Lattice Dynamics
of
Relaxor Ferroelectrics

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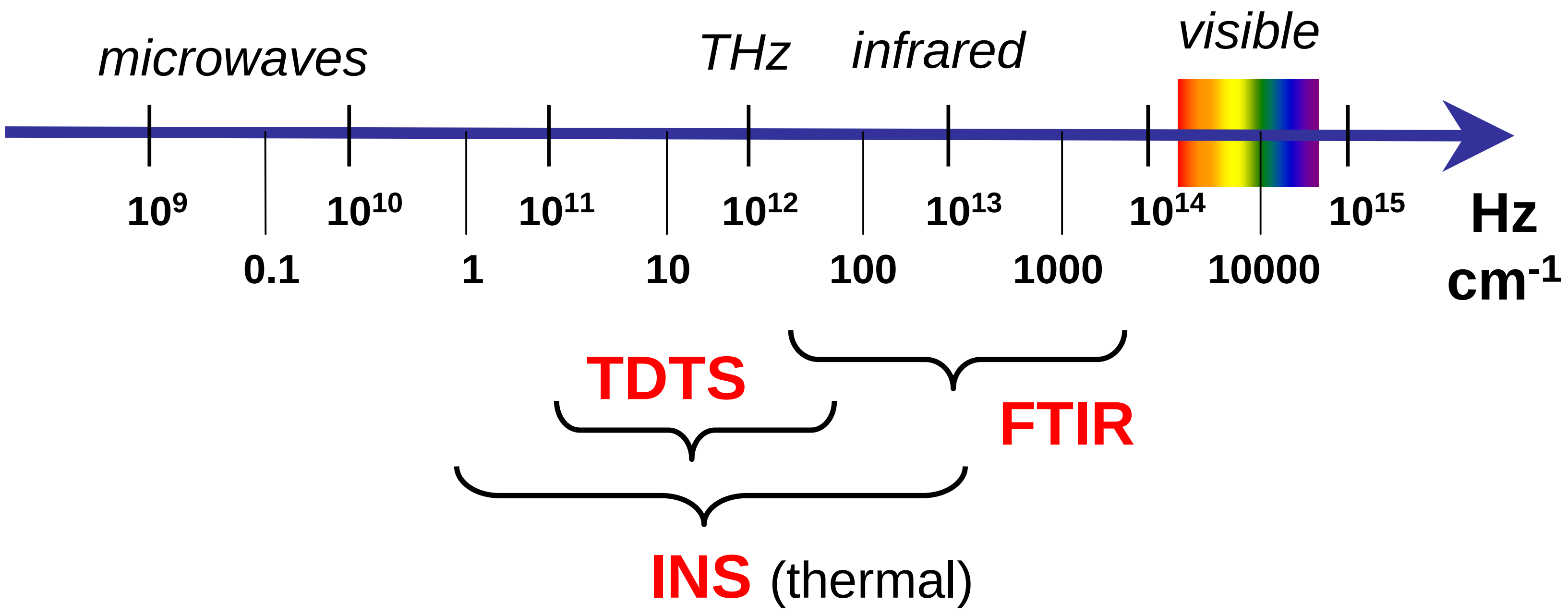
Experimental Techniques



- Inelastic Neutron Scattering spectroscopy (**INS**)
- Fourier Transform Infrared Spectroscopy (**FTIR**)
  - conventional, high resolution, intensity of transmission / reflection
- Time Domain Terahertz Spectroscopy (**TDTS**)
  - both Re & Im part of permittivity

Relaxors: properties

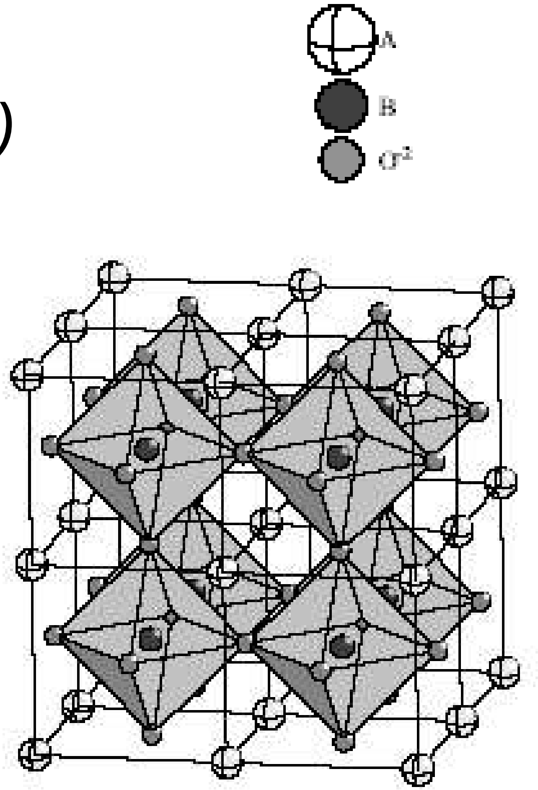
- In **relaxor ferroelectrics** (relaxors) the **ferroelectric** (FE) **state** originates only in **nanoscopic regions** – dynamical polar nanoclusters, related to the **structural disorder**
- Anomalously high material constants (permittivity; piezoelectric, pyroelectric, electrostriction coefficients...)
  ➔ interesting applications
  (e.g. piezoelectric devices, capacitors, FE-RAMs)
- Essential processes in relaxors:
  - lattice vibrations
  - relaxational dynamics

  ➔ dielectric dispersion in wide frequency and temperature ranges

Investigated materials

“Common features, similar properties”

- *(Disordered ferroelectric $BaTiO_3$)*
- Relaxor FEs – perovskite structure **ABO_3**
  (more B-sites: single ➔ complex perovskite)
  - $Pb(Zn_{1/3}Nb_{2/3})O_3$ – 8% $PbTiO_3$ (**PZN-PT**)
  - $Pb(Mg_{1/3}Nb_{2/3})O_3$ (**PMN**)
  - $Pb(Sc_{1/2}Ta_{1/2})O_3$ (**PST**)
    ➔ ordered
    ➔ disordered
    } with respect to B-sites



$PbTiO_3$: ferroelectric, tetragonal below T_c=760 K

Polar modes in perovskite relaxors

- TO1: soft mode
  - follows Cochran law $$\boxed{\omega_{SM}^2 = A(T_d - T)}$$

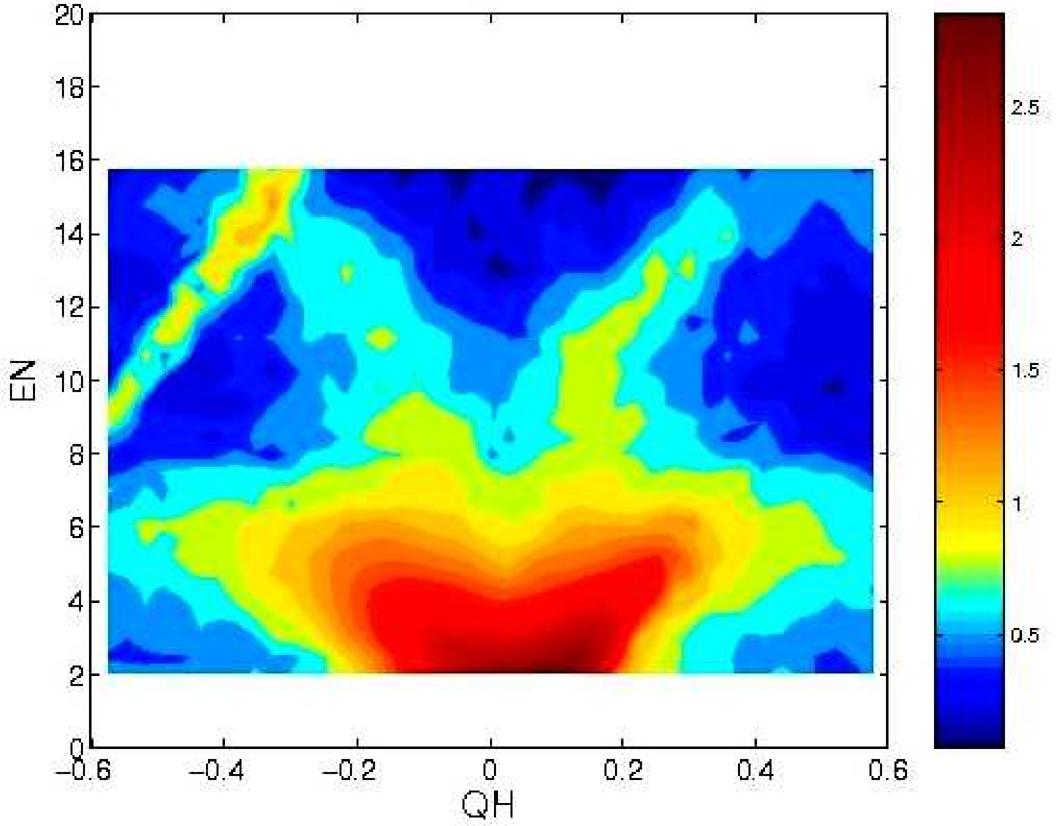
T_d … Burns temperature

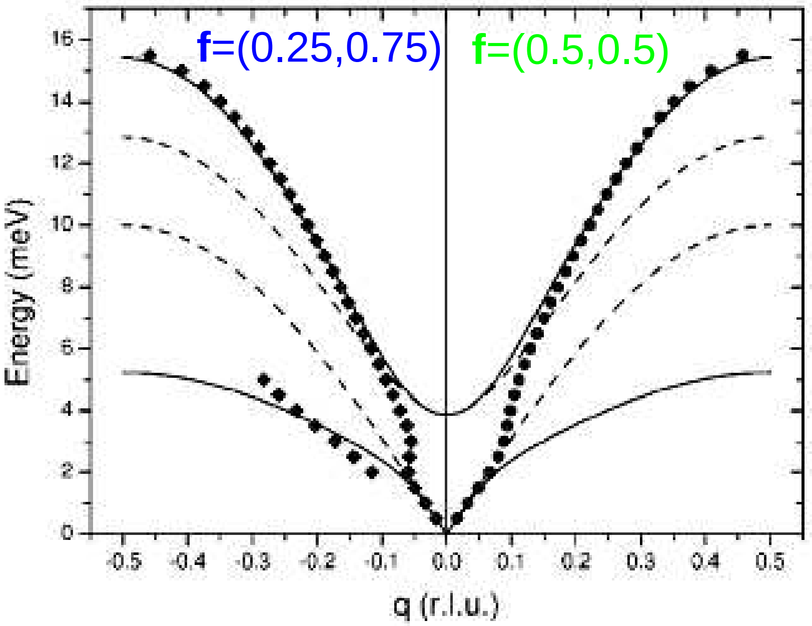
- CM: central mode
  - usually splits into 2 or 3 components
  - the mean relaxation time obeys Vogel-Fulcher law $$\boxed{\tau = \tau_0 \exp\left(\frac{U}{T - T_f}\right)}$$
- Other modes…

T_f … freezing temperature

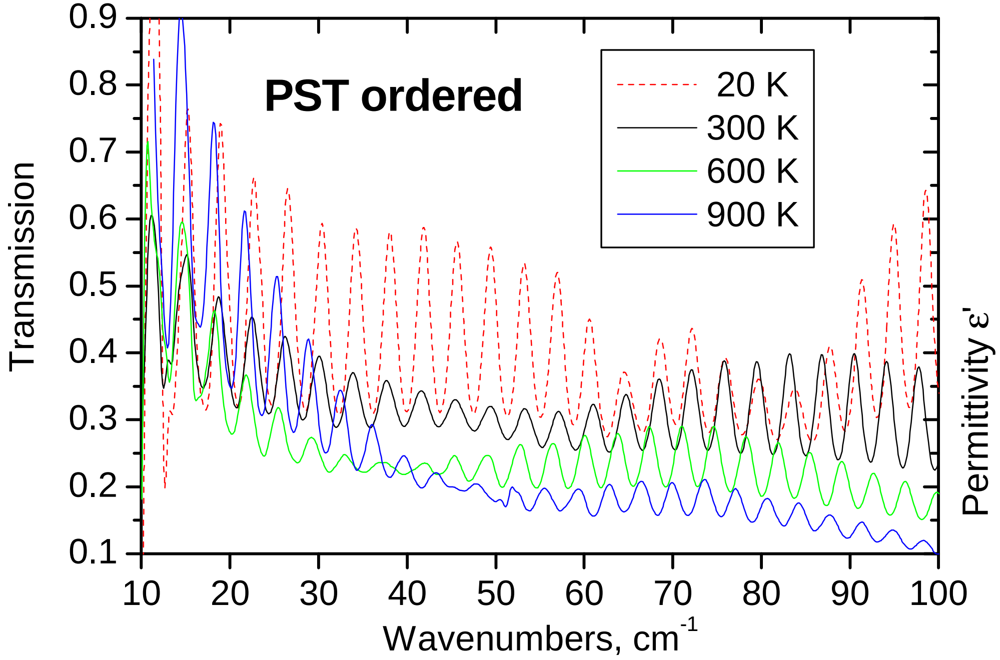
PZN-PT [$Pb(Zn_{1/3}Nb_{2/3})O_3$ – 8% $PbTiO_3$]

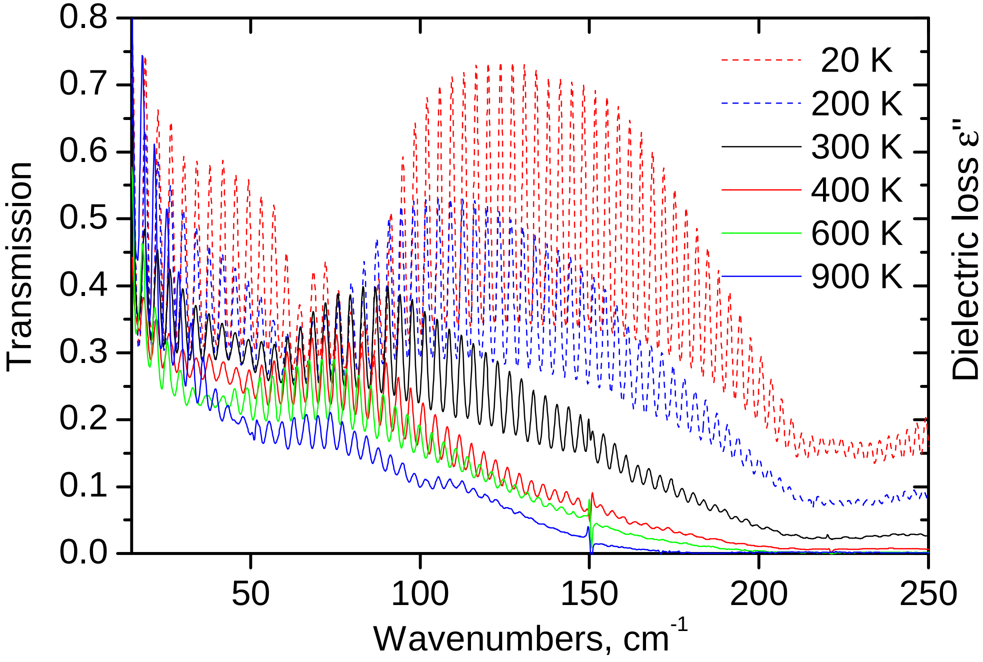
- "waterfall effect": upper branch rapidly drops into lower branch at a finite value of ***q***: $\boxed{q_{wf} \sim 0.2\ A^{-1}}$
- can be explained by classic interference of line shape anomalies due to the TA–TO coupling



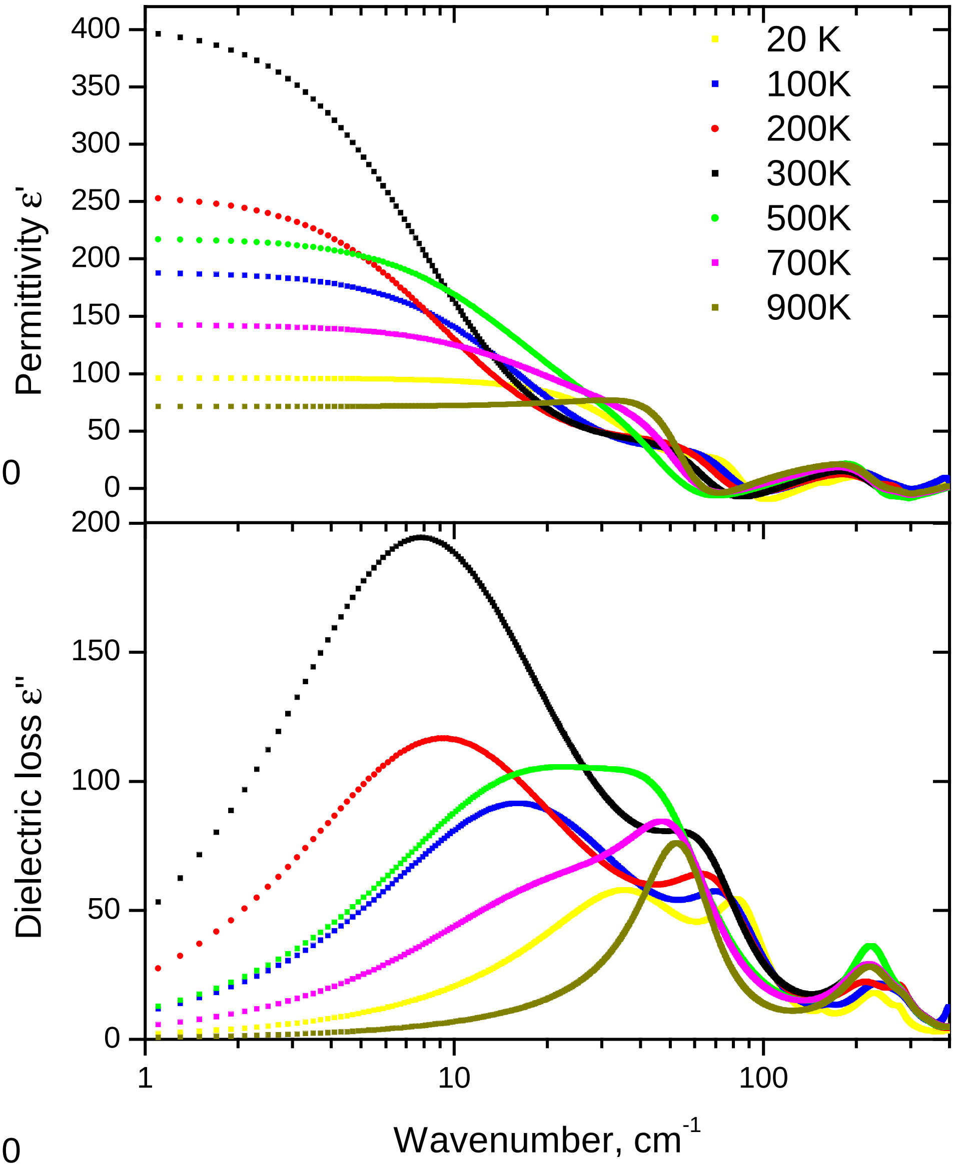


J. Hlinka et al.,
PRL **91**, 107602 (2003)


PST ordered
20 K
300 K
600 K
900 K
Transmission
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
Wavenumbers, cm^{-1}
10
20
30
40
50
60
70
80
90
100


20 K
200 K
300 K
400 K
600 K
900 K
Transmission
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Wavenumbers, cm^{-1}
50
100
150
200
250

PMN


20 K
100K
200K
300K
500K
700K
900K
Permittivity ε'
0
50
100
150
200
250
300
350
400
Dielectric loss ε''
0
50
100
150
200
1
10
100
Wavenumber, cm^{-1}

Relaxors: Future Research

- following INS experiments at ILL
- describe the “waterfall effect” in details
- assign the phonon branches
  (or phonon modes, respectively)
  from various methods
  to physical processes in relaxors
- characterize temperature dep. of the modes