LA-UR-20-23581
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Title: Ultrafast Acoustic Phonon Dynamics in the Weyl Semimetal TaAs Probed by Time-Resolved X-ray Diffraction

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Intended for: CLEO20, 2020-05-11/2020-05-15 (San Jose, California, United States)

Issued: 2020-05-13

Ultrafast Acoustic Phonon Dynamics in the Weyl Semimetal TaAs Probed by Time-Resolved X-ray Diffraction

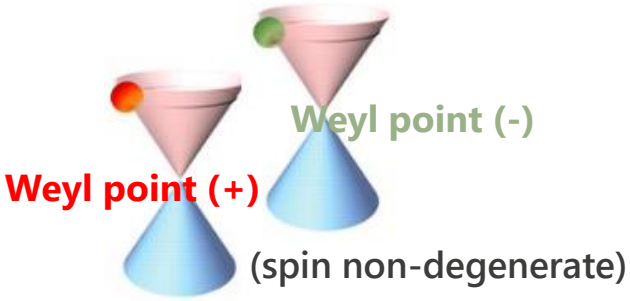
Min-Cheol Lee

May 14, 2020

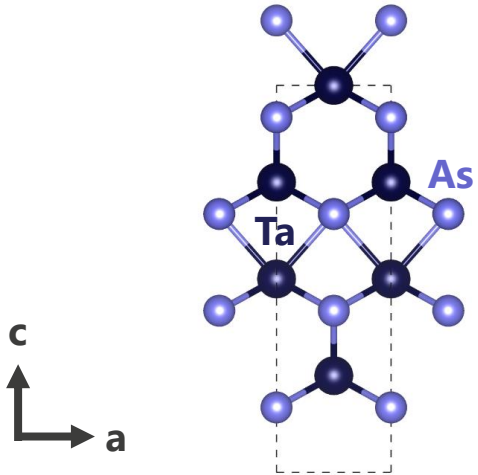
Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

Weyl Semimetal TaAs

Weyl semimetals



(spin non-degenerate)



Thermoelectricity
thermoelectric figure of merit

$$zT = \frac{S^2 \sigma T}{\kappa}$$

- σ: electric conductivity
- κ: thermal conductivity

TaAs
Good thermoelectricity!

High σ
due to massless dispersion

Low κ
due to heavy ions (Ta & As)

	TaAs*	Graphene**
σ ($\Omega^{-1}cm^{-1}$)	10^8	10^6
κ (W/mK)	22.00	3300
zT	0.15	0.00055

parameters @T = 300 K

*Nano Energy **30**, 225 (2016)
2D Mater. **4, 025019 (2017)

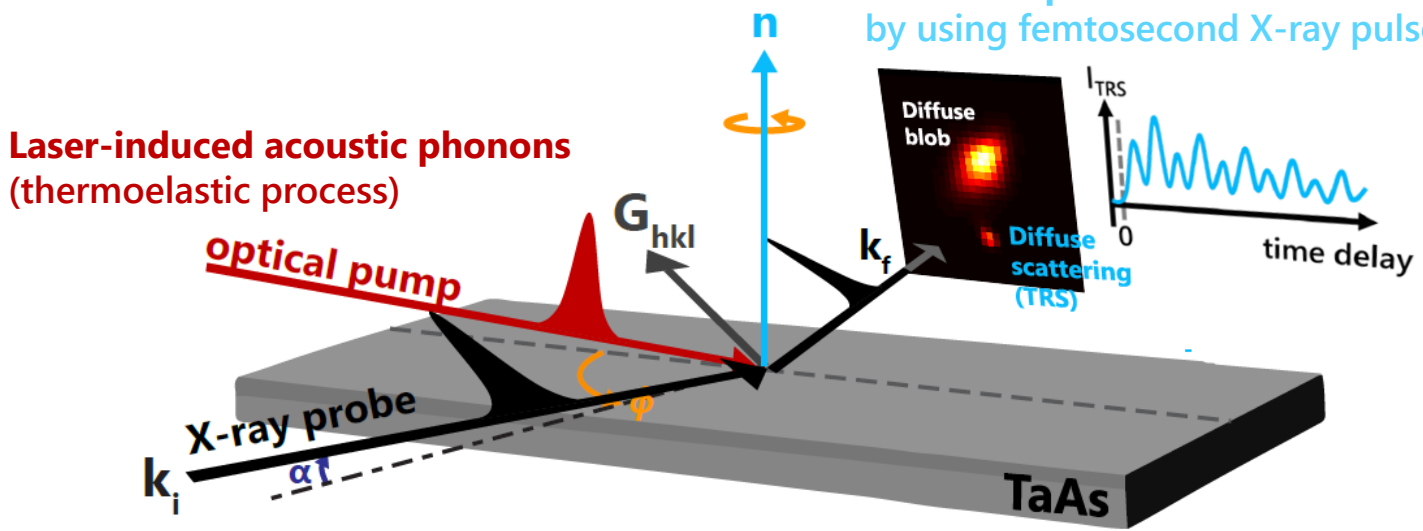
Experiment: optical-pump & X-ray-probe spectroscopy

Thermoelectricity

How are the electronic structure and the crystal lattice coupled in **TaAs**?

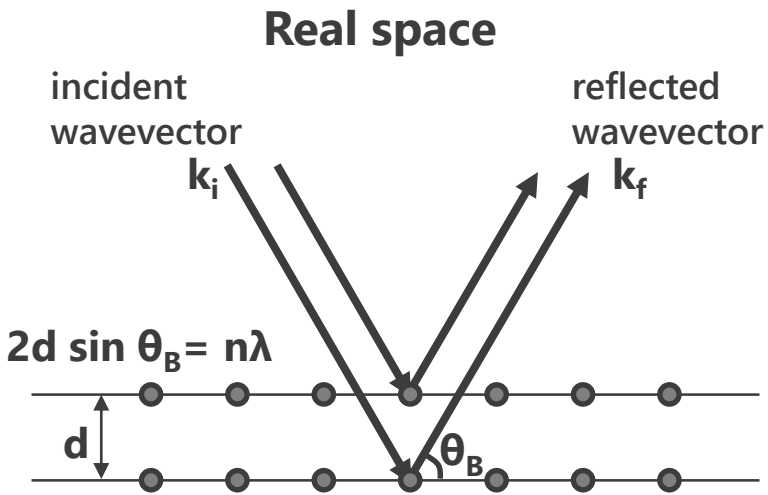
→ *acoustic phonon* + *electron-phonon coupling*

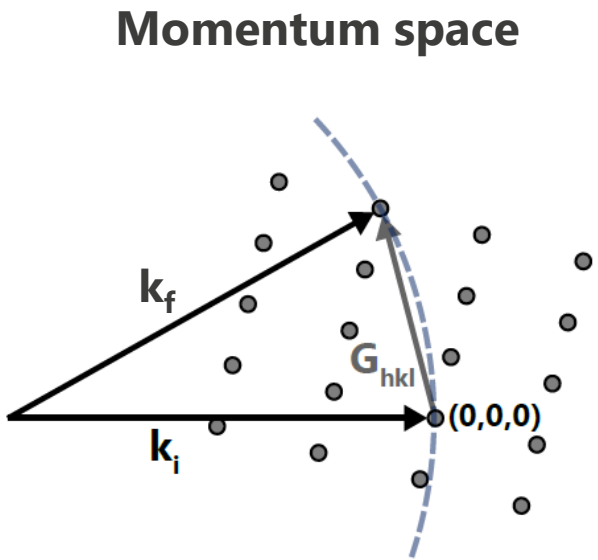
Real-time phonon observation
by using femtosecond X-ray pulses



Experiment @ SLAC / LCLS

Bragg Diffraction

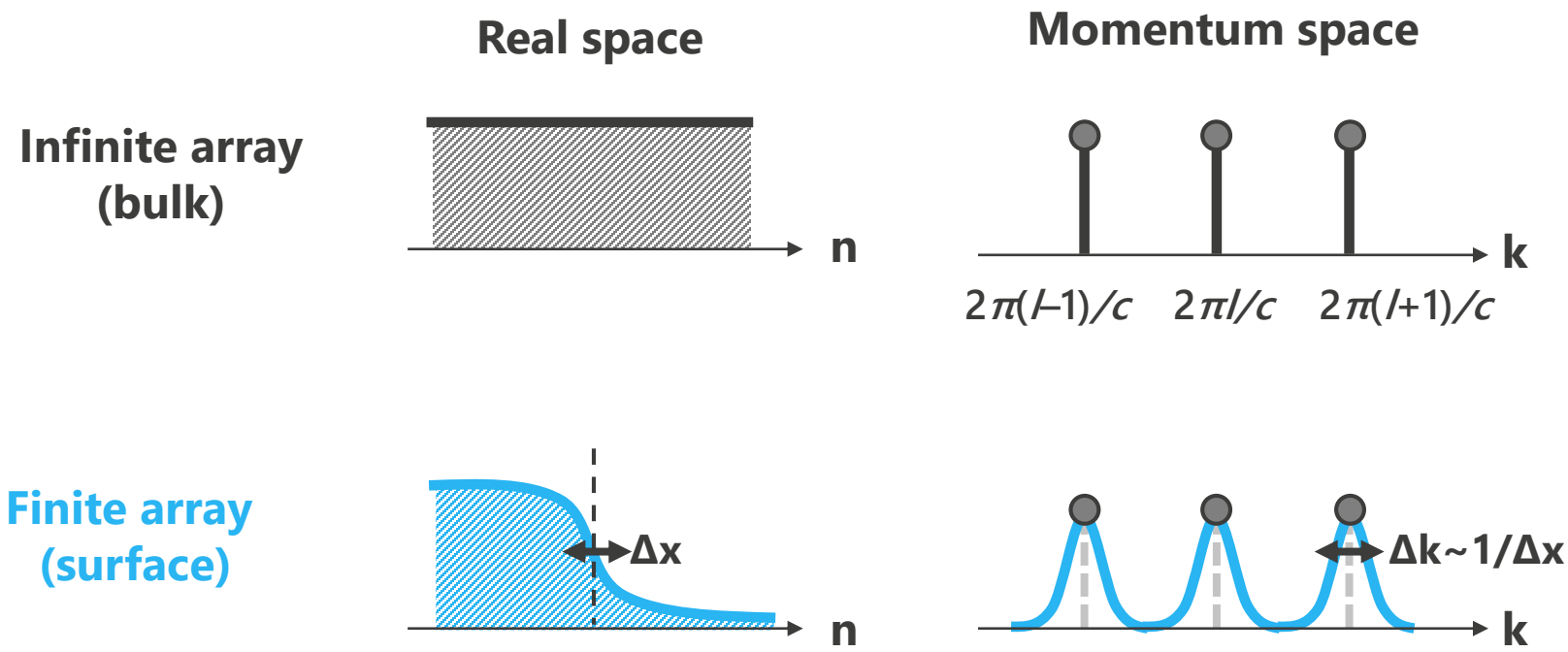




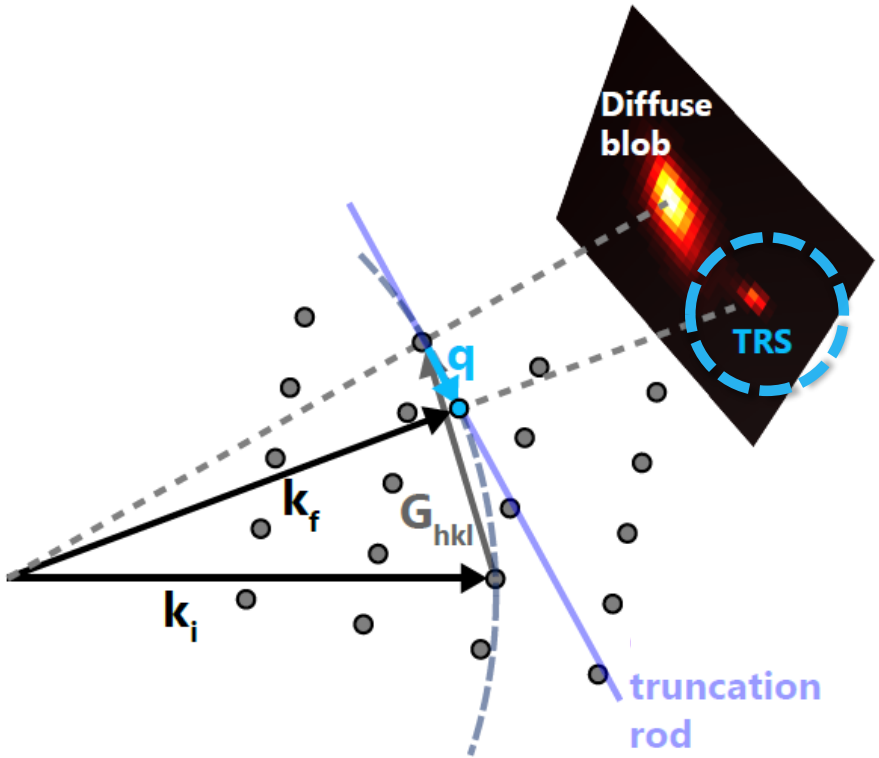
reciprocal
lattice vector

$$k_f - k_i = G_{hkl}$$

Bragg Rod (Truncation Rod) Scattering



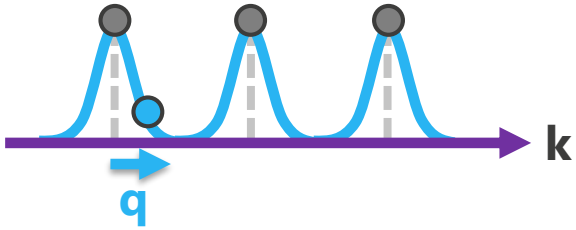
Bragg Rod (Truncation Rod) Scattering



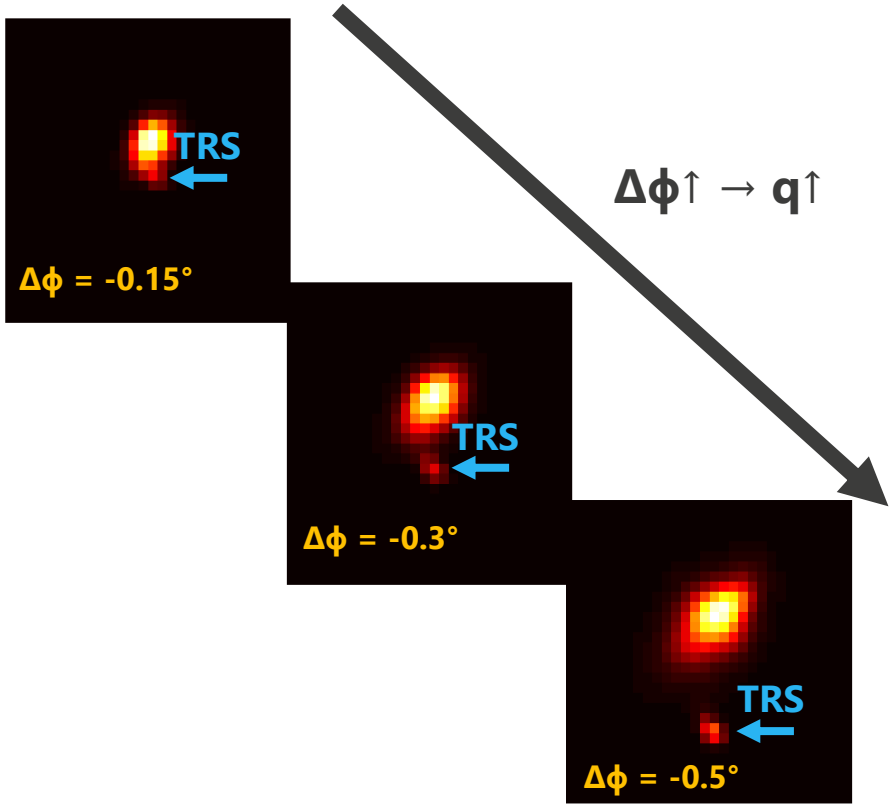
Momentum space

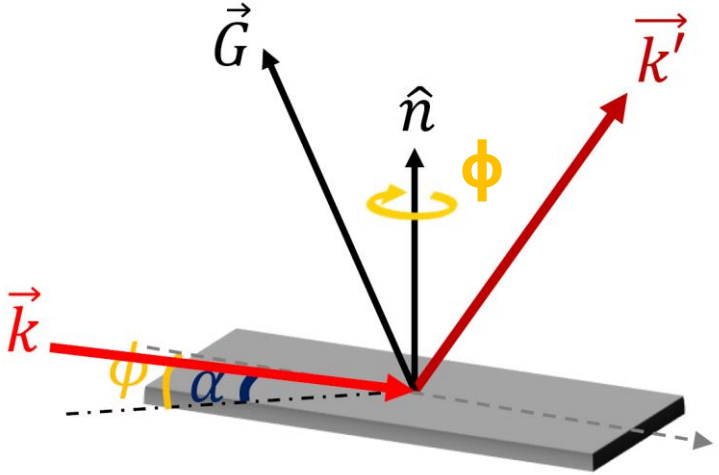
$$k_f - k_i = G_{hkl} + q$$

phonon momentum!



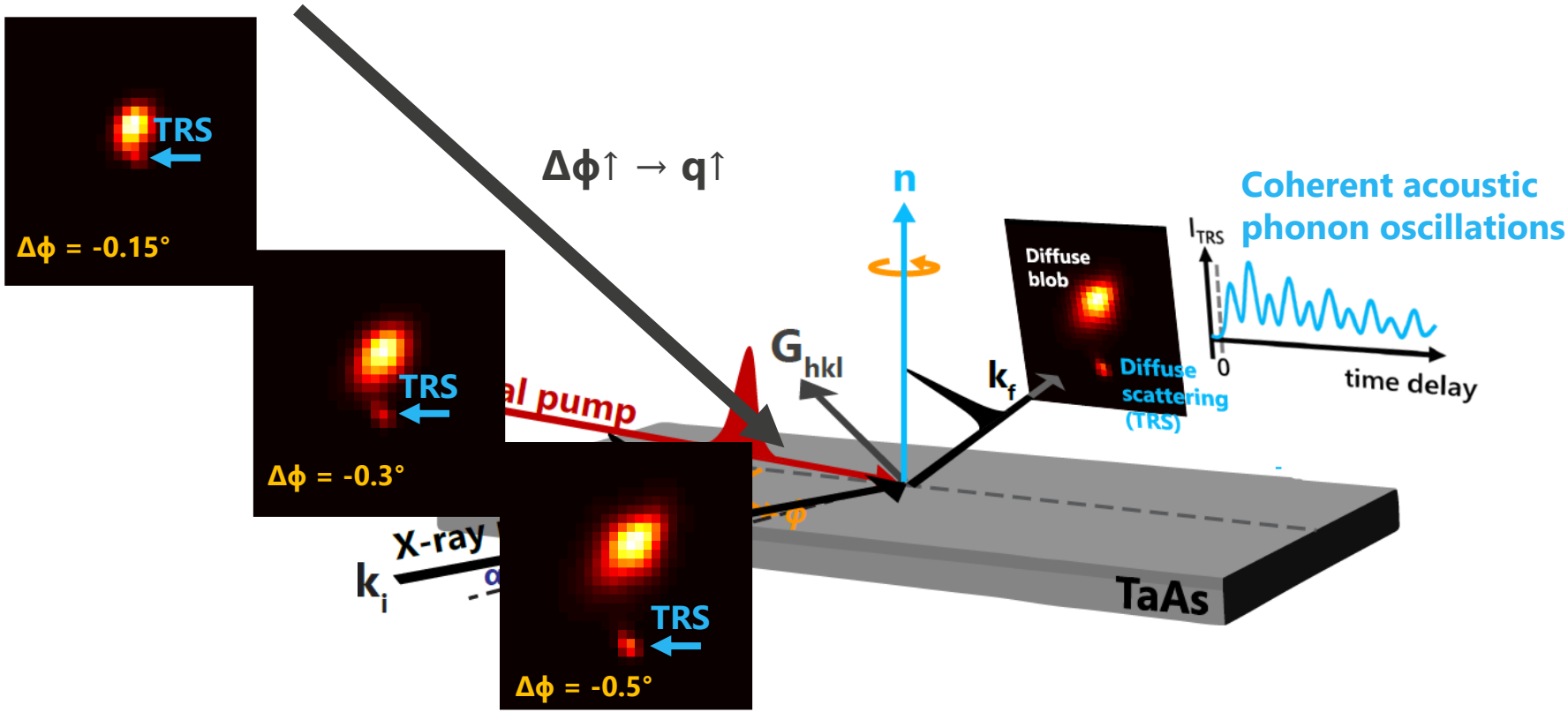
Truncation Rod Scattering in TaAs





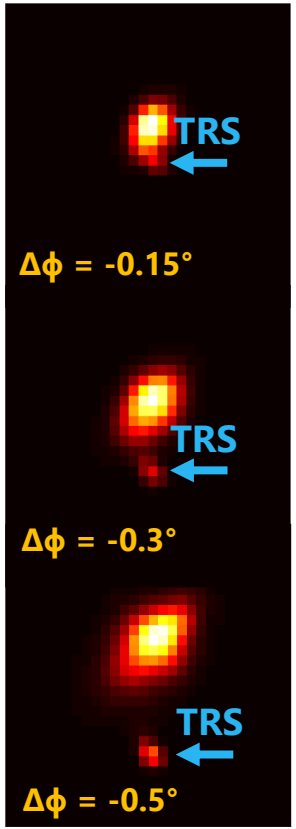
$Q = G_{hkl} + q = (1\ 0\ 3) + \xi(1\ 1\ 2)$

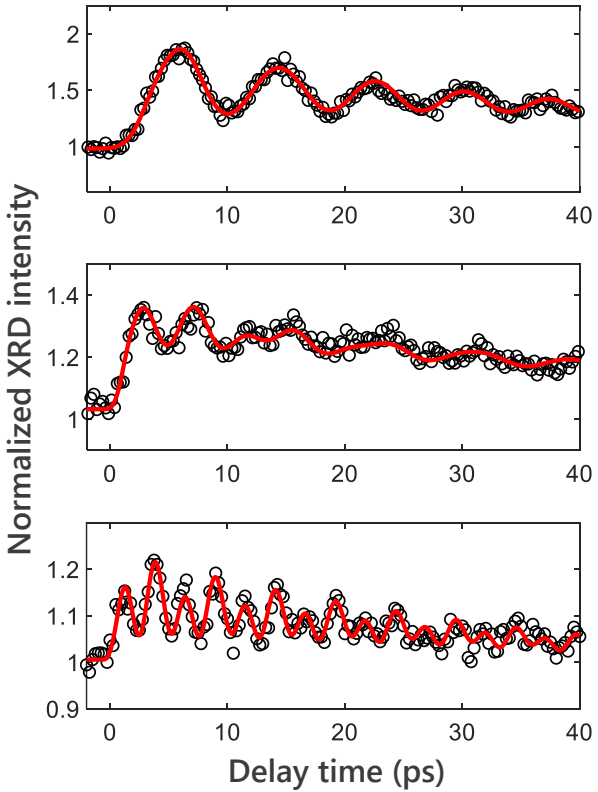
Truncation Rod Scattering in TaAs

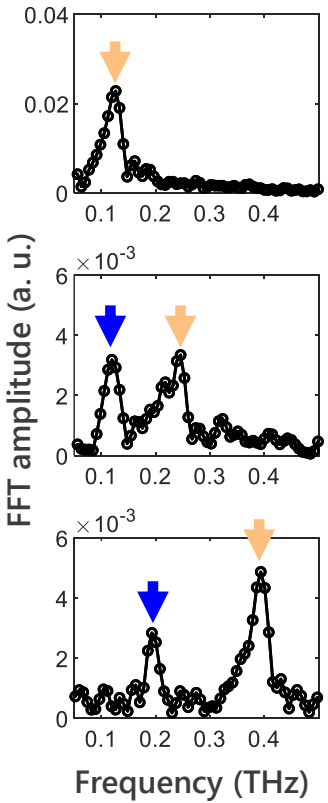


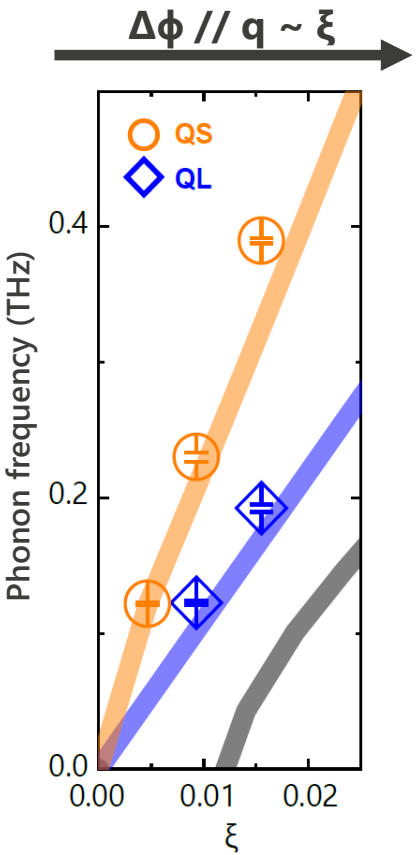
$Q = G_{hkl} + q = (1\ 0\ 3) + \xi(1\ 1\ 2)$

Coherent Acoustic Phonon Oscillations



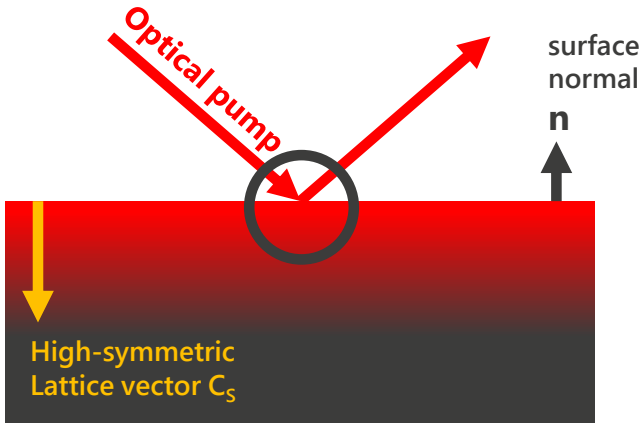


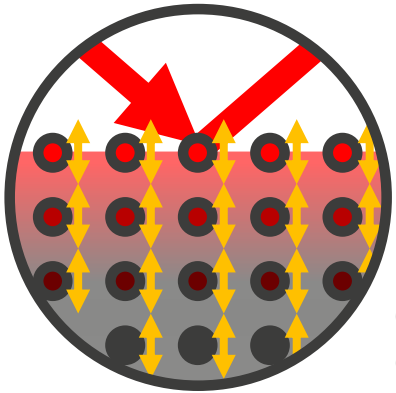




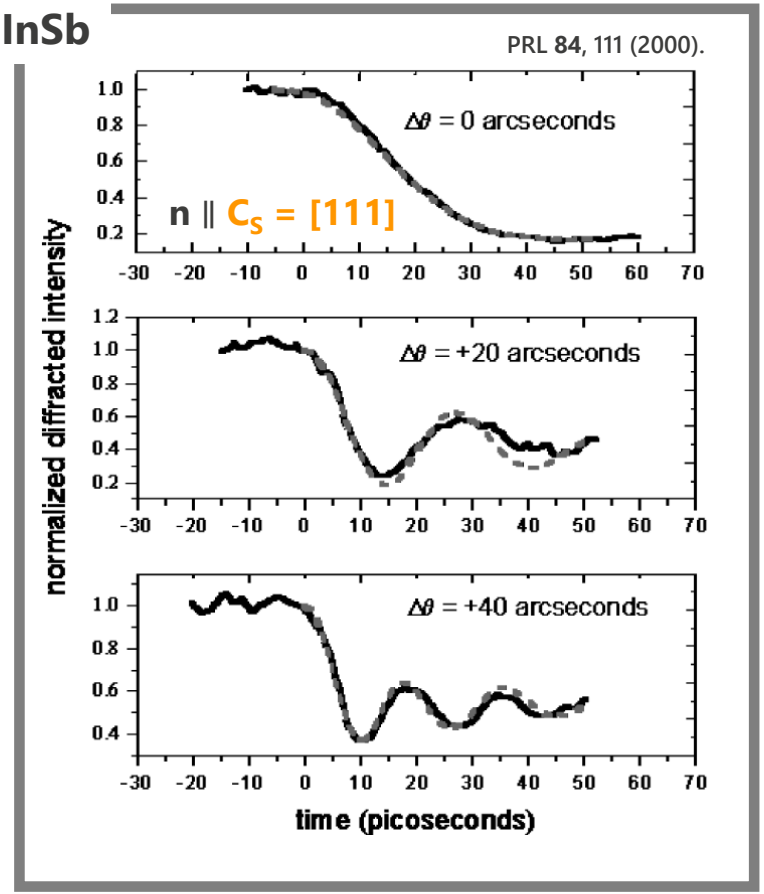
$Q = G_{hkl} + q = (1\,0\,3) + \xi(1\,1\,2)$

Acoustic Shear-mode Observation

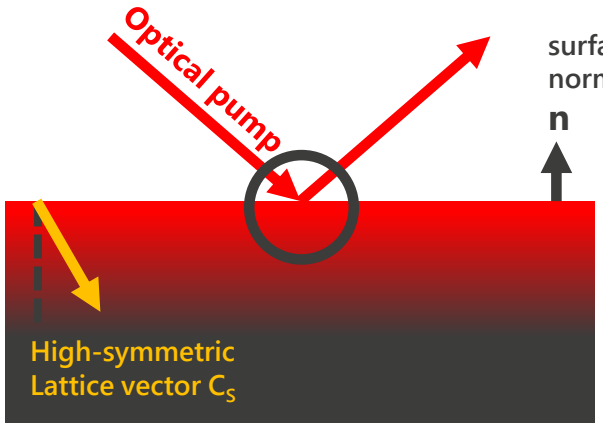


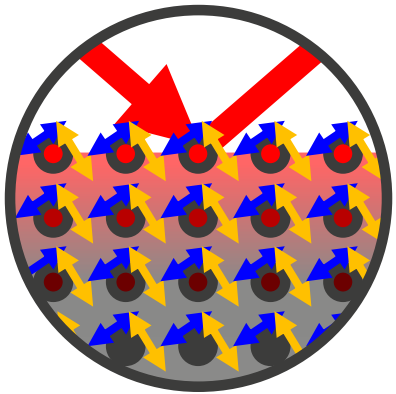


Only **Longitudinal mode** observed when **n** ∥ C_S



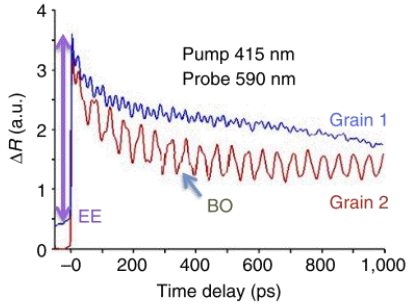
Acoustic Shear-mode Observation

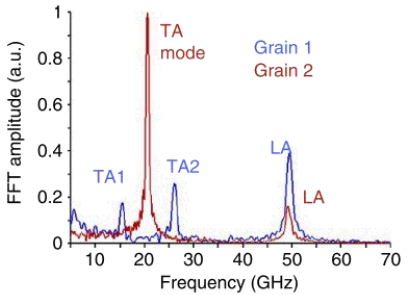




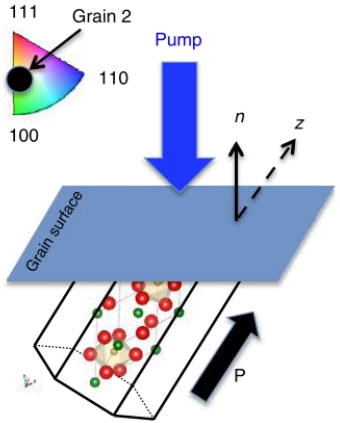
(Quasi-)Shear mode
also can be observed!

$BiFeO_3$



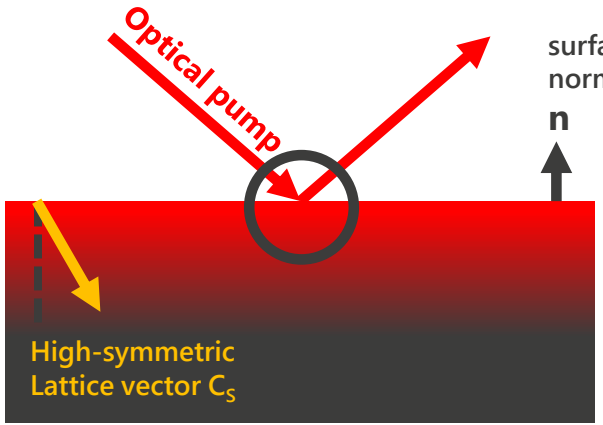


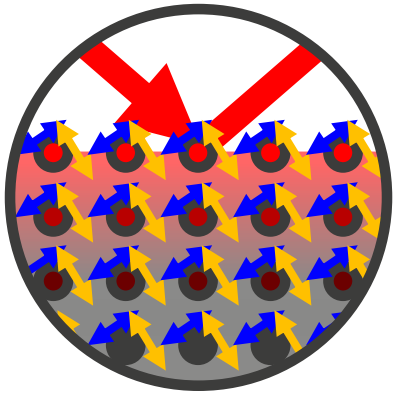
Nat. Commun. **5**, 4301 (2014).



The shear mode has been observed by optical probes

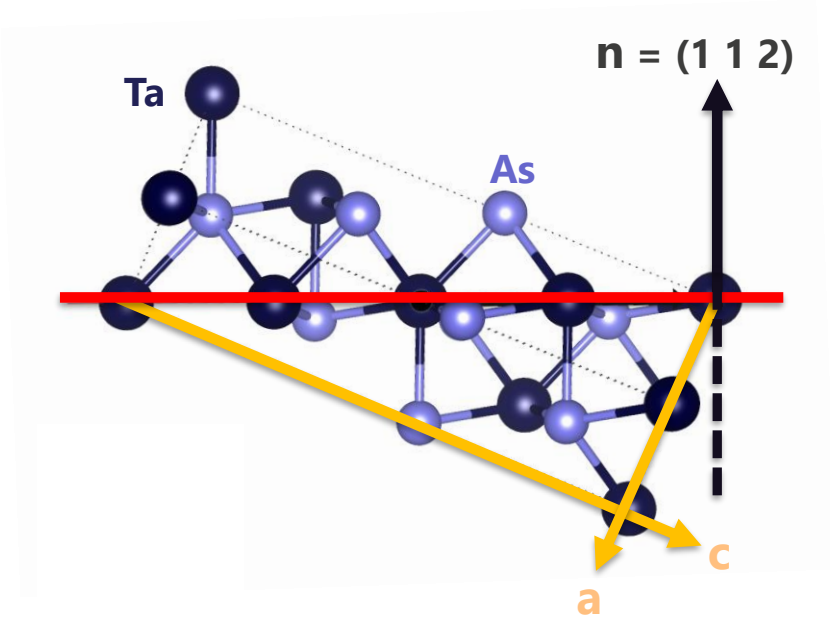
Acoustic Shear-mode Observation





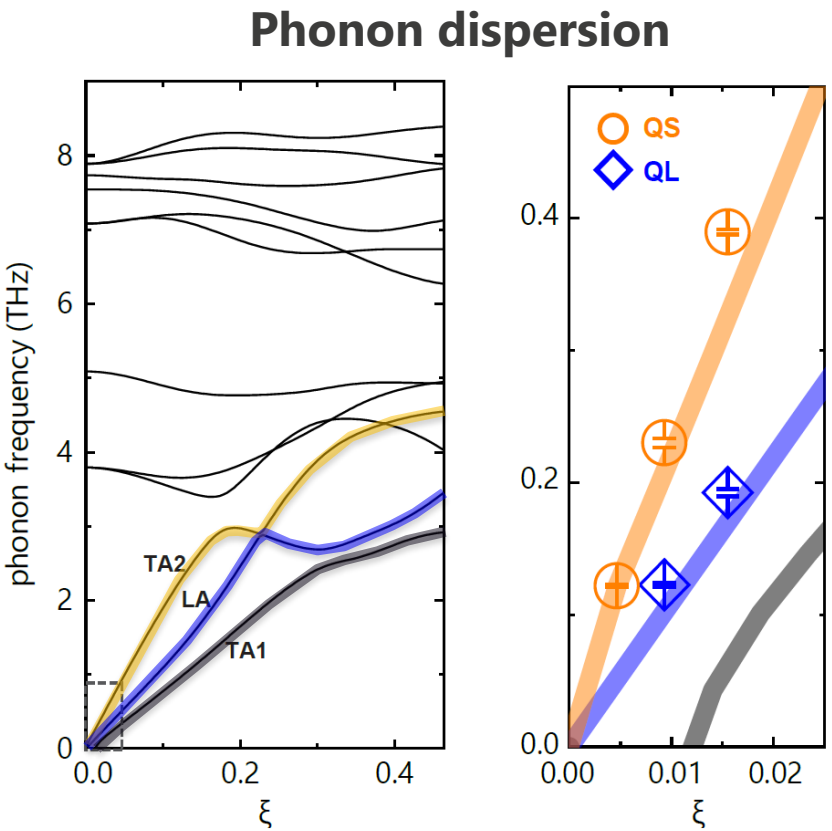
(Quasi-)Shear mode
also can be observed!

TaAs



First observation of QS mode from X-ray truncation rod scattering!

Simulation: Acoustic Phonons in TaAs

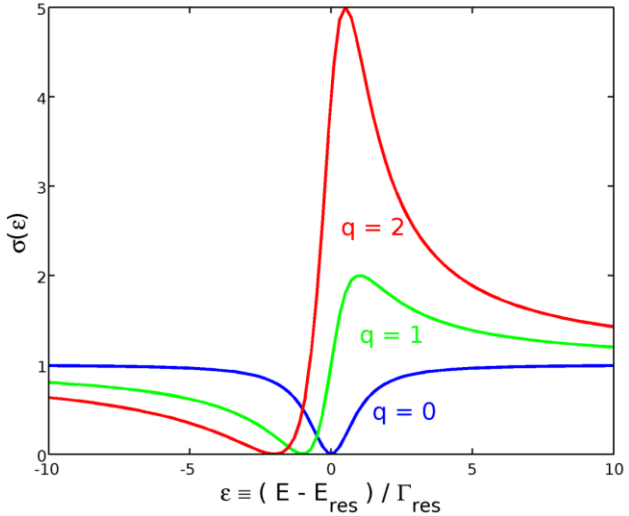


- Symbols: experiment
- Lines: simulation

Electron-phonon coupling in TaAs

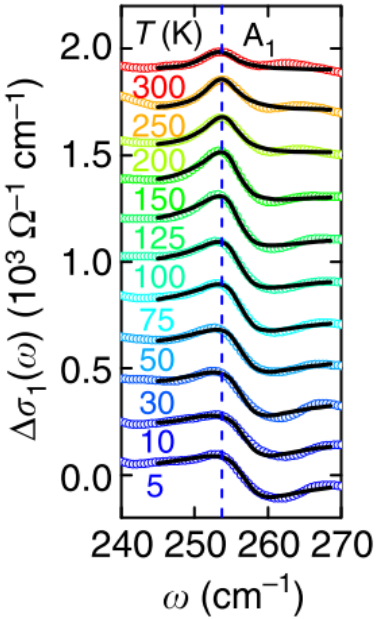
Fano-like asymmetric line shape

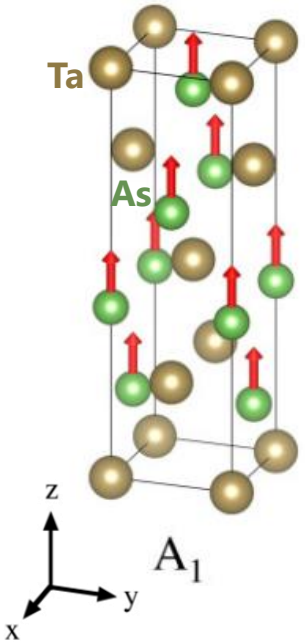
Evidence of el-ph coupling



$$\sigma = \frac{(\boldsymbol{q}\Gamma_{res}/2 + E - E_{res})^2}{(\Gamma_{res}/2)^2 + (E - E_{res})^2}$$

A_1 optical phonon in TaAs

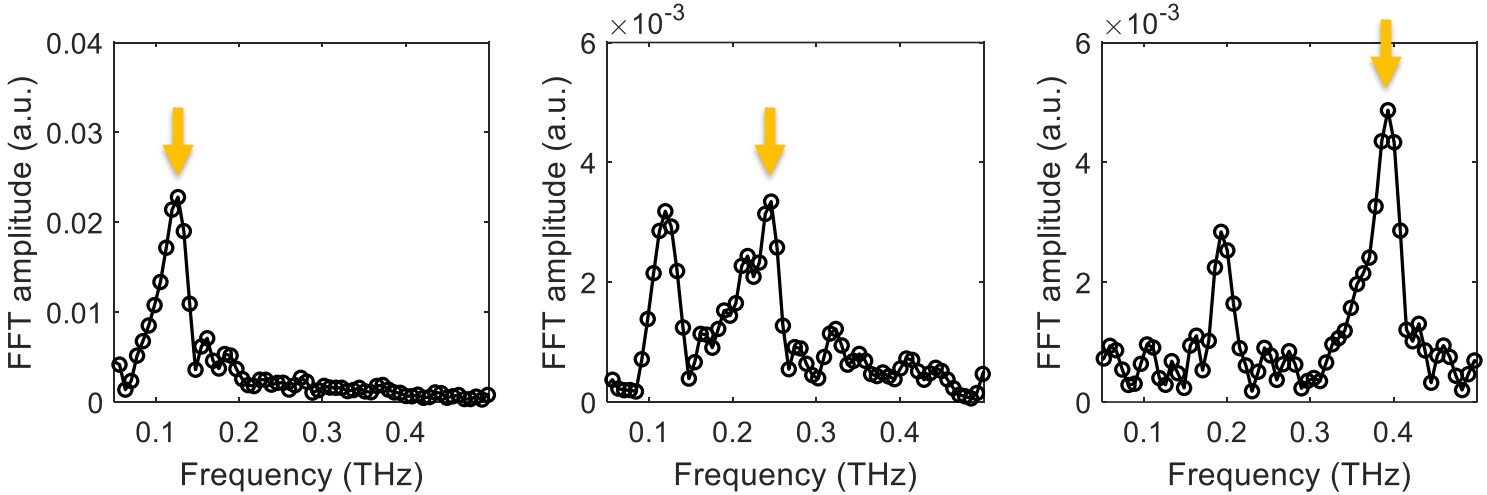




Nat. Commun. **8**, 14933 (2017).

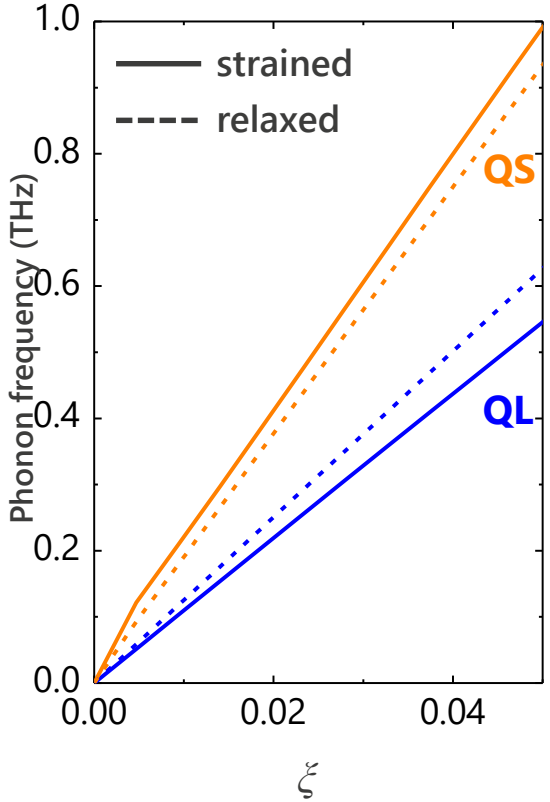
Electron-phonon coupling in TaAs

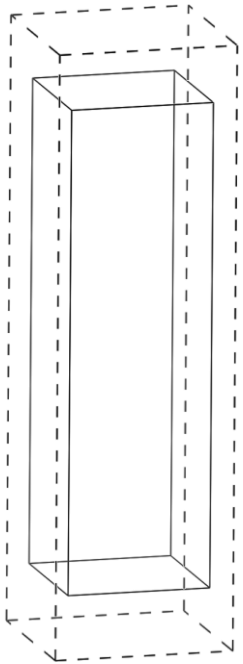
Quasi-shear acoustic phonon in TaAs



Strong el-ph coupling even at room temperature:
QS lattice motions → critical to modulate the electronic structure

Thermoelectricity control by strain





QS mode hardening
with strain effect

harder to vibrate
with spring constant ↑

thermal conductivity κ ↓
with heat capacity ↓

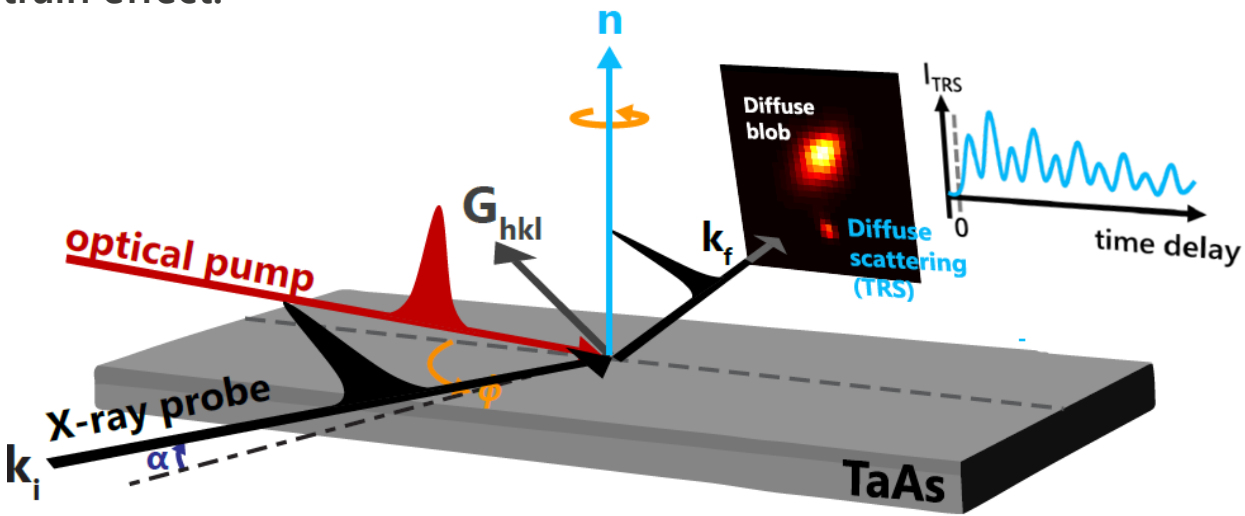
thermoelectricity increasing!

QS mode: possible pathway to thermoelectricity control

Conclusion

- By using optical-pump, X-ray probe spectroscopy in TaAs, we observed acoustic phonon oscillations and a quasi-shear acoustic mode from X-ray truncation rod scattering for the first time.

- We demonstrate that the quasi-shear acoustic mode is a signature of el-ph coupling, indicating that the quasi-shearing mode can be a pathway to control the thermoelectricity by a strain effect.



Acknowledgement

- Experiment

Min-Cheol Lee, N. Sirica, R. Prasankumar	Los Alamos National Laboratory
S. W. Teitelbaum, M. Trigo, D. Reis V. Krapivin, G. de la Pena, Y. Huang	SLAC National Laboratory
A. Maznev, K. A. Nelson	MIT

- Theory

R. Tutchton, J. Zhu	Los Alamos National Laboratory

- Sample

L. X. Zhao, G. F. Chen, B. Xu, R. Yang	Chinese Academy of Sciences