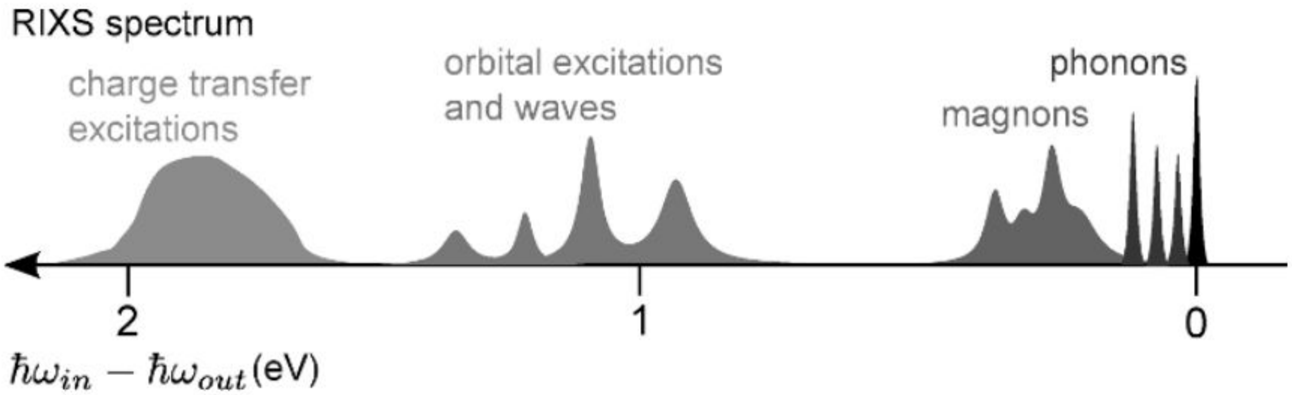
[††]

[†]T. Jo, X-Ray Absorption Spectroscopy. In: Encyclopedia of Condensed Matter Physics, *Elsevier*, 319-323 (2005). https://doi.org/10.1016/B0-12-369401-9/00670-7

[††]Tam, C.C., Choi, J., Ding, X. *et al.* Charge density waves in infinite-layer $NdNiO_2$ nickelates. *Nat. Mater.* 21, 1116–1120 (2022). https://doi.org/10.1038/s41563-022-01330-1

RIXS - Inelastic Scattering

Energy Transfer Spectrum



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†Chiuzbăian, S.G. (2013). A Student's Introduction to Resonant Inelastic Soft X-ray Scattering. In: Beaurepaire, E., Bulou, H., Joly, L., Scheurer, F. (eds) Magnetism and Synchrotron Radiation: Towards the Fourth Generation Light Sources. *Springer Proceedings in Physics*. 151. Springer, Cham. https://doi.org/10.1007/978-3-319-03032-6_6

RIXS - Significance

- **Range of Excitations**
  - Phonons and Magnons
  - Orbital Excitations and Waves
  - Charge Transfer Excitations
- **Low Energy Excitations**
- **Few Restrictions on Materials**
  - Solids, Liquids, and Gases
  - Thin Films and Single Crystals
- **Measurement Specificity**
  - Momentum
  - Element and Orbital
  - Polarization

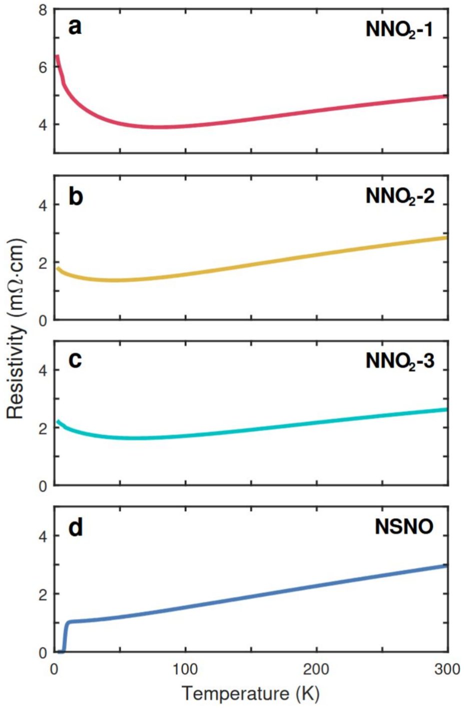
Methods and Key Findings

Unless noted, data and figures are taken from Tam, C.C., Choi, J., Ding, X. *et al.* Charge density waves in infinite-layer $NdNiO_2$ nickelates. *Nat. Mater.* 21, 1116–1120 (2022). https://doi.org/10.1038/s41563-022-01330-1

Methods - Meet the samples

- **$NdNiO_2$ - Parent Material**
  - 3 samples made, referred to as NNO_2-1, NNO_2-2, NNO_2-3
  - Each reduced at different temperatures
    - Reduction at 200 °C for NNO_2-1
    - Reduction at 220 °C for NNO_2-2
    - Reduction at 290 °C for NNO_2-3
- **$Nd_{0.8}Sr_{0.2}NiO_2$**
  - Referred to as NSNO
  - Reduced at 300 °C
- **No samples were capped with $SrTiO_3$ (Referred to as STO)**
  - Often done in many studies
  - This will become important later!

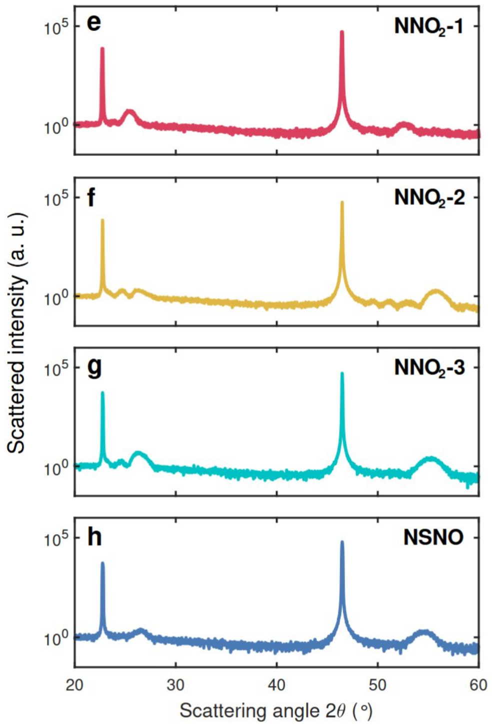
Methods - Initial Characterization (Resistivity)



- NNO_2-1, NNO_2-2, NNO_2-3 all exhibit weakly insulating behaviour
- NSNO exhibits superconductive behaviour at 10 K
  - Nickelate superconductivity predicted by substituting the copper of high Tc cuprate superconductors for nickel, seems to work![†]

[†]Tam, C.C., Choi, J., Ding, X. *et al.* Charge density waves in infinite-layer $NdNiO_2$ nickelates. *Nat. Mater.* 21, 1116–1120 (2022). https://doi.org/10.1038/s41563-022-01330-1

Methods - Initial Characterization (XRD)

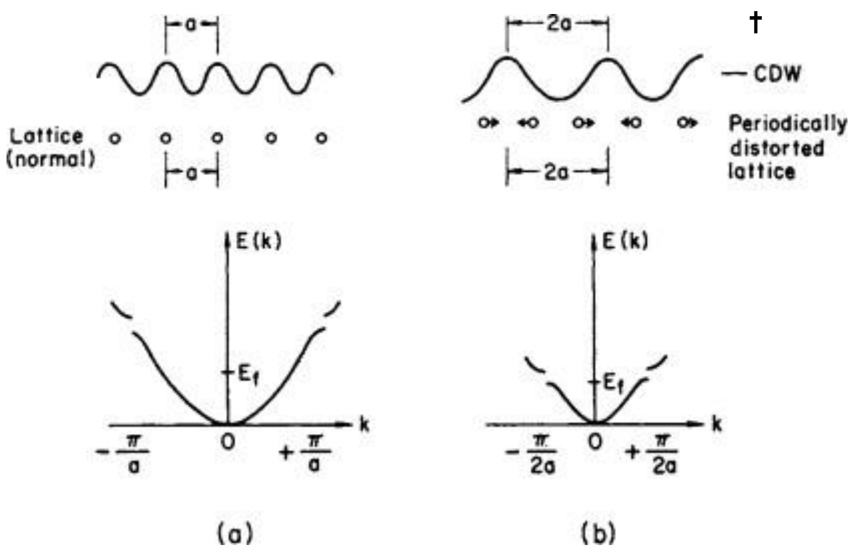


- Lattice Parameters determined using X-Ray Diffraction

Sample name	c lattice parameter (Å)
NNO_2-1	3.475
NNO_2-2	3.295
NNO_2-3	3.326
NSNO	3.363

Note - What are Charge Density Waves (CDWs)?

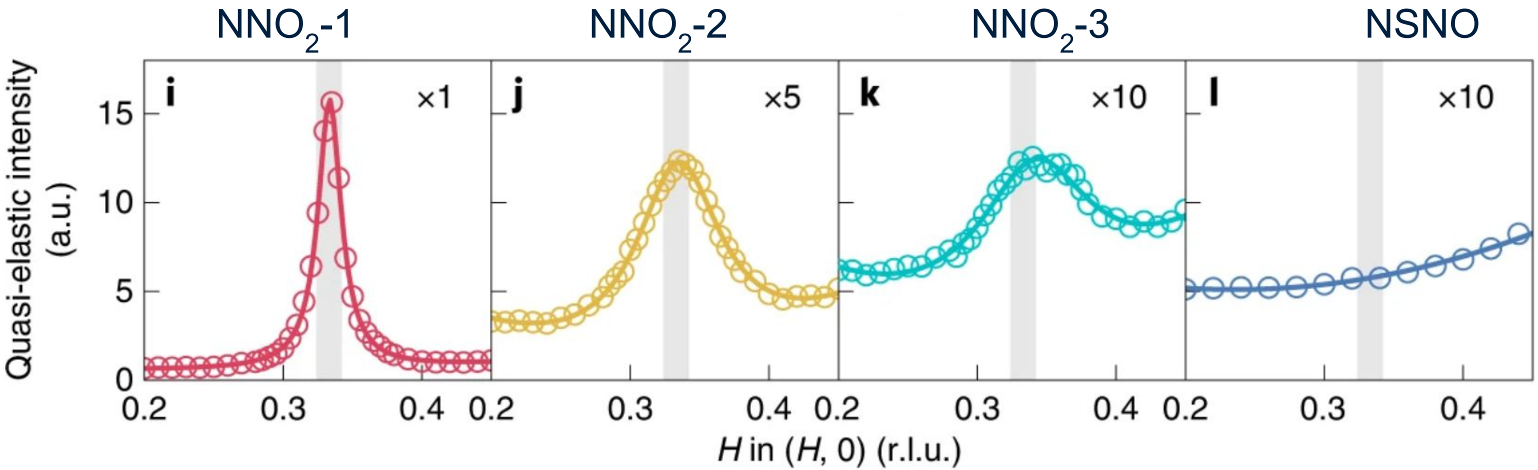
- "A charge density wave (CDW) is a static modulation of conduction electrons"†
- Distortions in the lattice lead to charge carriers (electrons or electron holes) grouping up periodically
- Lowers the Fermi energy
- Happens when energy "gain" from lowering Fermi energy outweighs energy "loss" from the strain on the lattice
- Why is this important? They show up in Cuprates††! What about Nickelates?



†Wayman, C. M., & Bhadeshia, H. K. D. H. (1996). CHAPTER 16 - PHASE TRANSFORMATIONS, NONDIFFUSIVE. In R. W. Cahn & P. Haasen† (Eds.), *Physical Metallurgy (Fourth Edition)* (Fourth Edition, pp. 1507–1554). doi:10.1016/B978-044489875-3/50021-1

††Tam, C.C., Choi, J., Ding, X. *et al.* Charge density waves in infinite-layer NdNiO2 nickelates. *Nat. Mater.* 21, 1116–1120 (2022). https://doi.org/10.1038/s41563-022-01330-1

Key Findings - Charge Density Waves in Nickelates?



- Momentum-dependent RIXS performed on samples, looking at only reciprocal lattice vectors in the (H, 0) direction (along r.l.v. h or k) or along (H, H) direction (along h+k)
- Peaks correspond to charge density waves corresponding to specific periodicities
- No peaks found for any (H, H)
- Any peaks for NSNO? NS**NO** peaks!
    - Why? Electronic structural shifts because of the doping! Nd 5d e^- → Ni 3d e^-

Key Findings - The Implications

- "The results for both parent and superconducting samples suggest that the Nd 5d hybridized orbital actively contributes to CDW ordered states in infinite-layer nickelates."[†]
- The Nd atom's orbitals contributes to charge density waves in Nickelates!
  - This doesn't occur in Cuprates - "conventional CDWs are normally hosted in the CuO_2 layers rather than in the spacer-layers, and are quasi-two dimensional"[†]
- Examination of these CDWs along L direction (c direction) shows dependence
  - CDWs may be 3D!
- Inversely proportional to temperature, same as Cuprates
- Previous RIXS studies on STO-capped $NdNiO_2$ films showed no CDW signals
- Maybe a connection between CDWs and superconductivity?
  - If Nd 5d states are important, then CDW may compete with superconductivity!

[†]Tam, C.C., Choi, J., Ding, X. *et al.* Charge density waves in infinite-layer $NdNiO_2$ nickelates. *Nat. Mater.* 21, 1116–1120 (2022). https://doi.org/10.1038/s41563-022-01330-1

Any Questions?
We may have answers!

Thank you for listening!