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Microscopy of Interfaces and Crystal Defects in Materials

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DOE Academies Creating Teacher Scientists (ACTS)

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Outline/Agenda

- Microscopy in materials science
  - -Focus on transmission electron microscopy
- Research examples:
  - -Interfaces and Crystal Defects
  - -Thermoelectric materials
- Lab tour:
  - -Atom probe tomography
  - -Scanning tunneling microscope
  - -Transmission electron microscope
- Discussion

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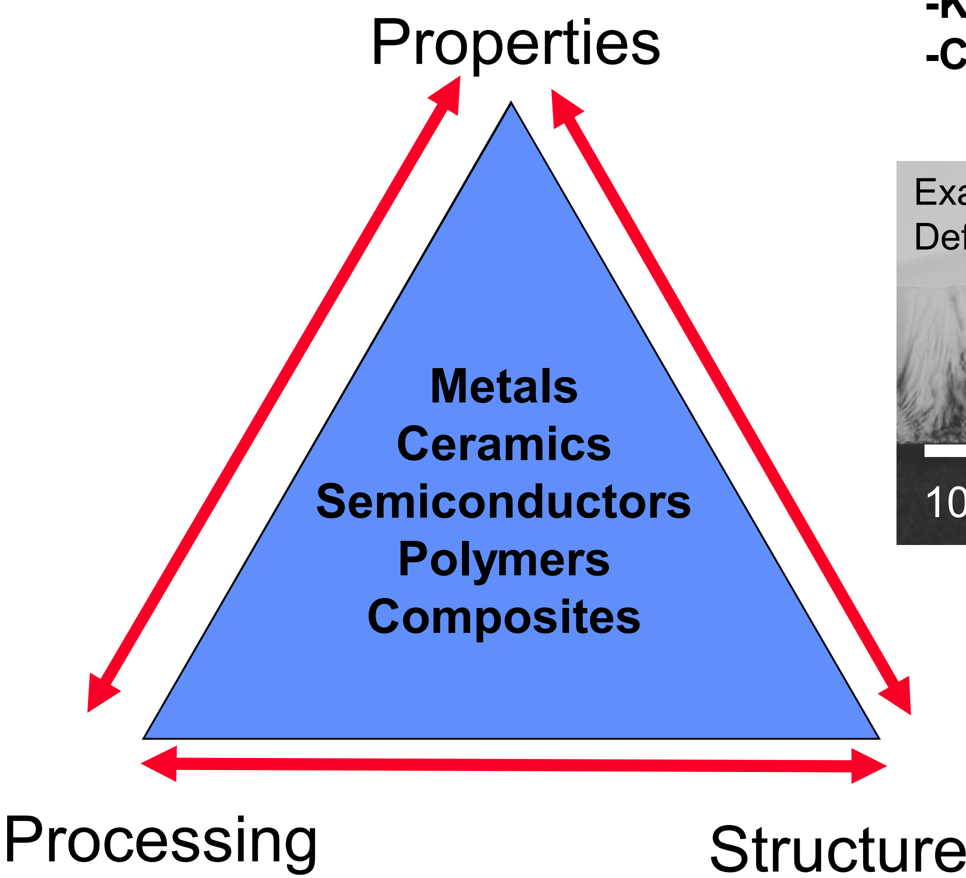
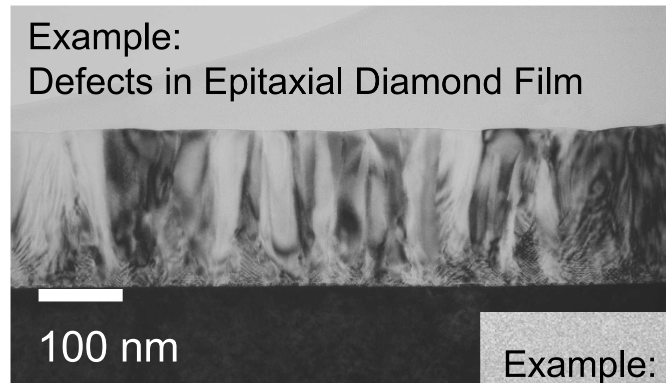
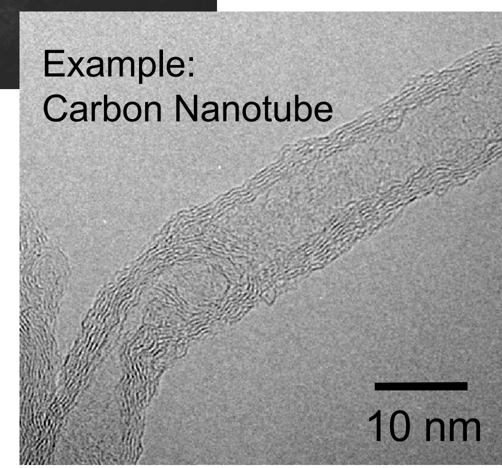
Materials Science and Engineering

Microscopy:
-Key to Understanding Materials Structure
-Critical tool for discovery







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Wide range of microscopies in materials science:

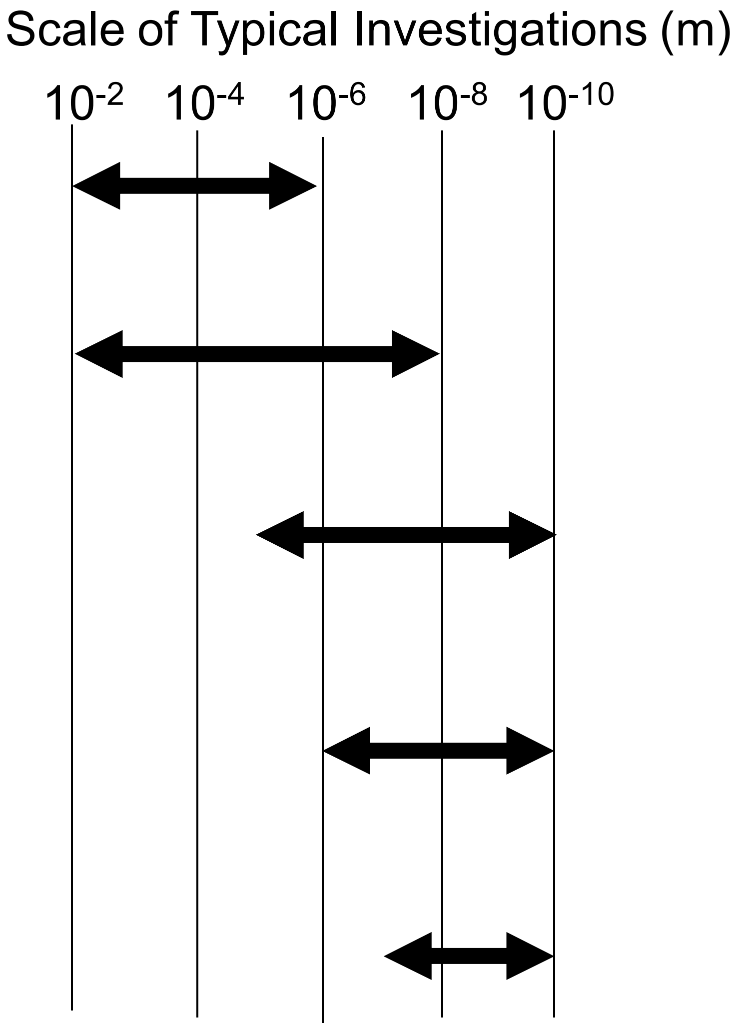
Optical Microscopy

Scanning Electron Microscopy (SEM)

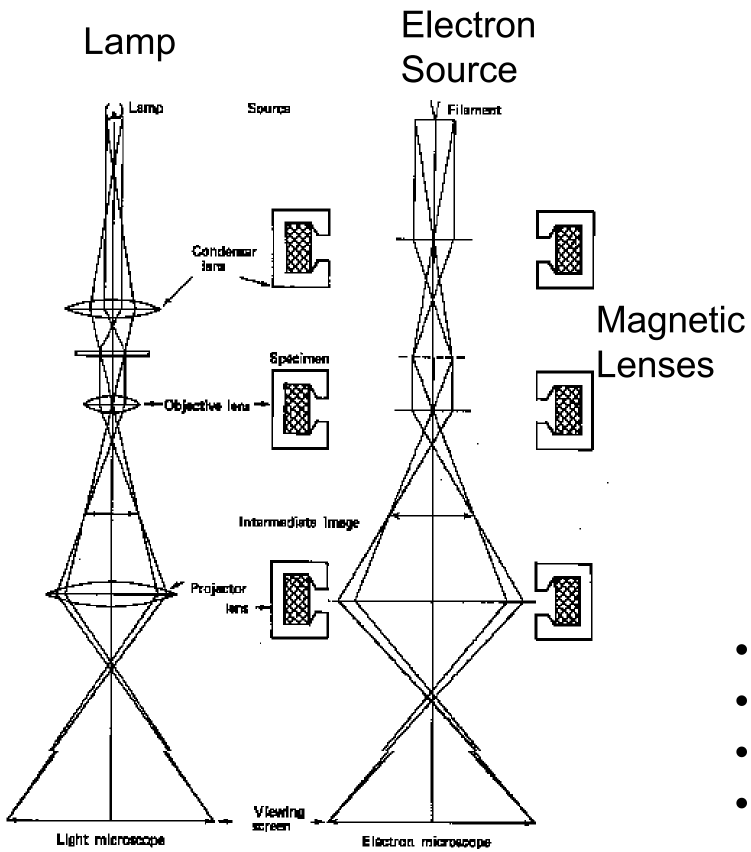
Transmission Electron Microscopy (TEM)

Scanning Probe Microscopies (STM, AFM)

Atom Probe Tomography



Transmission Electron Microscopy: Analogies to Light Optical Microscopy



Light Microscope

Electron Microscope

- Electrons accelerated through high voltage
- Magnetic lenses to focus electrons
- Specimens are thin: ~10 nm - 200 nm
- Electrons have wavelength:==> Diffraction

	λ (10^{-12} m)
100 kV	3.7
200 kV	2.5
400 kV	1.7

- Electron and x-ray detectors for imaging and spectroscopy

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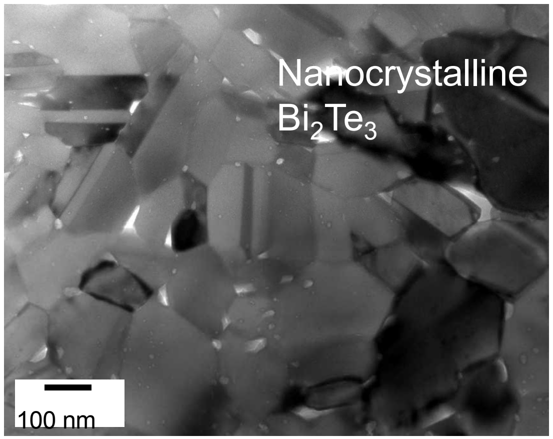
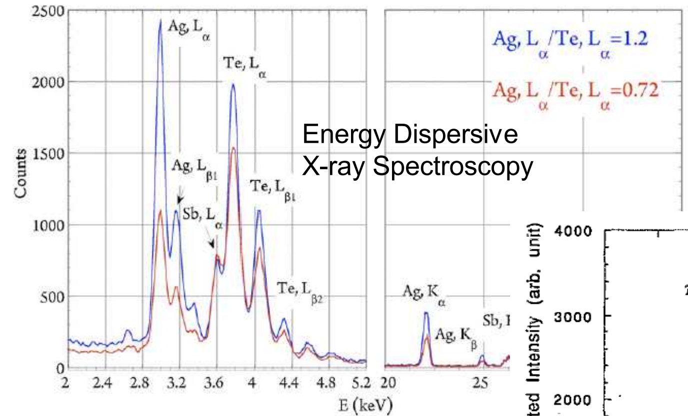
TEM Provides Comprehensive information about materials

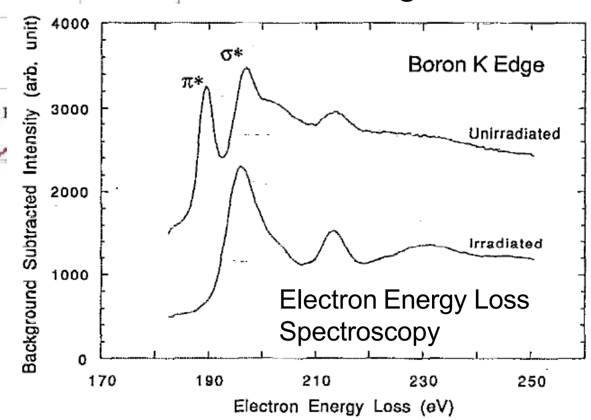
Microstructure



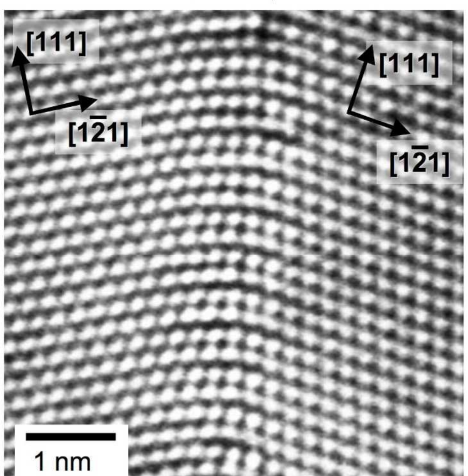
Composition



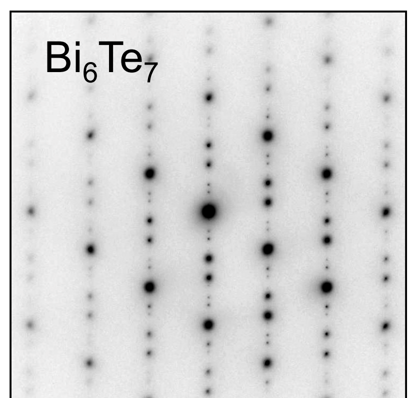
Bonding



Atomic structure



Crystallography



Electron Diffraction

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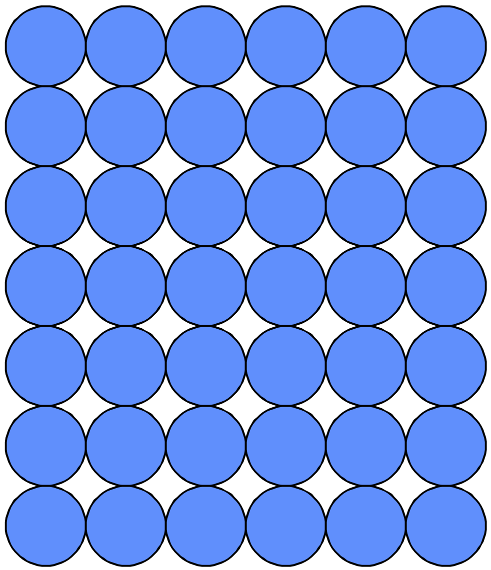
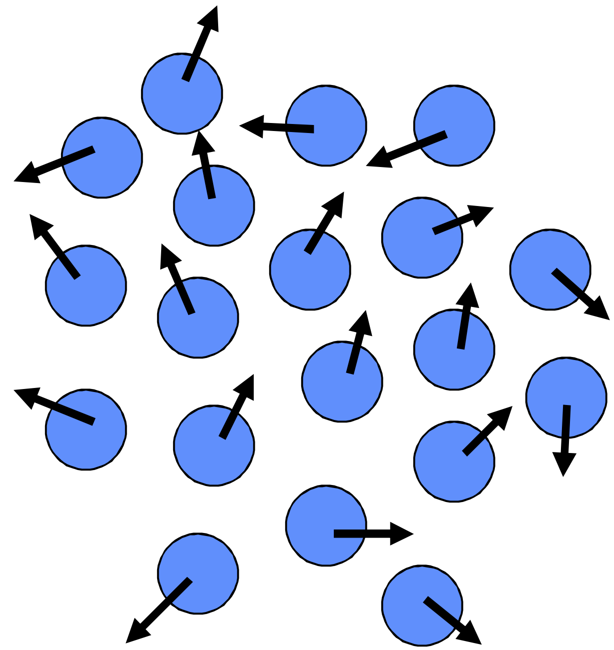
Many materials are crystalline

Atoms in a Crystal

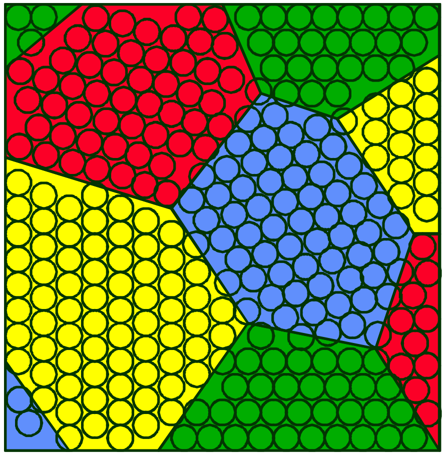


Atoms in a Liquid or Gas

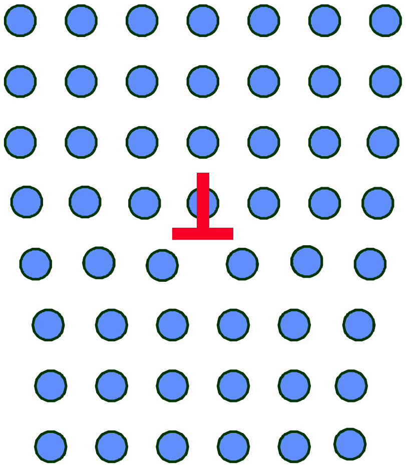


Interfaces and Crystal Defects control many materials properties

Grain Boundaries



Dislocations



Mechanical properties:

Strength and ductility

Fracture

Electronic properties:

Carrier mobility

Charge trapping, recombination

Thermal properties:

Phonon scattering, reduced thermal conductivity

Materials Stability

Corrosion, Fatigue

Want to understand influence of defects on materials properties

and

How to form desired defect arrangements

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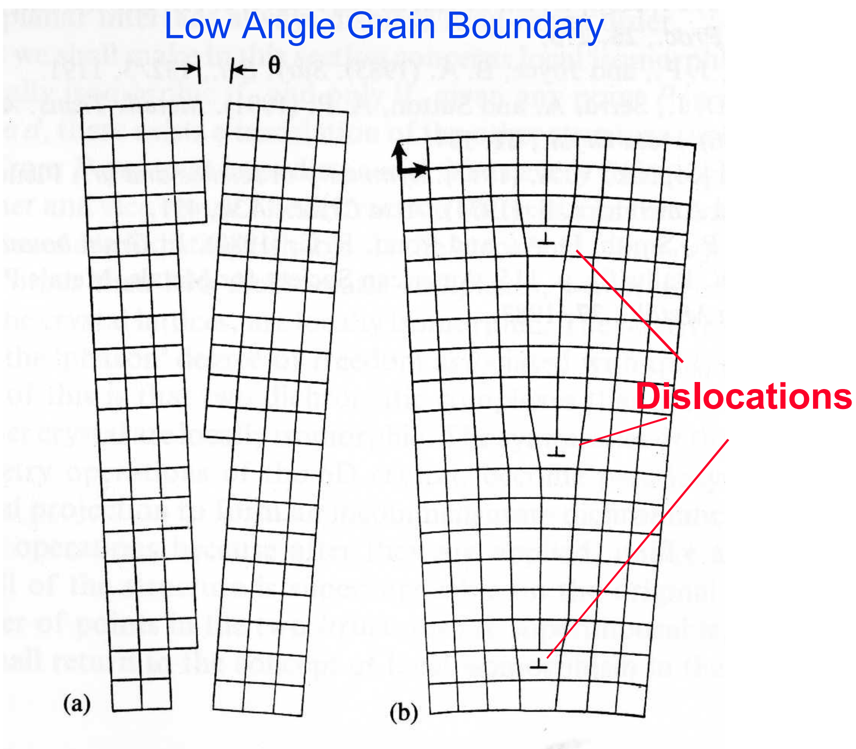
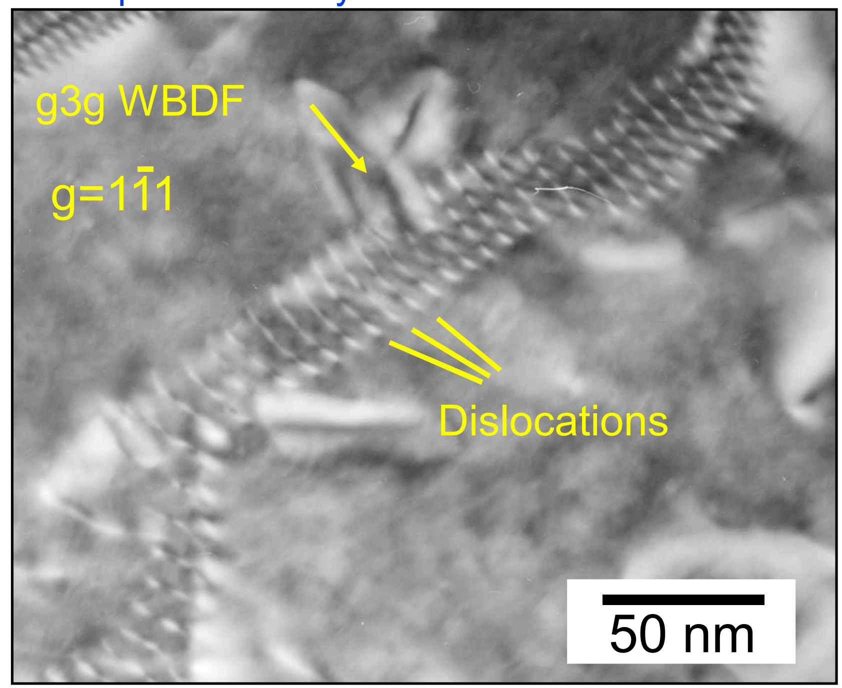
Imaging crystal defects in TEM



Example: Grain boundary in aluminum composed of array of dislocations.



Elastic distortions at dislocation cores scatter (diffract) electrons differently than in the bulk, perfect crystal.

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In situ microscopy: Material Dynamics

Example: motion of dislocations at grain boundary in gold

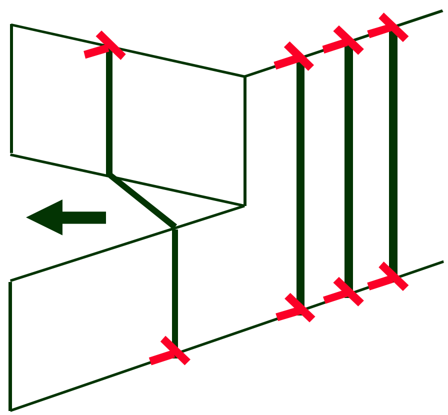
Au $\Sigma=3$ grain boundaries

QuickTime™ and a
Compact Video decompressor
are needed to see this picture.

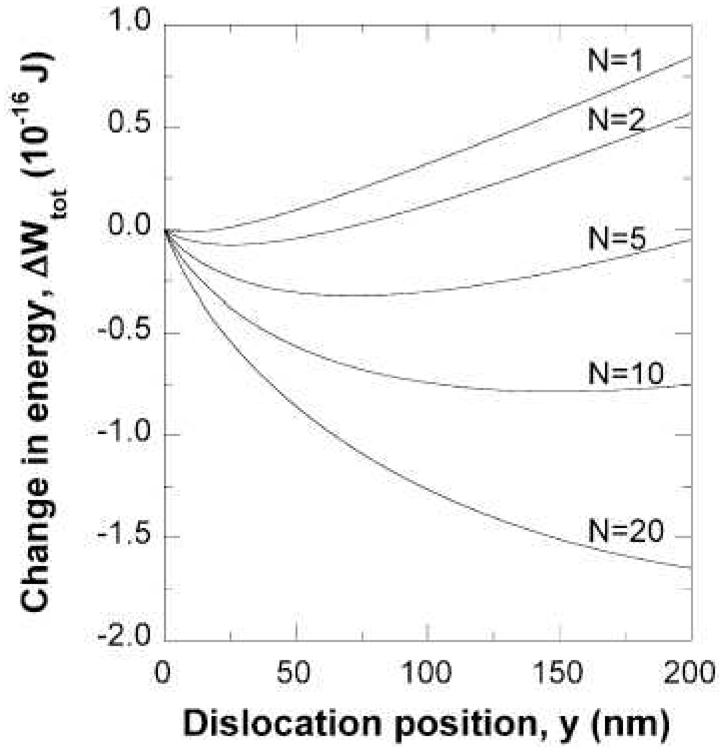
T=550° Δt=400 sec

Au $\Sigma=3$ thin film bicrystal

20 nm



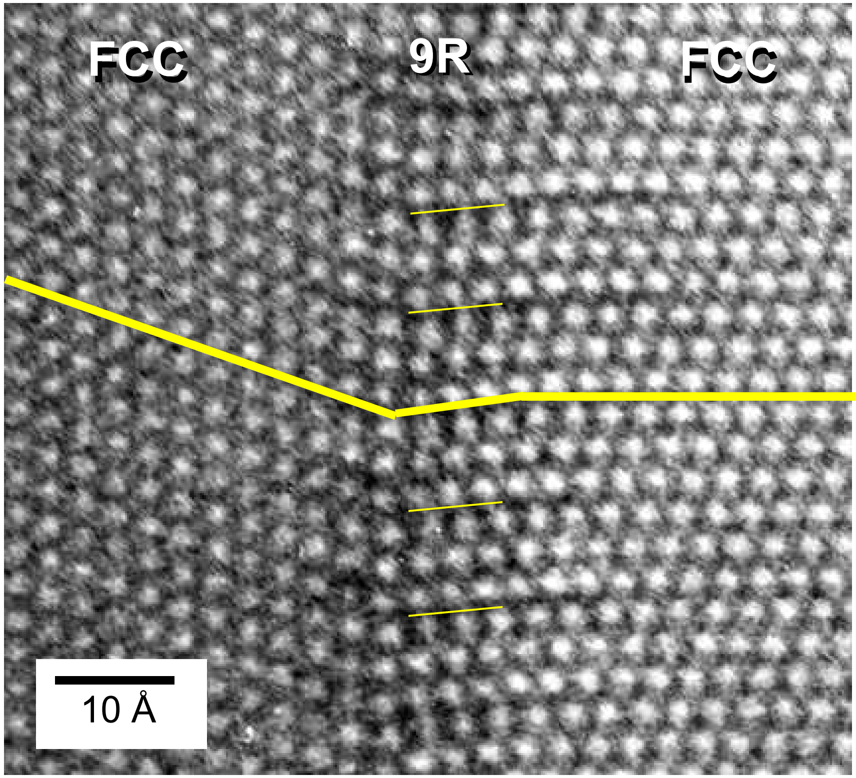
Balance of elastic repulsion
and increase in line energy



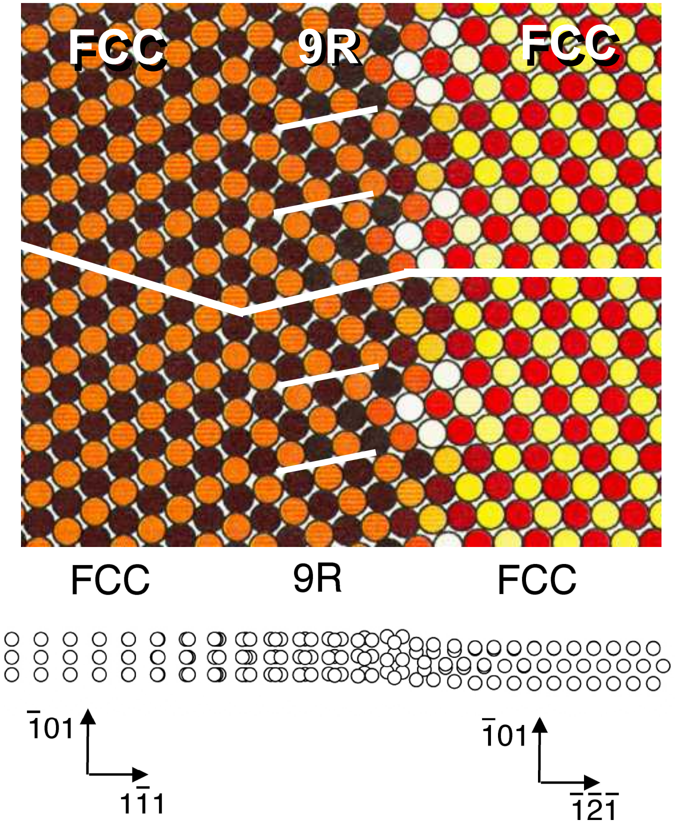
G. Lucadamo and D.L. Medlin, Acta mat. 50 (2002)

We can study defect structures at atomic resolution

HRTEM Observation of Au {111}/{112} Interface



Atomistic Calculation (EAM)



A new phase of gold is stabilized at interface

- Model strained to produce coherent interface.
- 1/8[101] shift in calculated structure.
- Similar results for unstrained calculation.

D.L. Medlin, S.M. Foiles, D. Cohen, Acta mater. 49 (2001) 3689.

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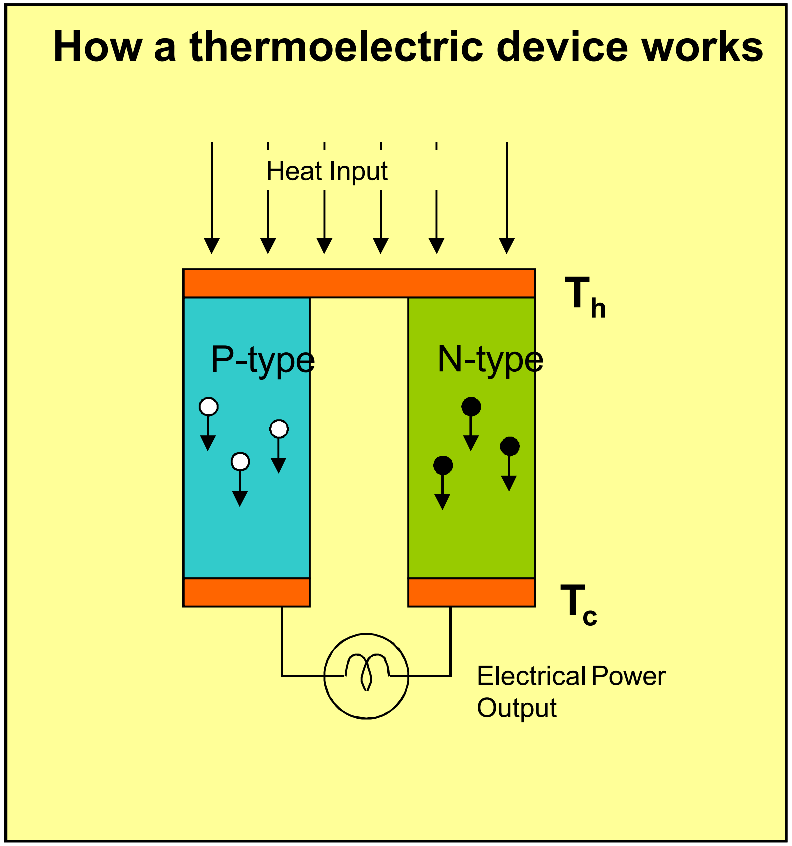
Sandia has a large effort in thermoelectric materials



Many Applications:

-Cooling

-electronics, detectors

-portable and rugged refrigeration

-Power Generation:.

-Waste-heat recovery.

-Power scavenging.

Key Challenge:

Improving energy conversion efficiency.

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Interfaces can improve thermoelectric performance

Energy conversion efficiency of thermoelectric material characterized by figure of merit

Seebeck Coefficient — Electrical Conductivity — Thermal Conductivity

$$ZT = \frac{\alpha^2 \sigma}{\kappa} T$$

Interfacial strategies to enhance ZT:

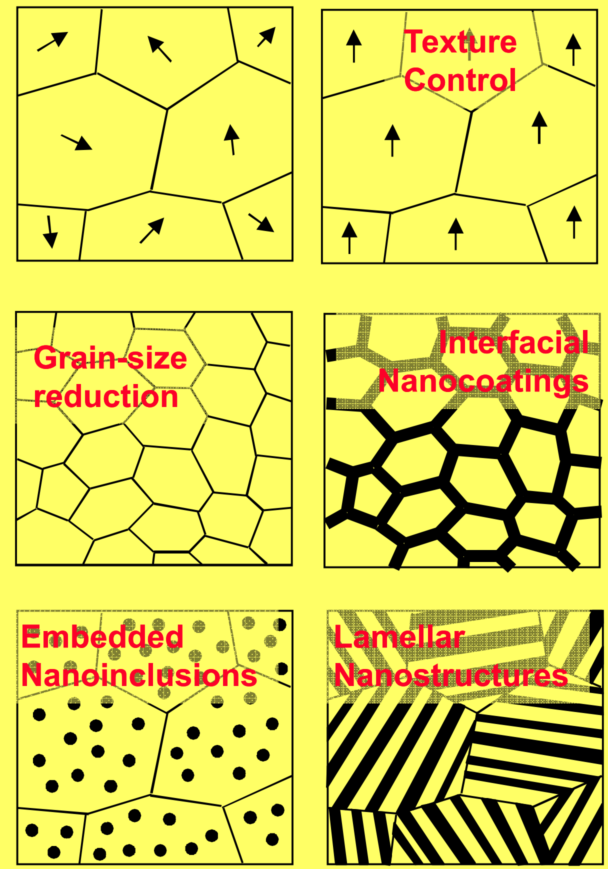
-phonon scattering:

$$\downarrow \kappa$$

-energy filtering:

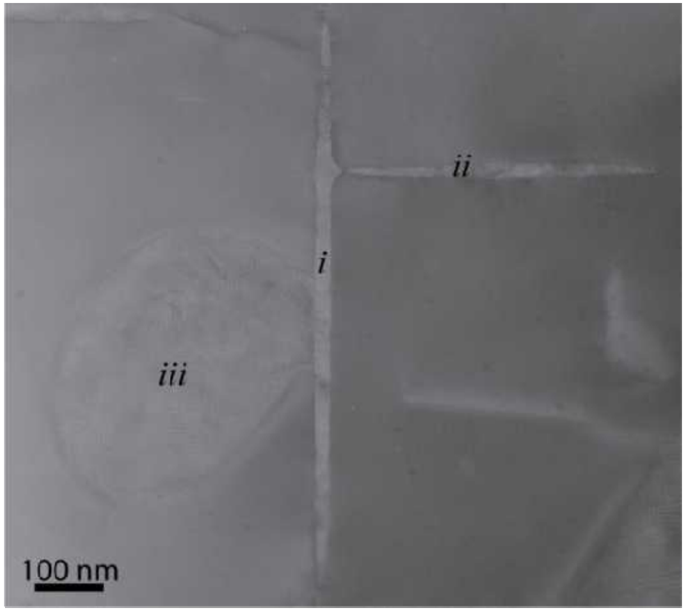
$$\uparrow \alpha^2 \sigma$$

Microstructural Strategies for Nanostructured Bulk Thermoelectrics

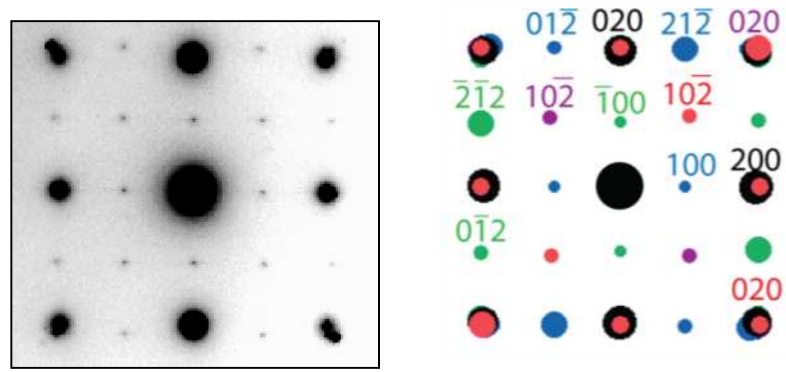


Medlin and Snyder, Current Opinion in Colloid and Interface Science, 2009

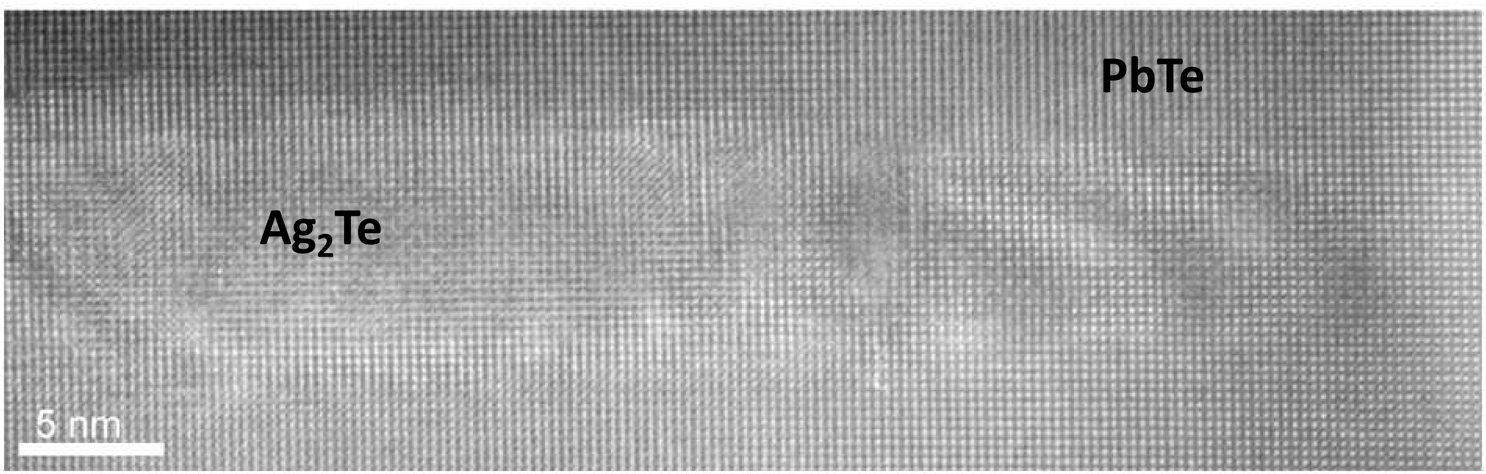
Example: Crystallographically Aligned Ag_2Te Precipitates in PbTe



[001] PbTe Zone



[201]monoclinic || [001]fcc
(-204)monoclinic || (2-20)fcc
+ symmetry-related variants



Lensch-Falk, Sugar, Hekmaty, Medlin, Journal of Alloys and Compounds, in press (2010)

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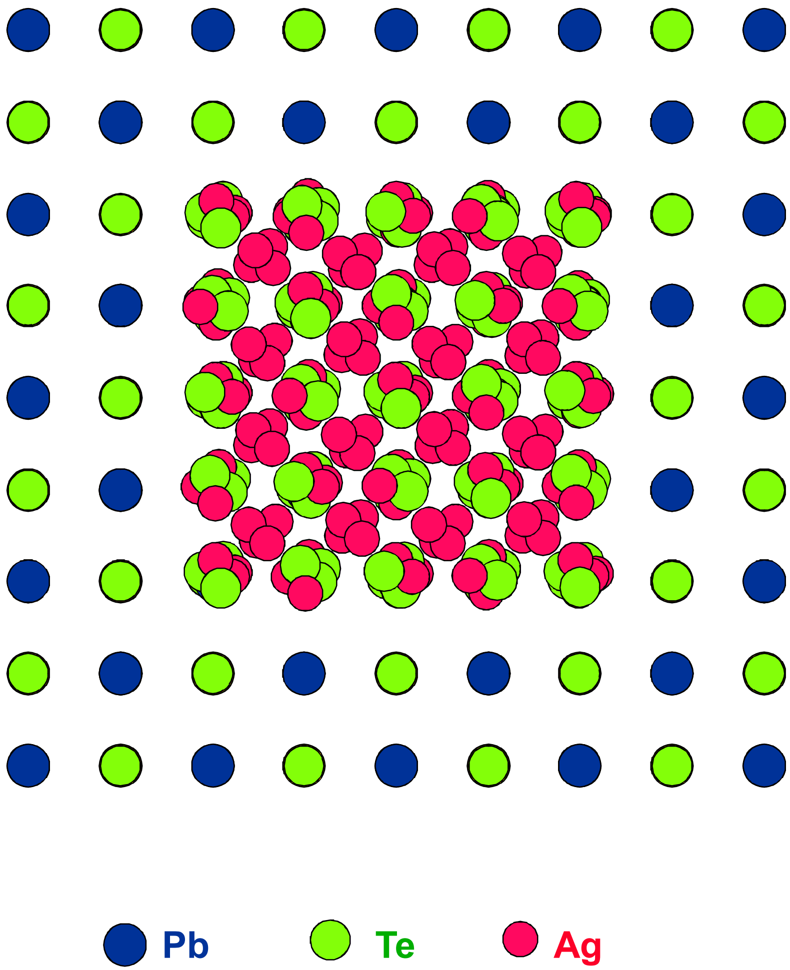
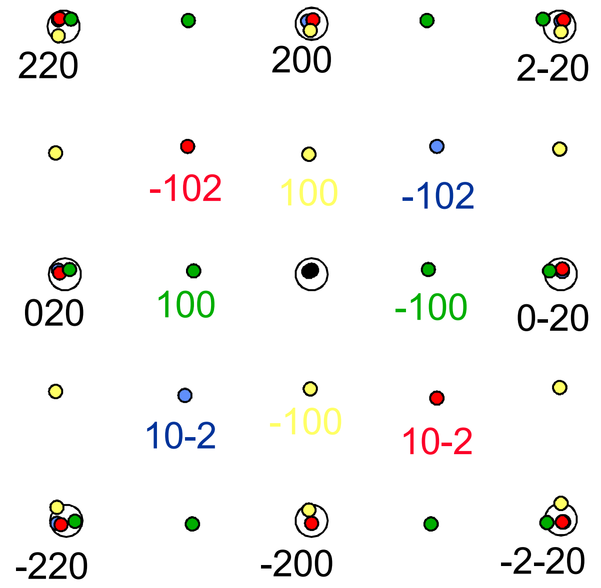
Ag_2Te: Orientation variants

PbTe [001] **Ag_2Te: [201]**



Electron Diffraction Pattern



Additional variants due to rotations about PbTe [100] and [010]

J.D. Sugar & D.L. Medlin, J. Alloys & Compounds (2009).

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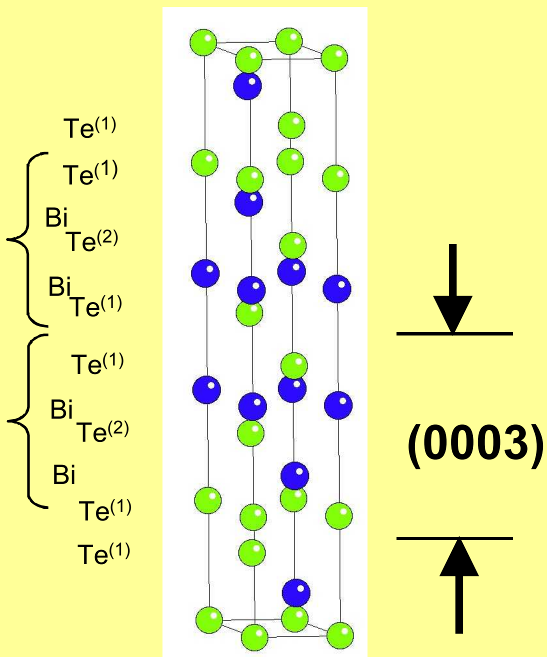
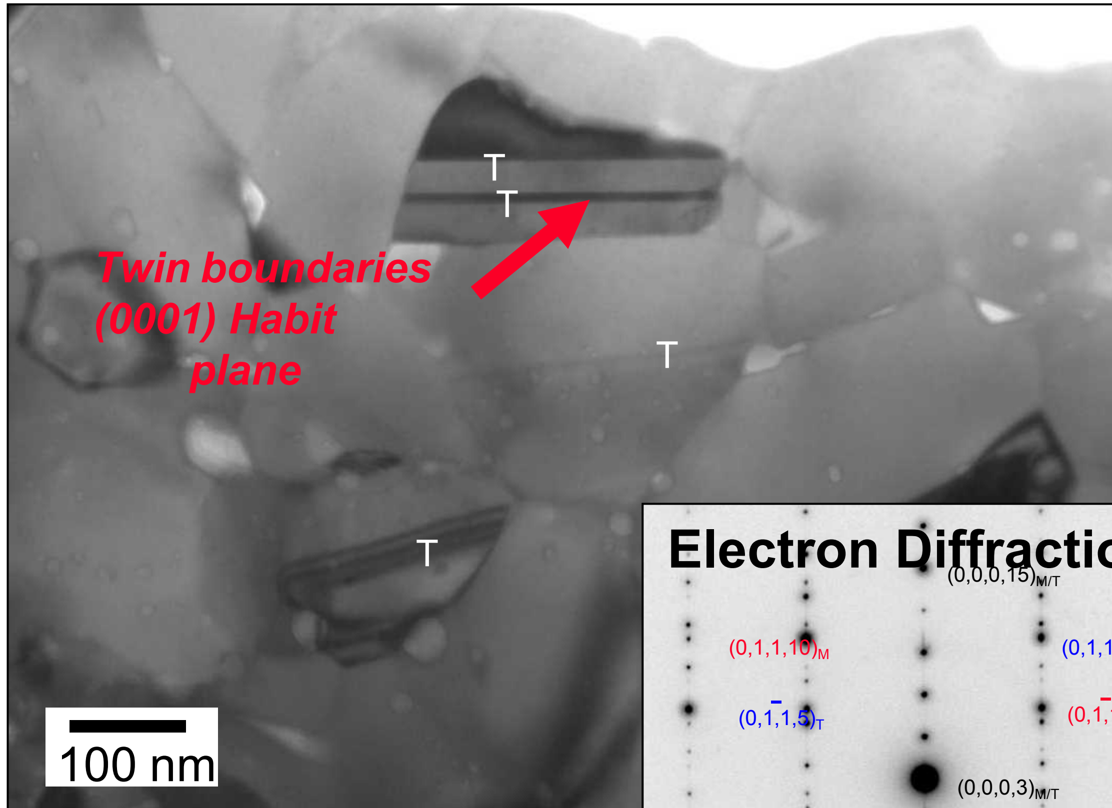
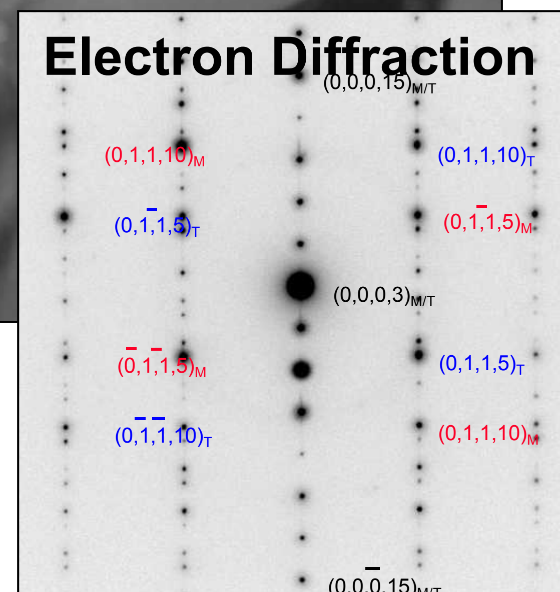
Example: Twin Boundaries in Bi_2Te_3

Bi_2Te_3 Crystal Structure



a=4.380 Å   c=30.480Å





Orientation Relationship:
(0001)//(0001)
[2-1-10]//[-2110]

60° rotation about c-axis

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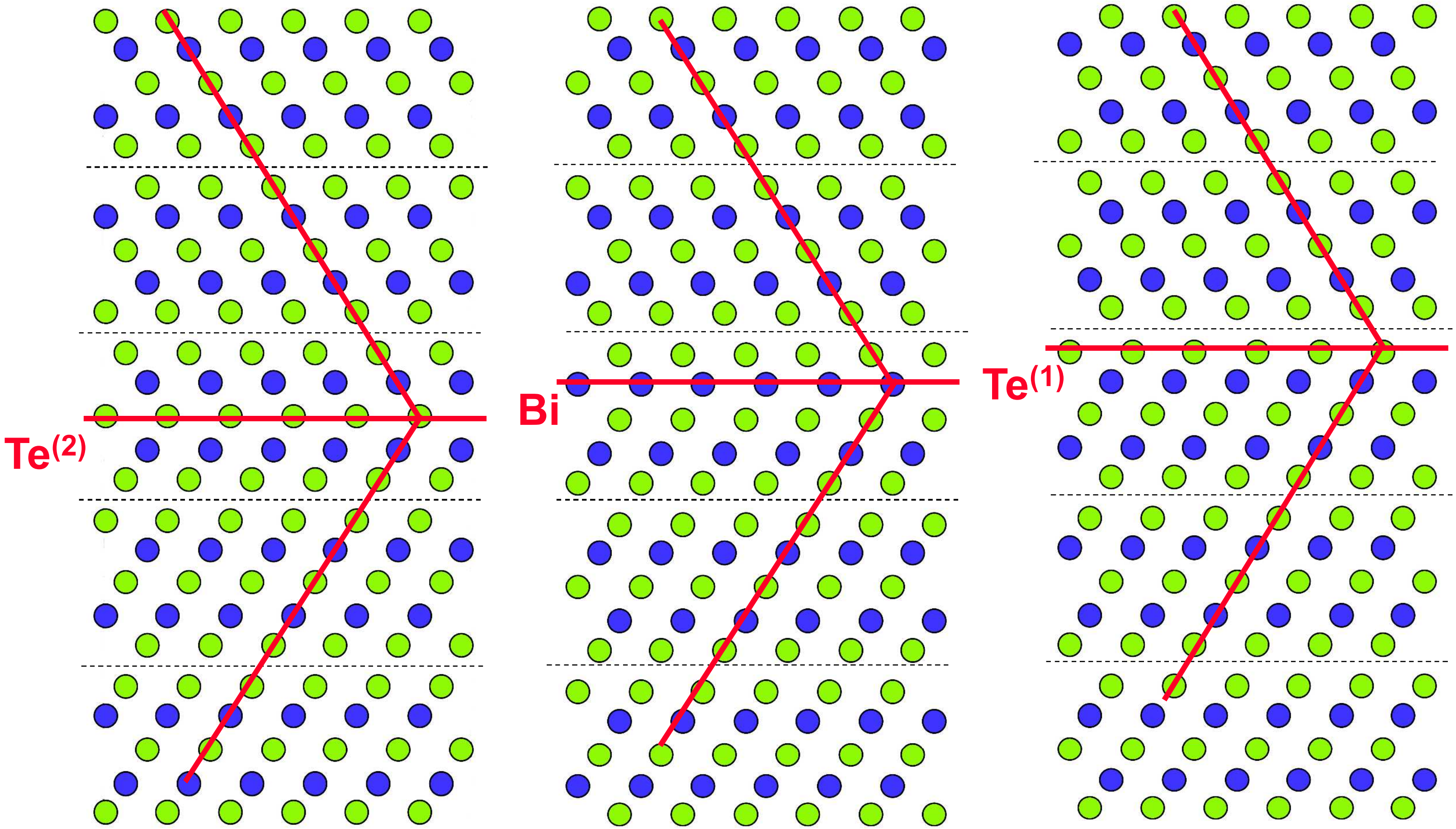
Question: How is twin boundary terminated?



DFT-LDA: 60.1 mJ/m^2 303.0 mJ/m^2 **40.7 mJ/m^2**

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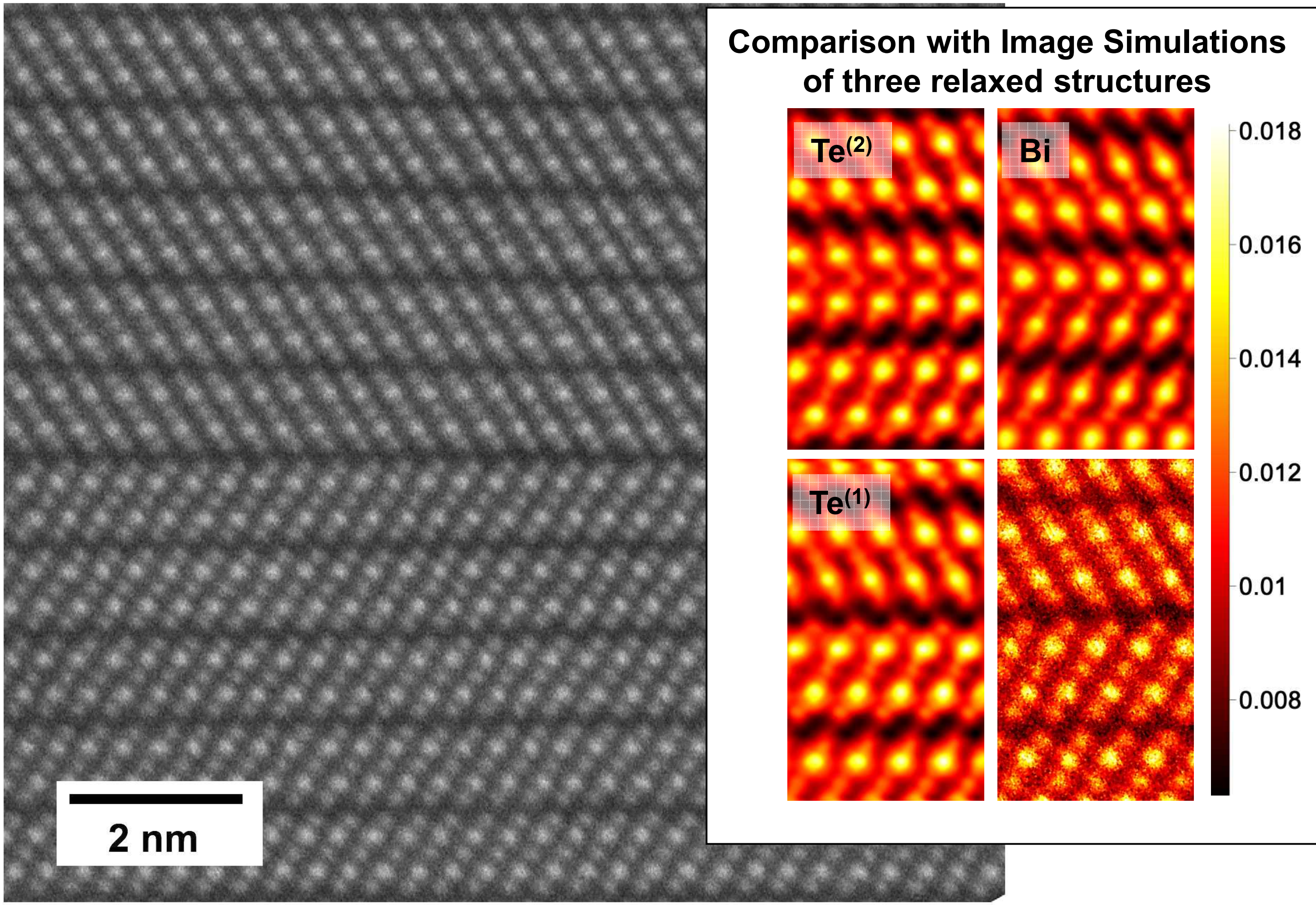
Observations:
Twin terminated at $Te^{(1)}$-$Te^{(1)}$ layer



Bi: Z=83
Te: Z=52

Bi is bright because it scatters electrons more strongly than Te

Medlin, Ramasse, Spataru, Yang, in press, J. Appl. Phys (2010)

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Outline/Agenda

- A bit about microscopy in materials science

  -Focus on transmission electron microscopy

- Research examples:

  -Interfaces and Crystal Defects

  -Thermoelectric materials

- Lab tour:

  -Atom probe tomography

  -Scanning tunneling microscope

  -Transmission electron microscope

- Discussion

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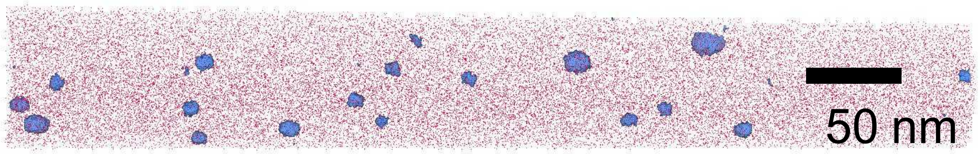
Lab Tour

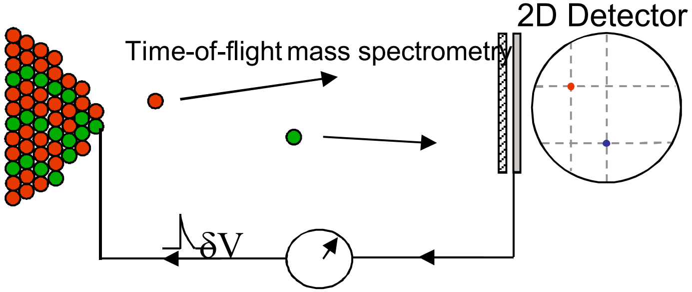
•Atom Probe Tomography

(Jessica Lensch-Falk, Michelle Hekmaty)

Example: Ag_2Te nanoprecipitates in PbTe thermoelectric



Lensch-Falk et al. J. Alloy Cmpds, (2010) in press.

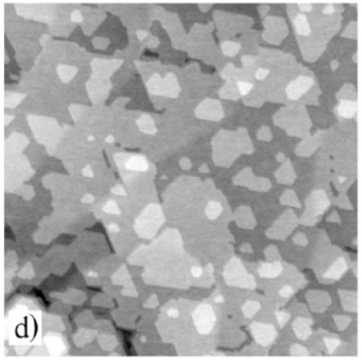


• Scanning Tunneling Microscope

(Konrad Thürmer))

Example:
Islands of ice on platinum

Nie, Bartelt, Thürmer, Phys. Rev. Lett. (2009)



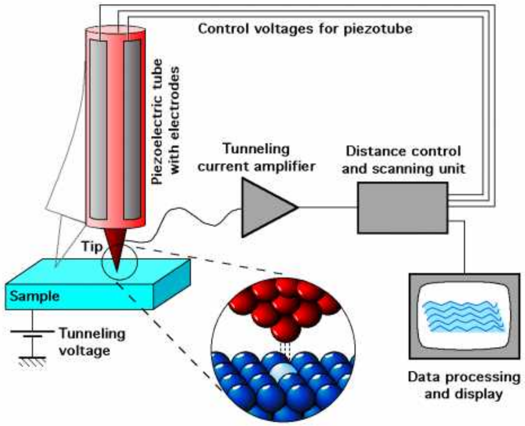


Figure: Michael Schmid, TU Wien

• Transmission Electron Microscope

(Ben Jacobs)

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Microscopy Resources

Microscopy Society of America (MSA)

http://www.microscopy.org/resources/laboratories.cfm

Microscopic Explorations:A GEMS Festival Guide

(LHS “Great Explorations in Math and Science”)

Grades 4-8

http://lhsgems.org/GEMmicro.html

National Center for Electron Microscopy

http://ncem.lbl.gov/
DOE Funded National User facility.
Links to all major microscopy resources.

San Joaquin Delta College:

http://www.deltacollege.edu/dept/electmicro/whatis.html
2-year AA degree in electron microscopy
Preparation for technologist positions in bio- and materials.

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Resources-
Materials Science and Engineering

ASM Materials Education Foundation:

http://asmcommunity.asminternational.org/portal/site/www/Foundation/

-"Materials Camps" for high-school students and teachers.
-Links to all US and Canadian College MS&T programs by state/province.

National Resource Center for Materials Technology Education

http://www.materialseducation.org/

NSF-funded resource for Materials Science Education
Good set of materials science demos and lab-projects.

Materials Research Society

http://www.mrs.org/s_mrs/index.asp

http://www.strangematterexhibit.com/

NISE (Nanoscale Informal Science Education) Network

http://www.nisenet.org/community/k-12-teachers

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