

Intrinsic Quasi 1-D Lattice Instability and Thermoelectricity in $\text{In}_4\text{Se}_{3-\delta}$

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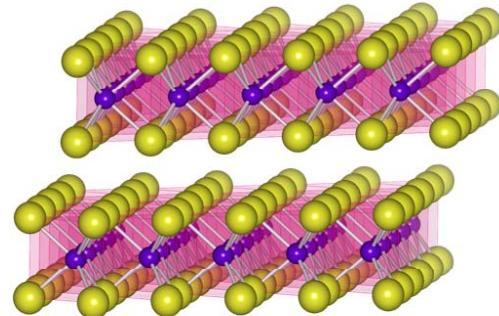
³**Dept. of Physics and Astronomy, Rutgers University, USA**



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Low Thermal Conductivity and CDW

Extremely low thermal conductivity

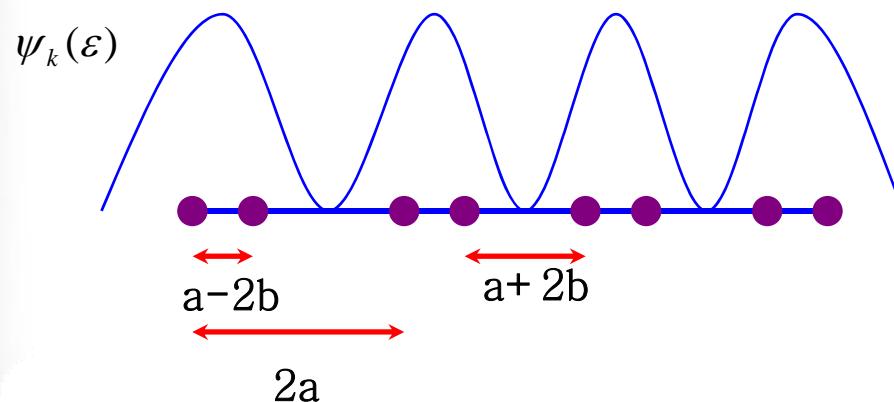


Crystal structure of WSe₂
C. Chitescue et al. Science (2007)

- 2-D layered WSe₂ thin film
- Disordered layered structure
- $\kappa=0.04$ W/mK

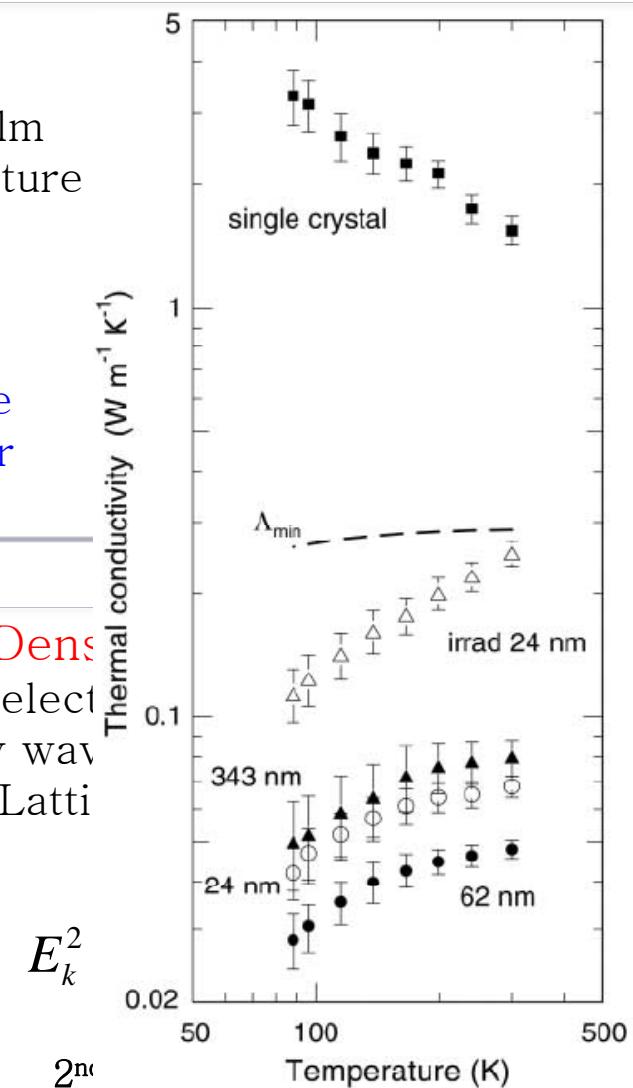
- * Limitations
 - Thin film structure
 - Electrical insulator

Charge Density Wave



Charge Dens

- Strong elect
- Density wav
- Low D Latti

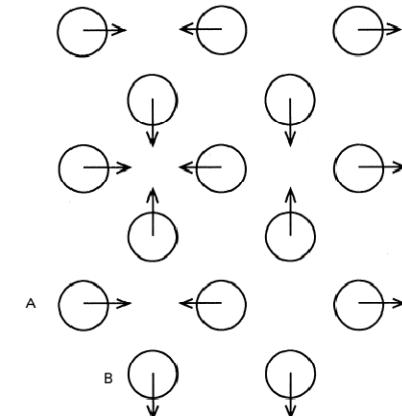
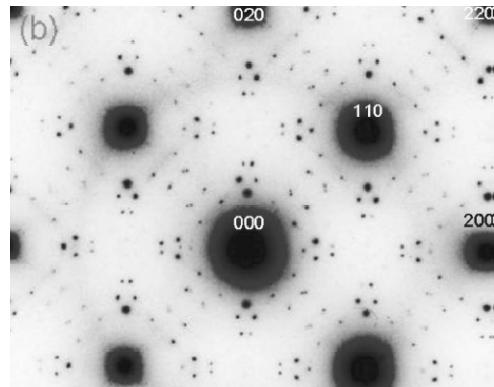
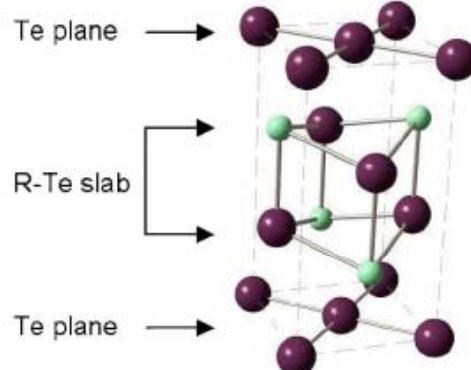


Thermoelectric properties of CDW



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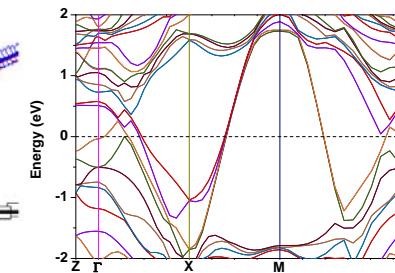
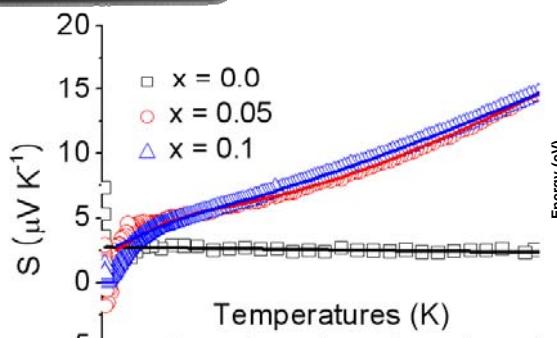
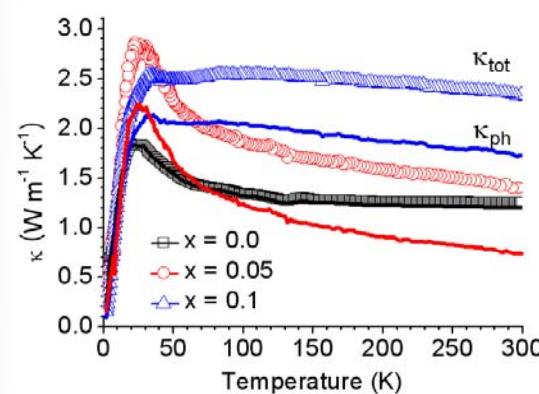
Toy model – CeTe₂



CeTe₂
- High T_{CDW}
- Lattice distortion along the plane of CDW

K. Y. Shin et al.
Phys. Rev. B (72) 85132 (2005)

Thermoelectricity in CeTe₂



- Low thermal conductivity
- Low Seebeck coefficient

J. S. Rhyee et al.
J. Appl. Phys. (105) 53712 (2009)

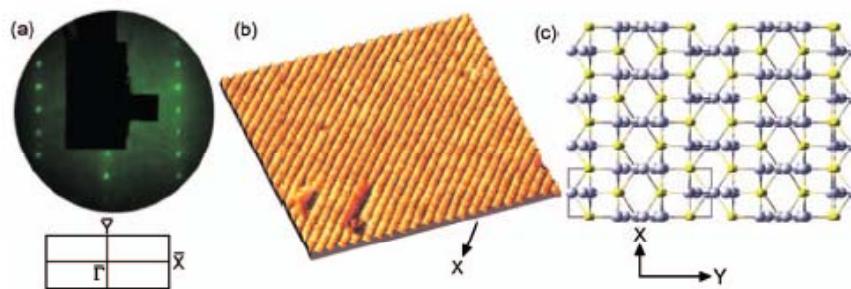
Thermal conductivity (left) and Seebeck coefficient of CeTe_{2-x}Sn_x

Peierls distortion and Thermoelectricity



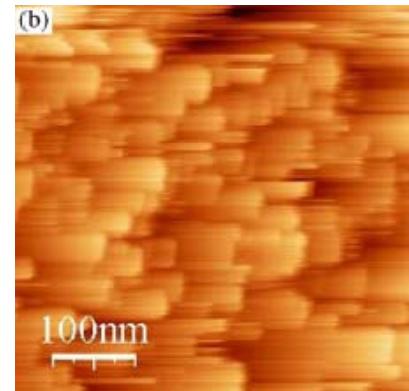
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Quasi-1D Bulk crystal

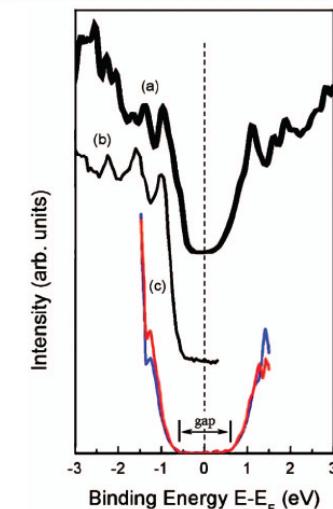


Quasi 1-D In chain in In_4Se_3 (100) plane

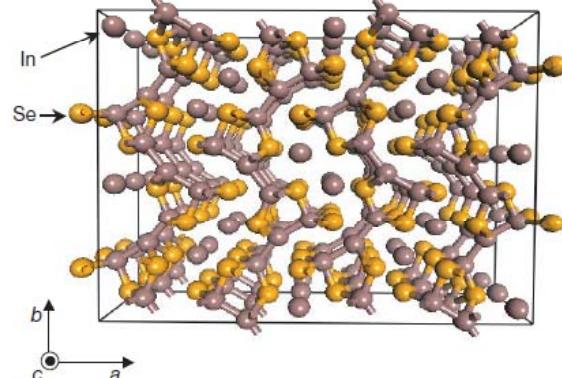
Y. B. Losovyj et al. *Appl. Phys. Lett.* (92) 122107 (2008)



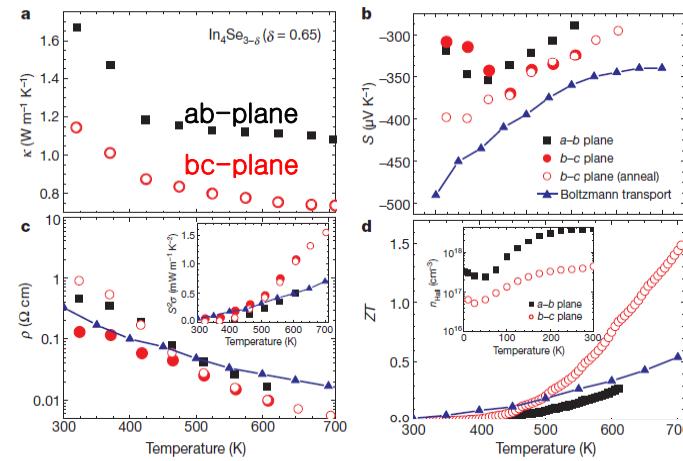
O. A. Balitskii et al.
Physica E (22) 921 (2004)



Crystal structure and TE properties of In_4Se_3



In_4Se_3 crystal structure



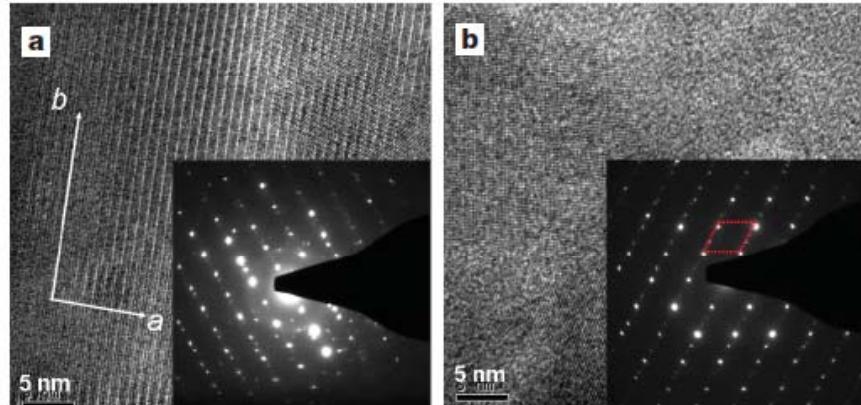
- Se-deficiency induced Peierls distortion
 - Low thermal conductivity along the plane of Peierls instability
 - High ZT (1.48 @705 K) for n-type materials
- J.S. Rhyee et al. *Nature* (2009)

Peierls distortion and Thermoelectricity

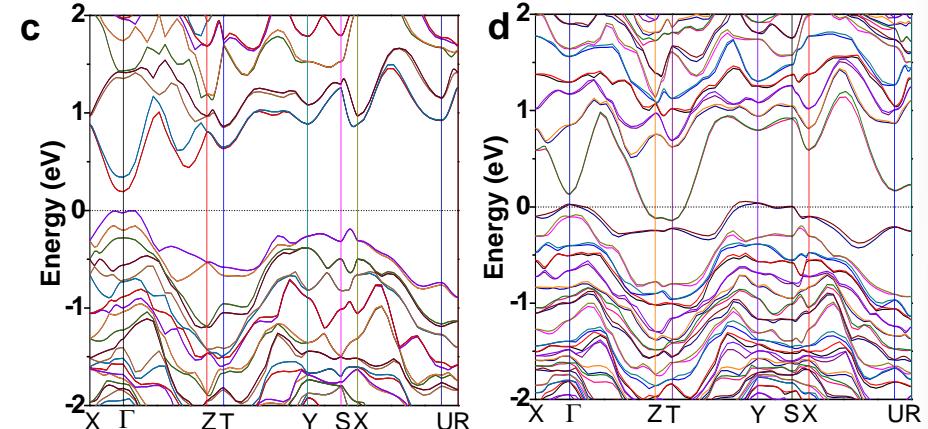


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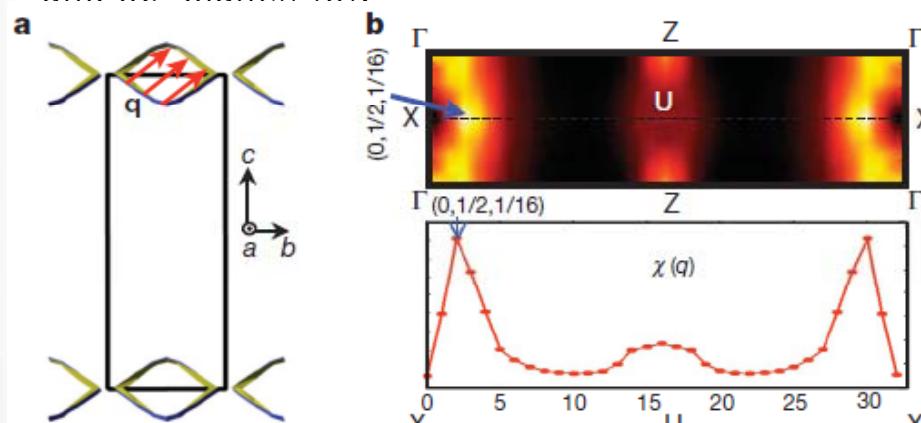
Band structure and Peierls distortion



TEM and ED of $\text{In}_4\text{Se}_{2.78}$ along the ab- (a) and bc-planes (b).



(c) In_4Se_3 and (d) $\text{In}_4\text{Se}_{2.75}$ band structure



Fermi surface (a) and generalized electron susceptibility (b) of $\text{In}_4\text{Se}_{2.75}$

- Quasi 1-D lattice distortion along the b-axis
- Lattice doubling in electron diffraction and generalized electron susceptibility calculation
- Semiconducting band gap of In_4Se_3
- Dispersive electron band and localized hole band of $\text{In}_4\text{Se}_{2.75}$

J. S. Rhyee et al.
Nature (2009)
APL (2009)

Summary and Conclusions



Summary

1. Low thermal conductivity
 - Extremely low thermal conductivity in the layered structure of disordered plane
 - CDW is an effective way to realize the disordered and layered structure
2. Band structural property of $\text{In}_4\text{Se}_{3-\delta}$
 - Asymmetric electron-hole band; hole localization
3. High thermoelectric performance and Peierls distortion
 - Peierls distortion of $\text{In}_4\text{Se}_{3-\delta}$
 - High thermoelectric figure-of-merit (ZT 1.48 @ 705 K)

Conclusions

Possible practical application for waste heat power generation of $\text{In}_4\text{Se}_{3-\delta}$

Peierls distortion is a new pathway of thermoelectric materials development