

Atomic Scale Investigation of Interfaces and Dislocations in Telluride-Based Thermoelectric Materials

SAND2013-5011C

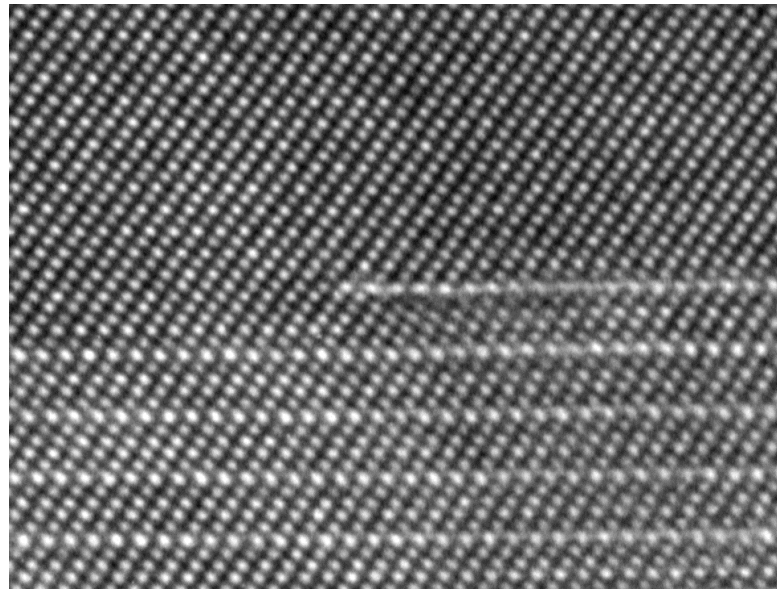
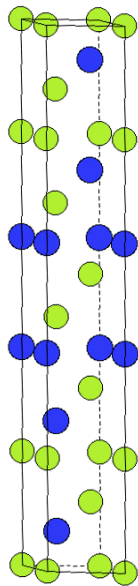
Douglas L. Medlin

Sandia National Laboratories

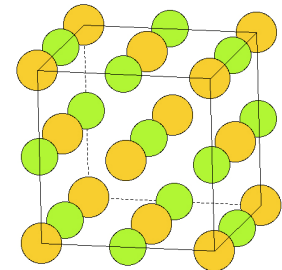
Livermore, CA 94551

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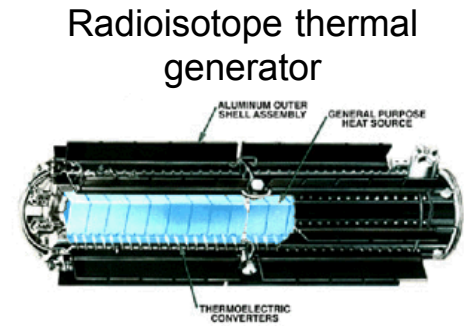
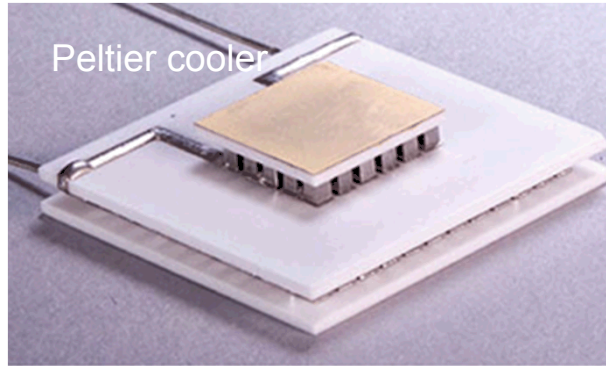
Tetradymite



Rock-Salt



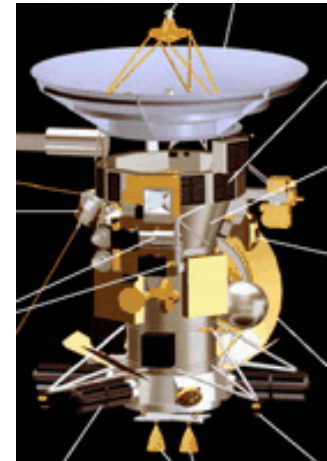
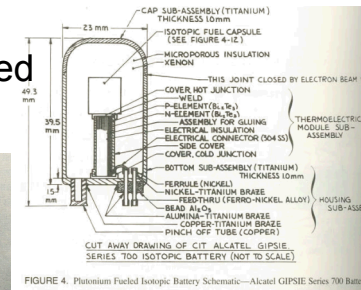
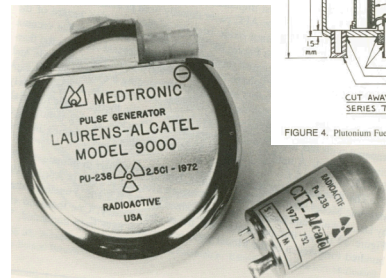
Thermoelectrics have many applications for cooling and power-generation



Automotive Climate Control

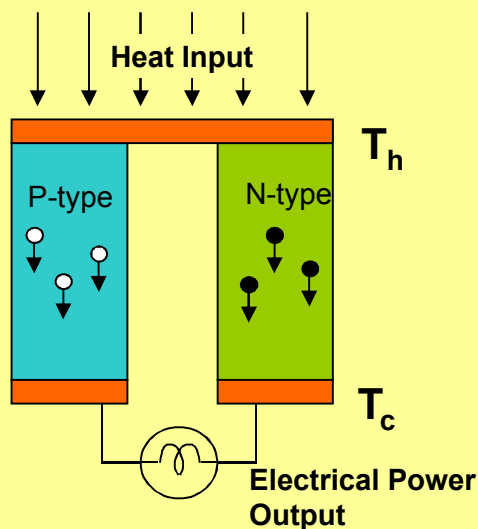


Plutonium powered pacemaker

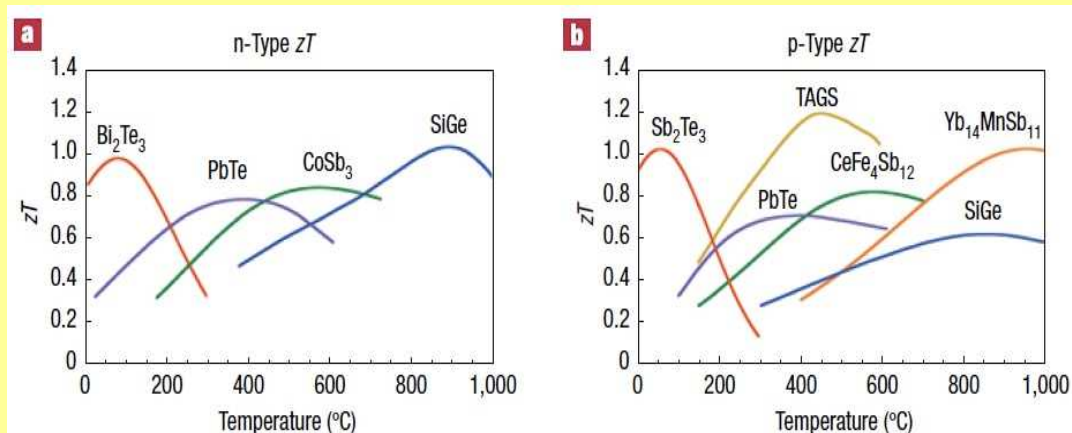


Thermoelectrics-Background:

TE Power Generation



Materials Performance Depends on Temperature



Snyder and Toberer, Nature Mat. 2008

Maximum Generator Efficiency

$$\eta = \underbrace{\frac{T_h - T_c}{T_h}}_{\text{Carnot}} \underbrace{\frac{\sqrt{1 + zT_m} - 1}{\sqrt{1 + zT_m} + T_c / T_h}}_{\text{Materials Term}}$$

Figure of Merit

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

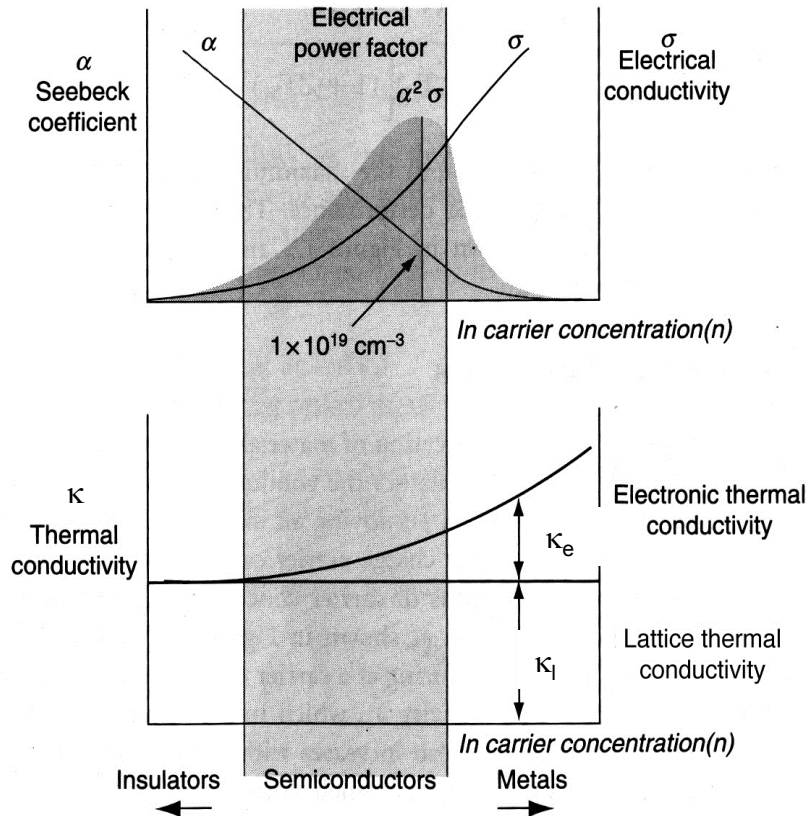
Seebeck Coefficient α , Electrical Conductivity σ , Thermal Conductivity κ

Important Roles for Interface Science:

- Improvement of TE properties through interfacial scattering.
- Materials Stability.
- Electrical contacts.

Challenge: Improving TE Materials Properties

Transport Properties are Interdependent



$$zT = \frac{\alpha^2 \sigma}{\kappa_e + \kappa_l} T$$

Traditional approaches:

- Alloy to scatter phonons, reducing κ_l
- Tune carrier concentration, by doping, to optimize power factor ($\alpha^2\sigma$)

Emerging approaches:

Embedded Nanoscale Interfaces

- Interfacial phonon scattering $\downarrow \kappa$
Most successful to date...
- Energy filtering $\uparrow \alpha^2\sigma$

Resonant State doping

- Enhanced power factor through peaks in DOS
- TI-doped PbTe; Sn-doped Bi₂Te₃
(Heremans, Science 2008; Jaworski, PRB, 2009)

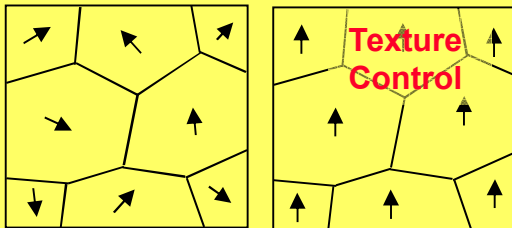
Quantum Confinement :

- Theoretical predictions of enhanced zT in nanowires.
(Hicks & Dresselhaus, 1993)
- Limited control of materials structure, composition.

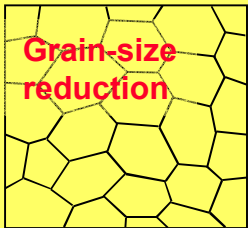
Bulk Thermoelectrics: Control of Microstructure to Improve Performance

Example: Ag_2Te nanoprecipitates in PbTe

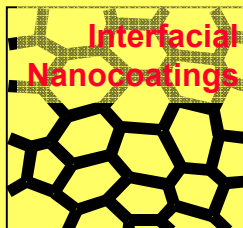
Microstructural Strategies for Nanostructured Bulk Thermoelectrics



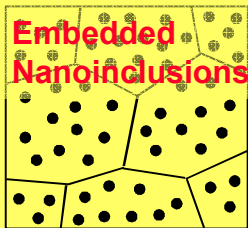
Texture Control



Grain-size reduction



Interfacial Nanocoatings



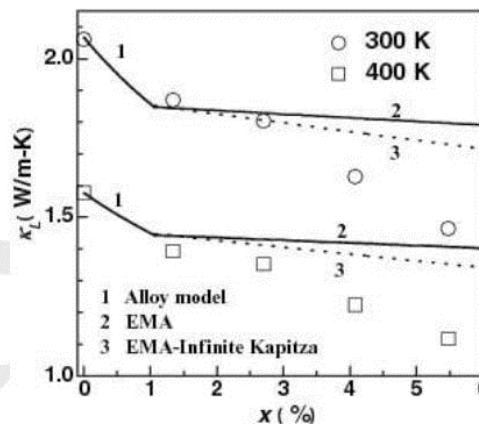
Embedded Nano-inclusions



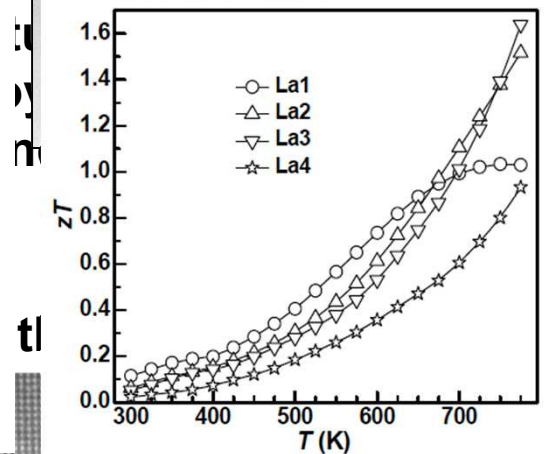
Lamellar Nanostructures

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

Phonon scattering on Ag_2Te precipitates lowers κ_L



T as high as 1.6 with suitable doping



Ag_2Te

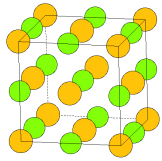
Y. Pei, J. Lensch-Falk, E.S. Toberer, D.L. Medlin, G.J. Snyder, *Advanced Functional Materials* (2010).

5 nm

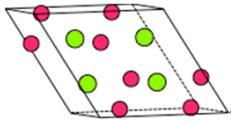
J. Lensch-Falk, J. Sugar, M. Hekmaty, D. Medlin, *Journal of Alloys and Compounds* (2010)

Focus for this talk: Interfacial structure in Thermoelectric Tellurides

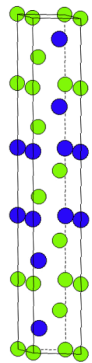
Rock-Salt
(PbTe, AgSbTe₂)



Monoclinic
(Ag₂Te)



Tetradymite
(Bi₂Te₃, Sb₂Te₃)



Rich set of structures and phase relations

Can we begin to make sense of interfaces in these complex systems?

• Grain boundary structure in Bi₂Te₃

-Low angle GB structure:

-array of individual, dissociated dislocations.

-High angle Grain boundaries

-(0001) basal twin

-Impact of weak bonding on Te(1)-Te(1) plane

-(0, -1, 1,13) boundary

-coherency of (0, -1, 5) planes

-local rocksalt coordination

•Rocksalt/Tetradymite Telluride Interfaces

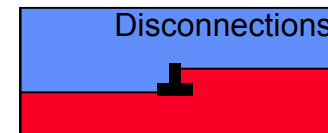
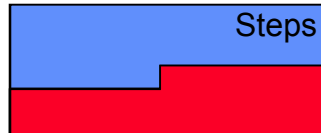
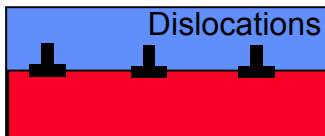
-AgSbTe₂/Sb₂Te₃

-PbTe/Sb₂Te₃

-Tetradymite plate formation.

-Interfacial strain accommodation.

Interfacial Line Defects: Building blocks to general understanding of interface structure and behavior.



Collaborators

Sandia/Livermore

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Sandia/Albuquerque

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LBNL/NCEM

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California Institute of Technology

N.A. Heinz, T. Ikeda, G.J. Snyder

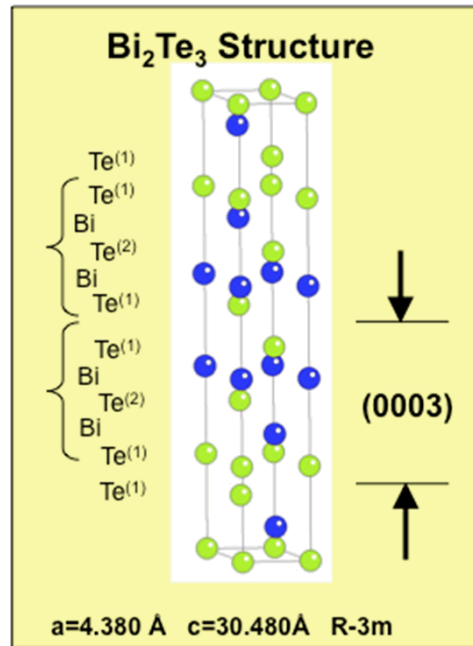
Special thanks to:

- LLNL: John Bradley, for use for LLNL's Titan 80/300 instrument
- LBNL: User program, National Center for Electron Microscopy
- UCD: Z. Zhang and E. Lavernia, for assistance with bulk Bi_2Te_3 processing

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Control of Grain Structure important to Bi_2Te_3 -Based Thermoelectrics

Microstructural Strategies applied to Bi_2Te_3 -based materials

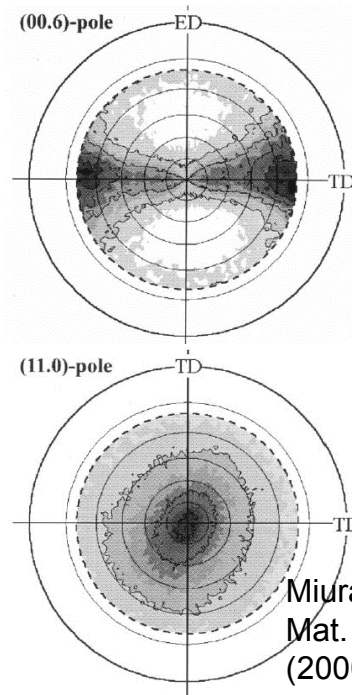


•Layered Crystal Structure

- anisotropic TE properties
- optimal zT parallel with basal planes
- easy fracture on basal planes

Control of crystal texture

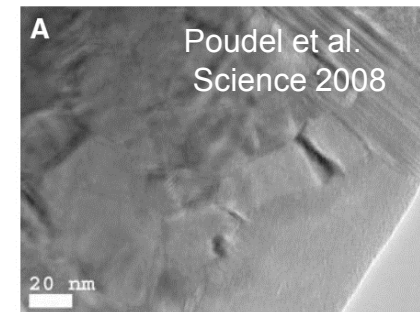
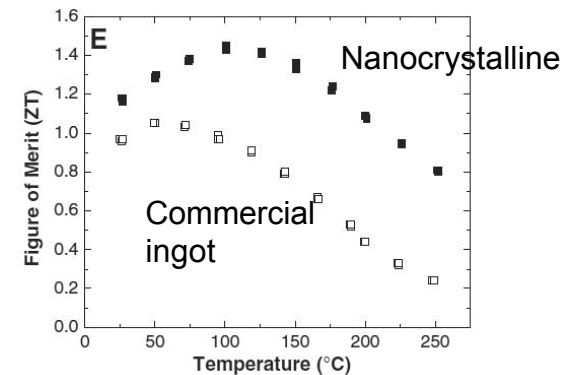
Example: Texture in Hot Extruded Bi_2Te_3



Miura et al.,
Mat. Sci. Eng. A
(2000)

Reduction of Grain Size

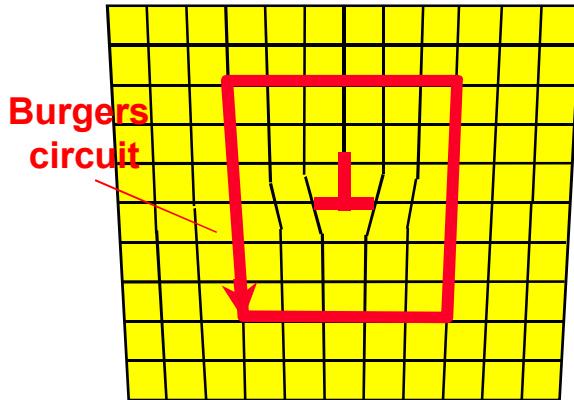
Example: Enhanced zT in nanocrystalline $(\text{Bi,Sb})_2\text{Te}_3$



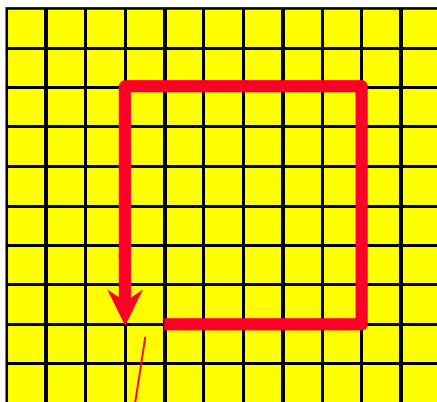
Little is known concerning the atomic scale structure of interfaces and line defects in Bi_2Te_3

Dislocations and Grain Boundaries

Dislocation

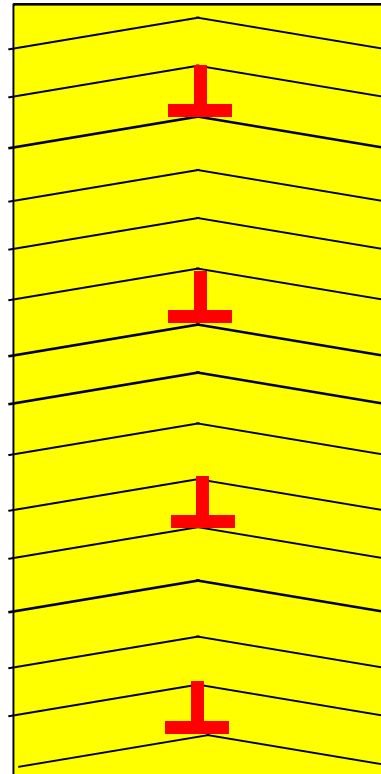


Perfect Crystal



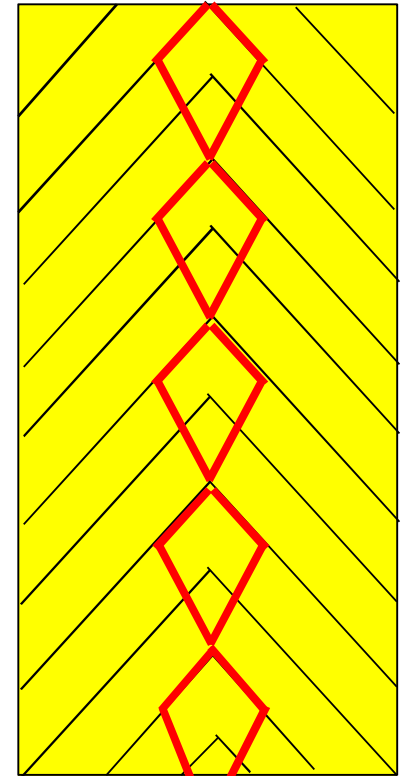
Closure Failure characterizes the Burgers vector, b

Low-Angle GB



-array of discrete dislocations

High-Angle GB

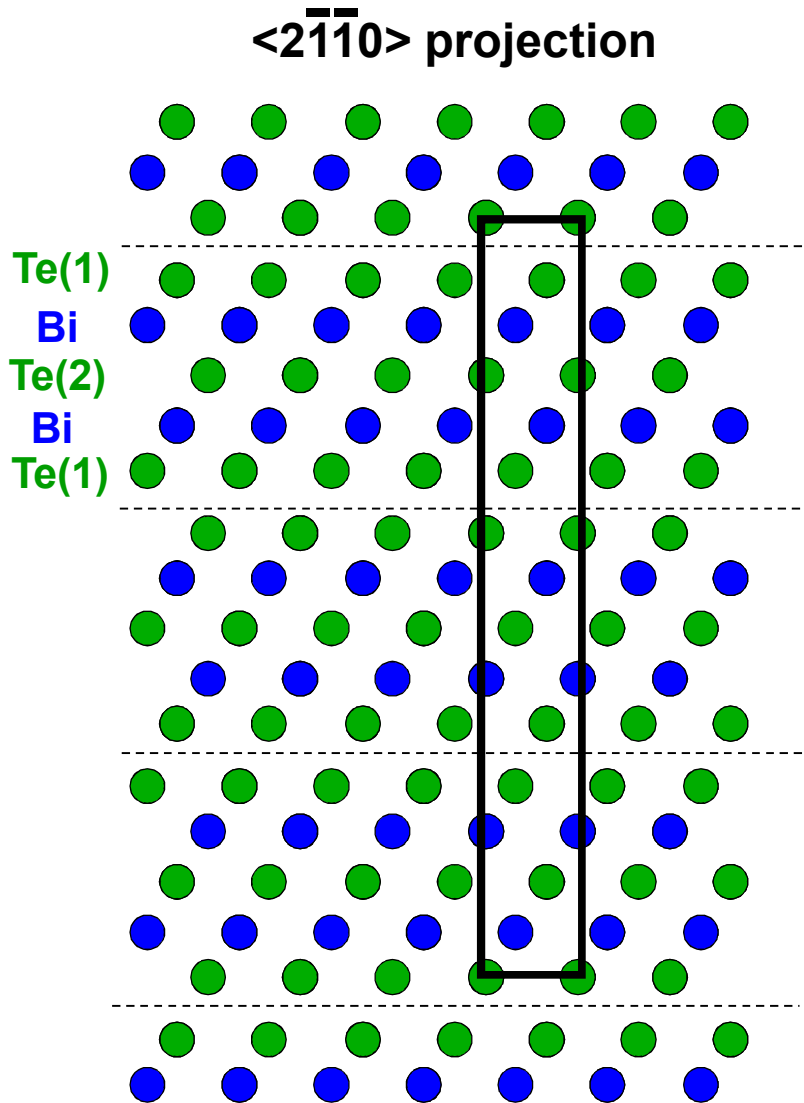


-dislocation description breaks down.
-individual structural units.

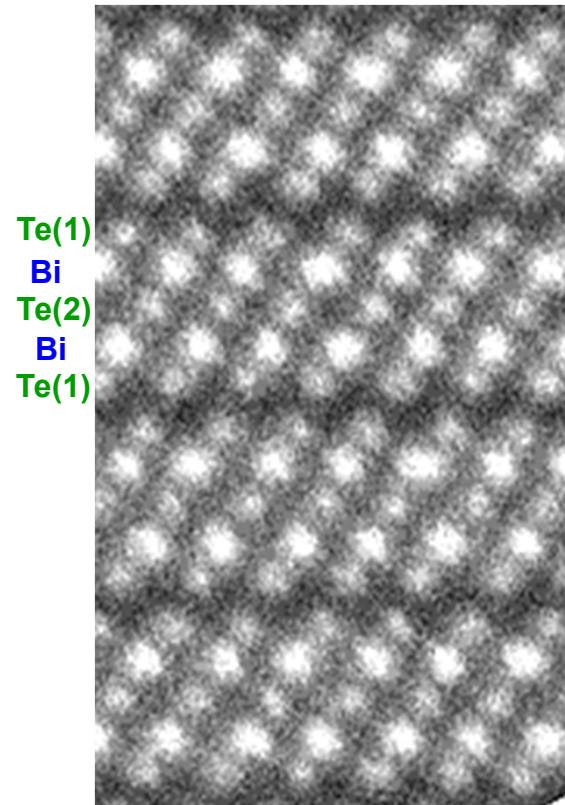
Increasing misorientation
➔

Bismuth Telluride (Bi_2Te_3): Crystal Structure

- Rhombohedral ($R\bar{3}m$) structure
- Based on tetradymite (Bi_2STe_2) prototype
- Three crystallographically distinct atomic sites



HAADF-STEM



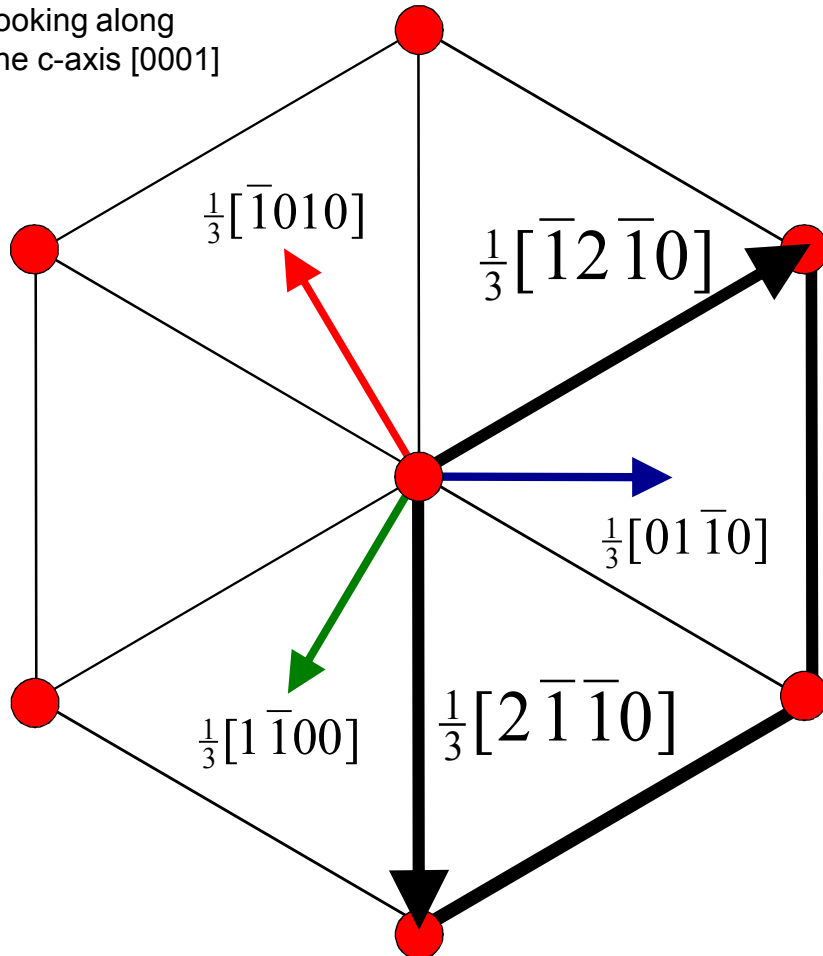
Bi: $Z=83$
Te: $Z=52$

Atomic number difference enables Bi and Te to be distinguished in HAADF-STEM

Dislocations in Bi_2Te_3

Burgers vectors lying in basal plane

Looking along
the c-axis $[0001]$

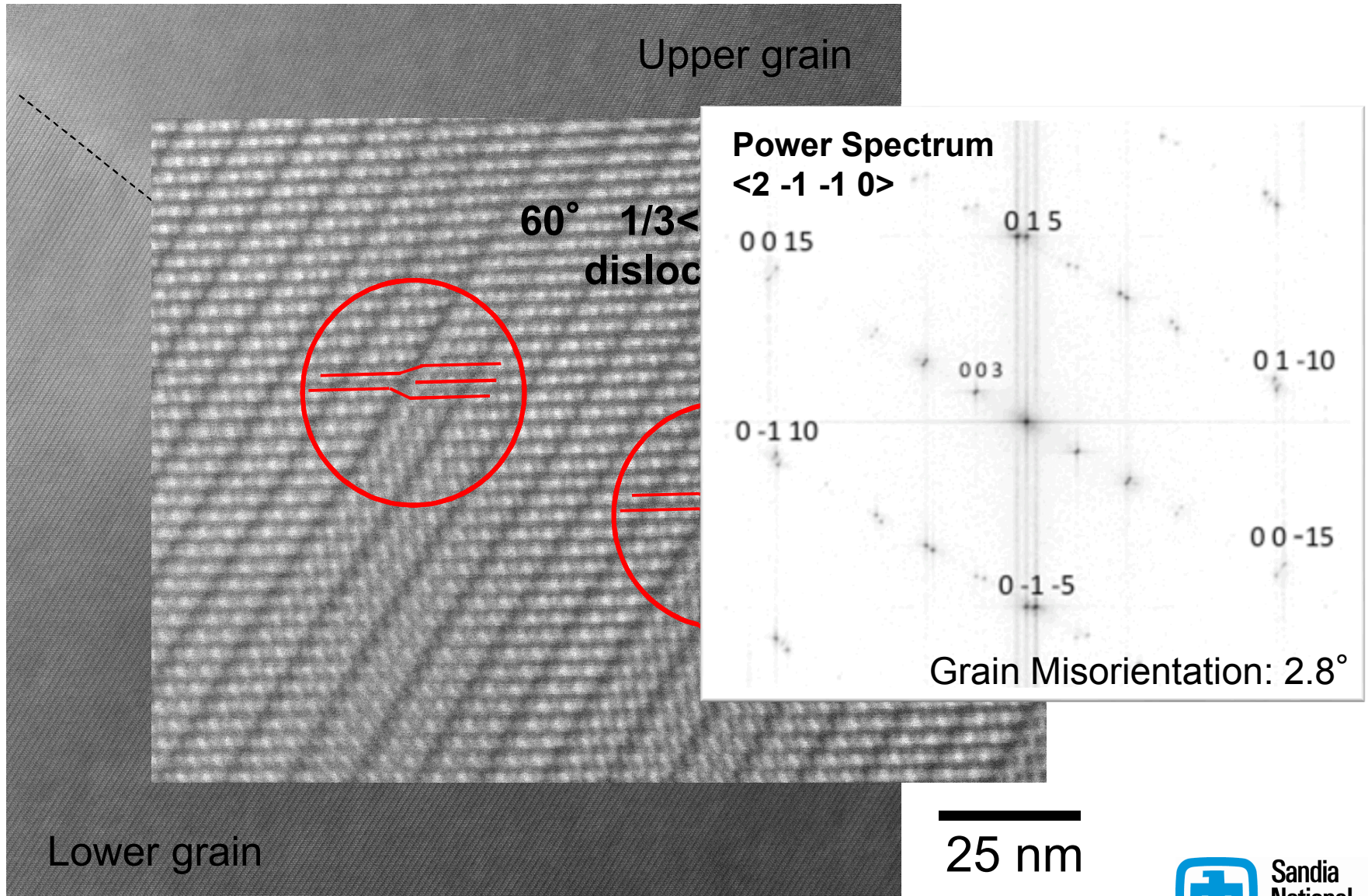


Array of $\frac{1}{3}\langle 2-1-1\ 0 \rangle$ Dislocations in Bi_2Te_3

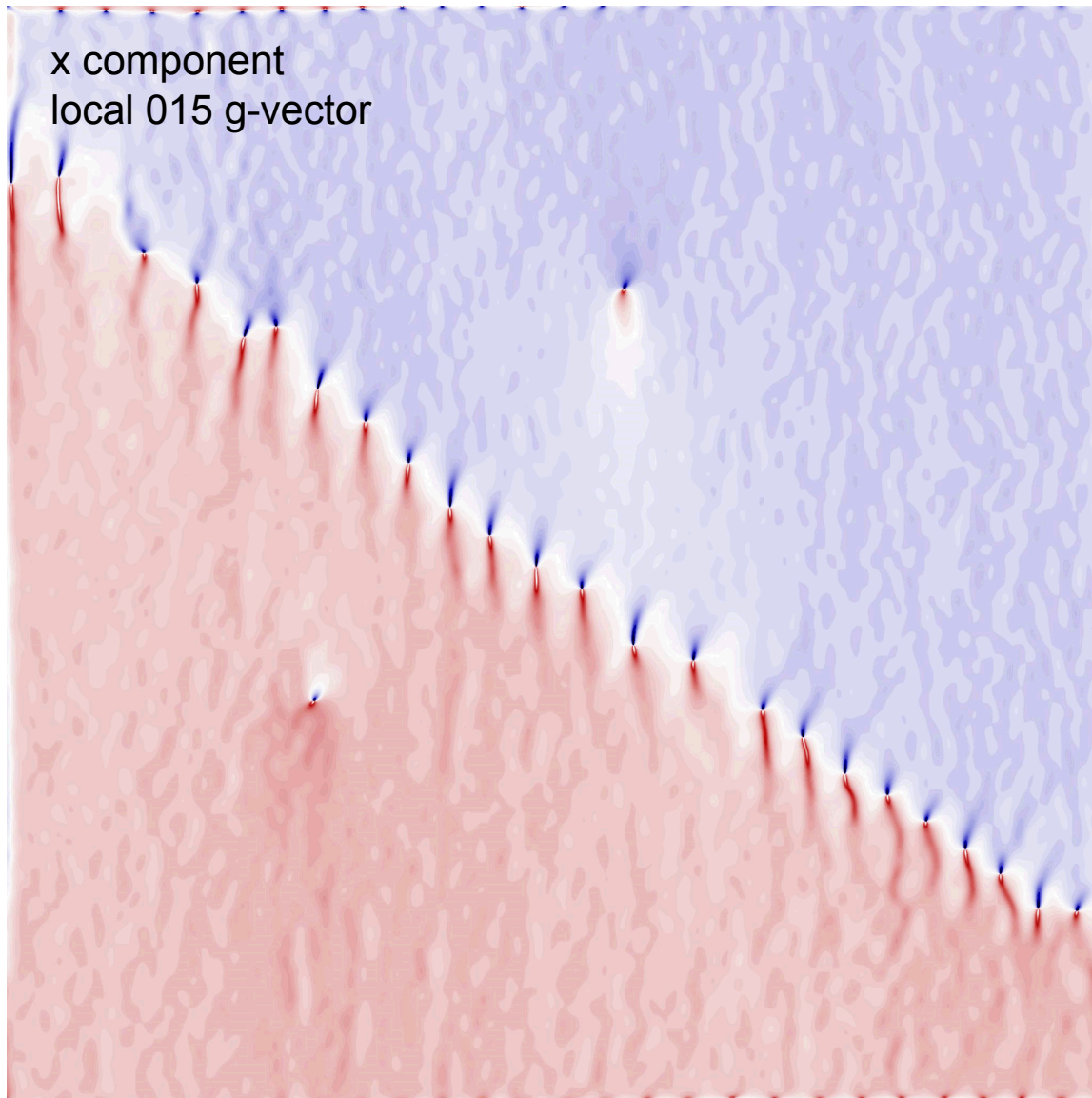


Fig. 1. Dislocation network in Bi_2Te_3 . Note that certain segments of dislocations and certain node-points have left the foil

A Low Angle Tilt Boundary



A Low Angle Tilt Boundary



Calculate tilt rotation
from dislocation density

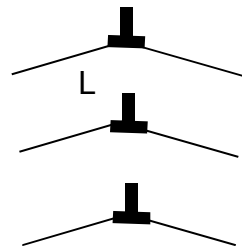
$$\theta = 2 \sin^{-1} \left(\frac{b_{edge}}{2L} \right)$$

= 3.2 ° (calculated)
(2.8° measured)

$$L_{avg} = 8.0 \text{ nm}$$

$$b_{edge} = 0.438 \text{ nm}$$

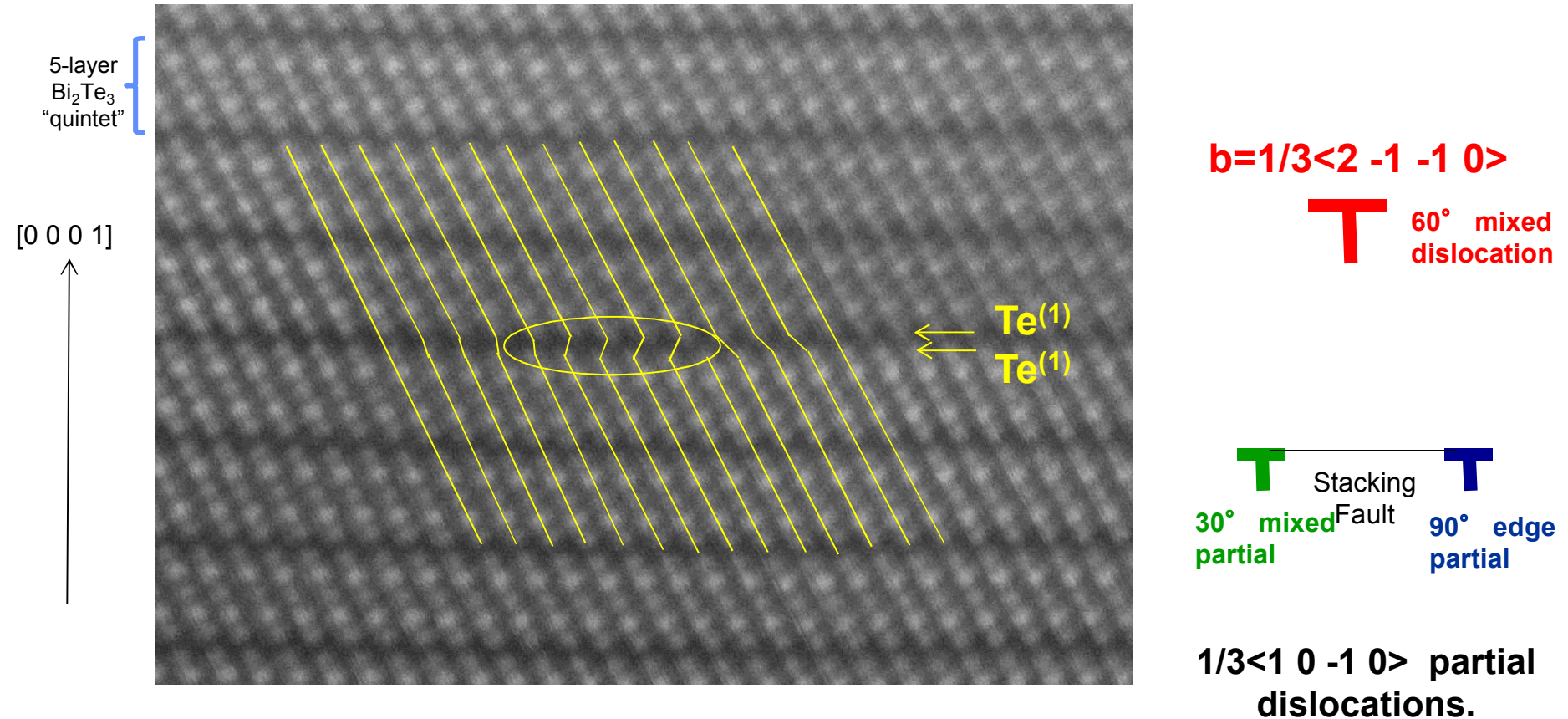
(60° 1/3<2-1-10>)



(for array of 60° dislocations,
to be pure tilt, screw components
must cancel)

25 nm

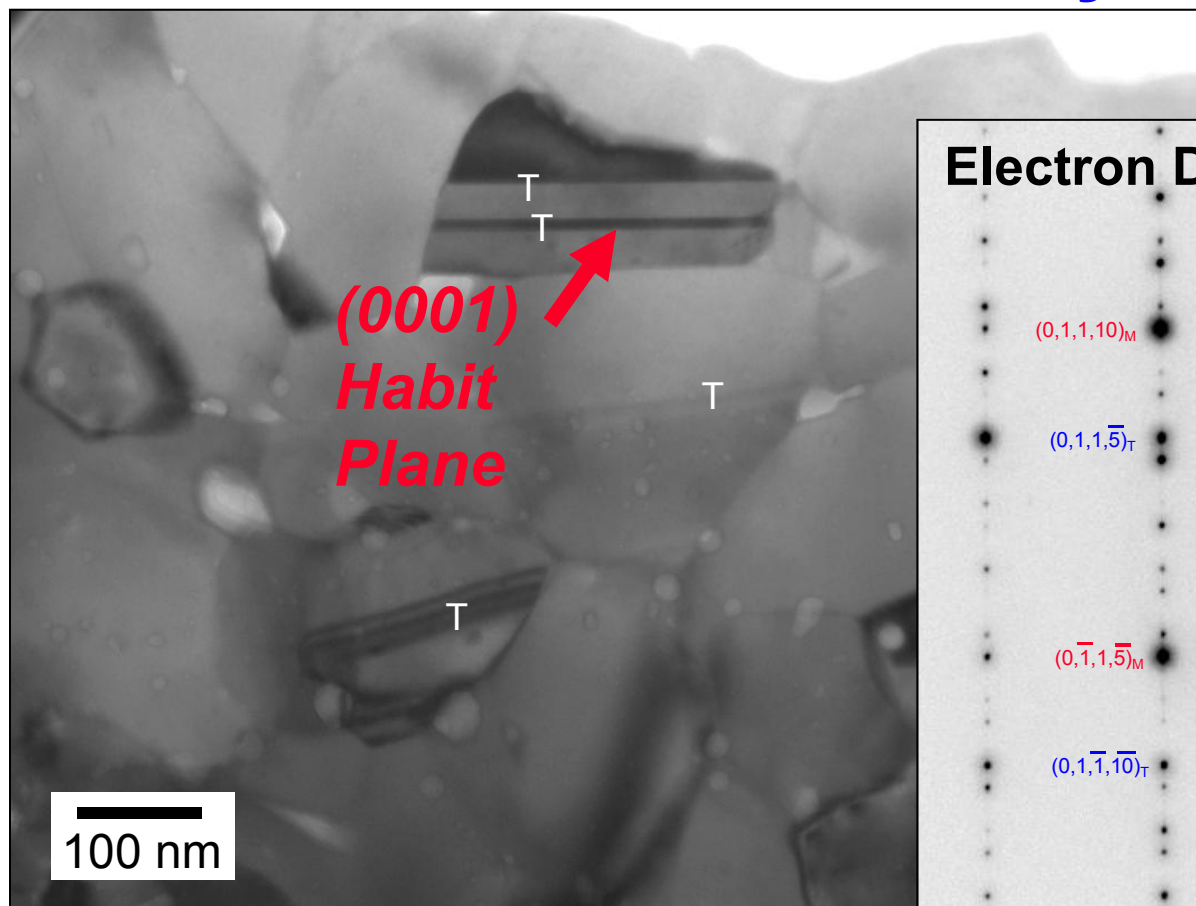
Dislocation Core structure: termination at $\text{Te}^{(1)}\text{-Te}^{(1)}$ layer, dissociation



LLNL-Titan
HAADF-STEM
300 keV

Weak, van der Waals bonding likely
favors dissociated dislocation core
at $\text{Te}^{(1)}\text{-Te}^{(1)}$ layer

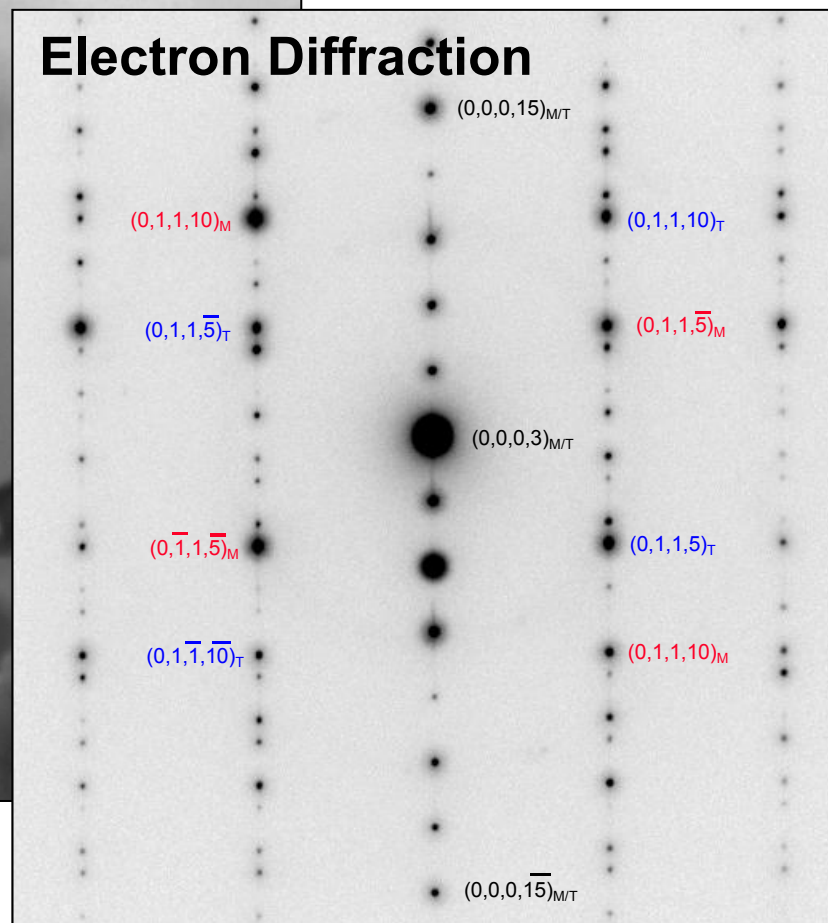
Bi₂Te₃ (0001) Basal Twin: Microstructure and crystallography



Bi₂Te₃: Powder consolidated
by spark plasma sintering

TEM Specimen Preparation:
Low voltage ion milling (1kV)
Cryo-cooling: <-100° C

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



**180° rotation
about c-axis**

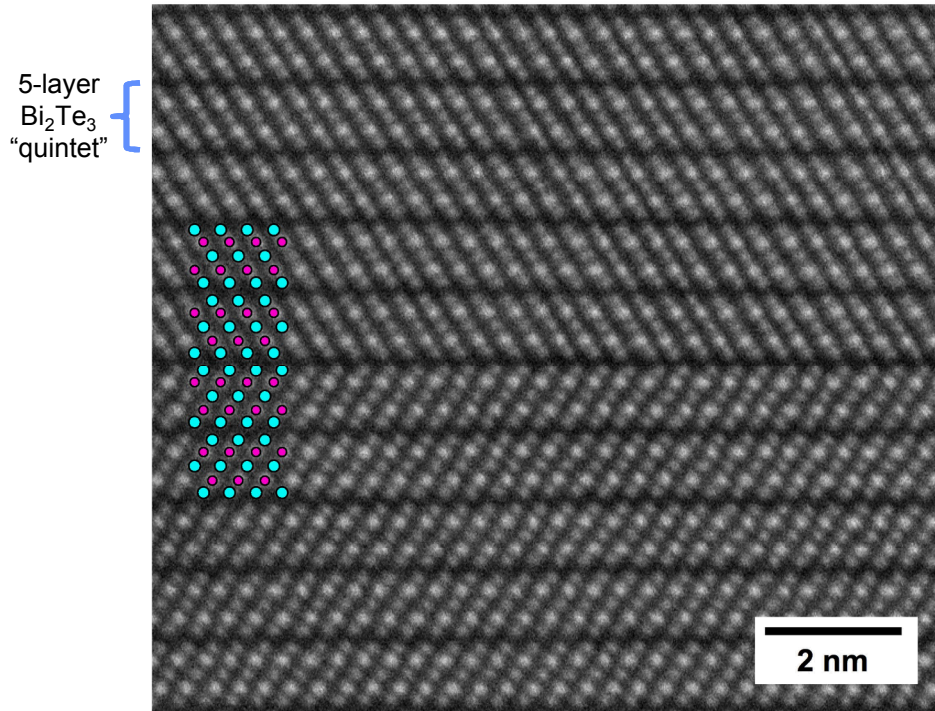


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Atomic Structure of the Bi_2Te_3 Basal Twin: Energetic preference for termination at $\text{Te}^{(1)}$ sites

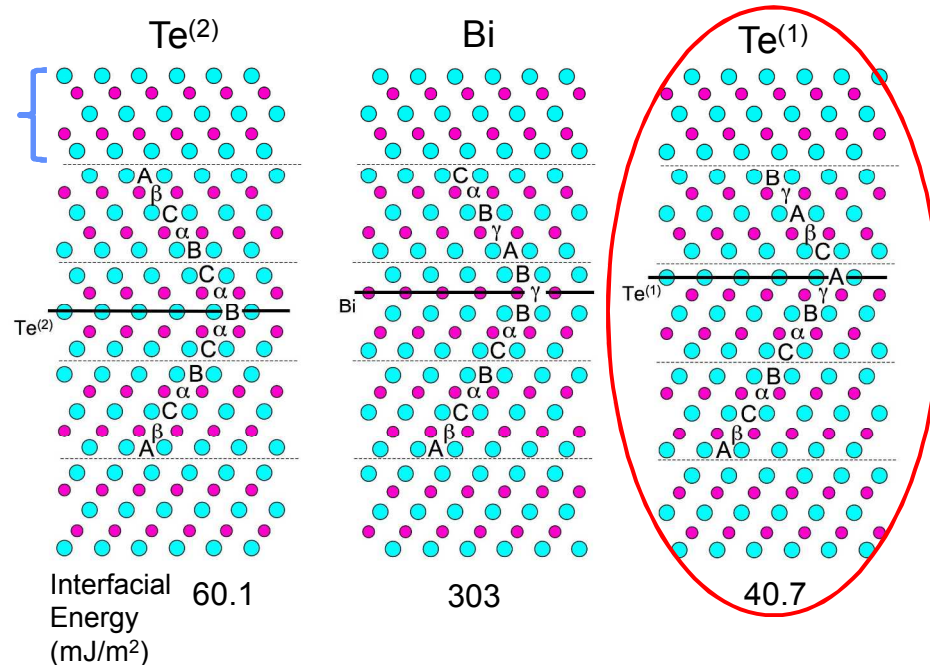
HAADF-STEM Imaging:

Twin Boundary Terminated at $\text{Te}^{(1)}$ layer



DFT Calculations:

Three Possible Compositional Terminations

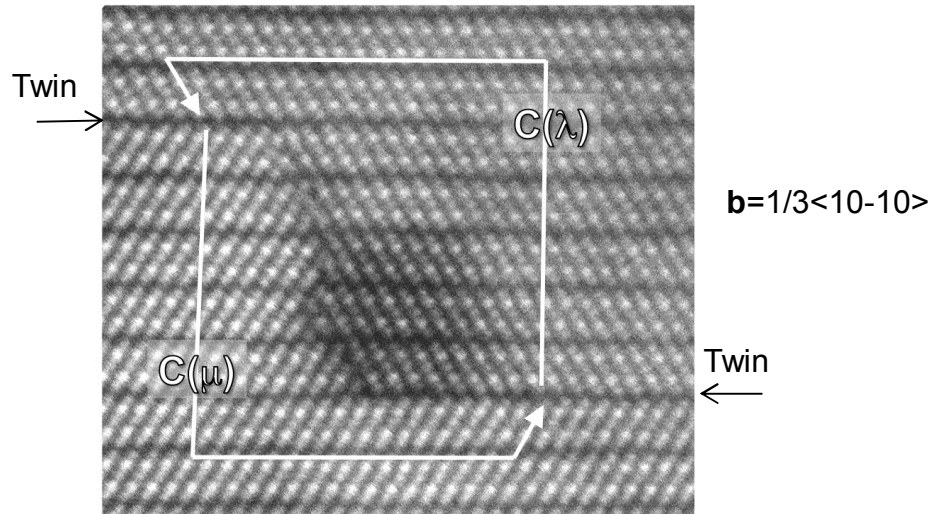


Collaboration with LBNL *National Center for Electron Microscopy*
TEAM 0.5 Microscope

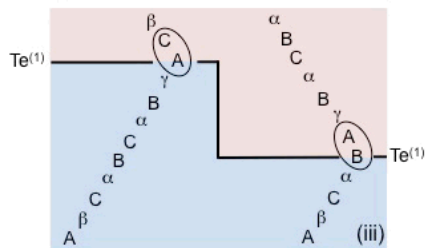
D.L. Medlin, Q.M. Ramasse, C. D. Spataru, N.C. Yang, J. Appl. Phys. (2010)

Preferential termination at $\text{Te}^{(1)}$ layers: Impact on boundary steps

Example: step in Bi_2Te_3 Basal Twin:
25 planes high (5 quintets)

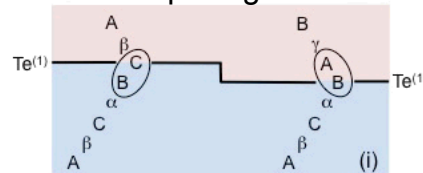


Step Height: 5

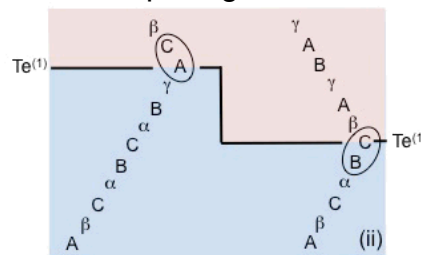


$b=1/3\langle 10-10 \rangle$

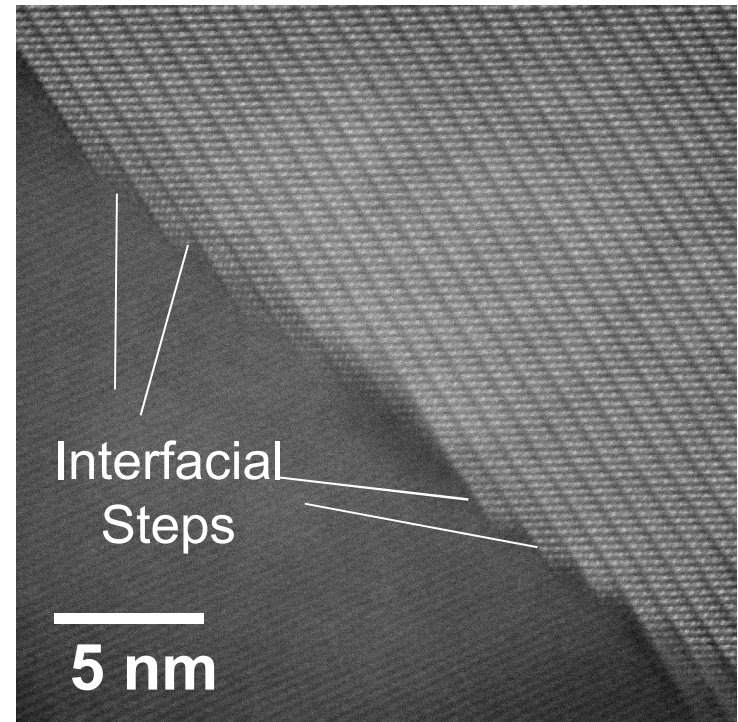
Step Height: 1



Step Height: 4



Grain boundary vicinal to (0001):
Steps of integral 5-plane Bi_2Te_3 Quintets

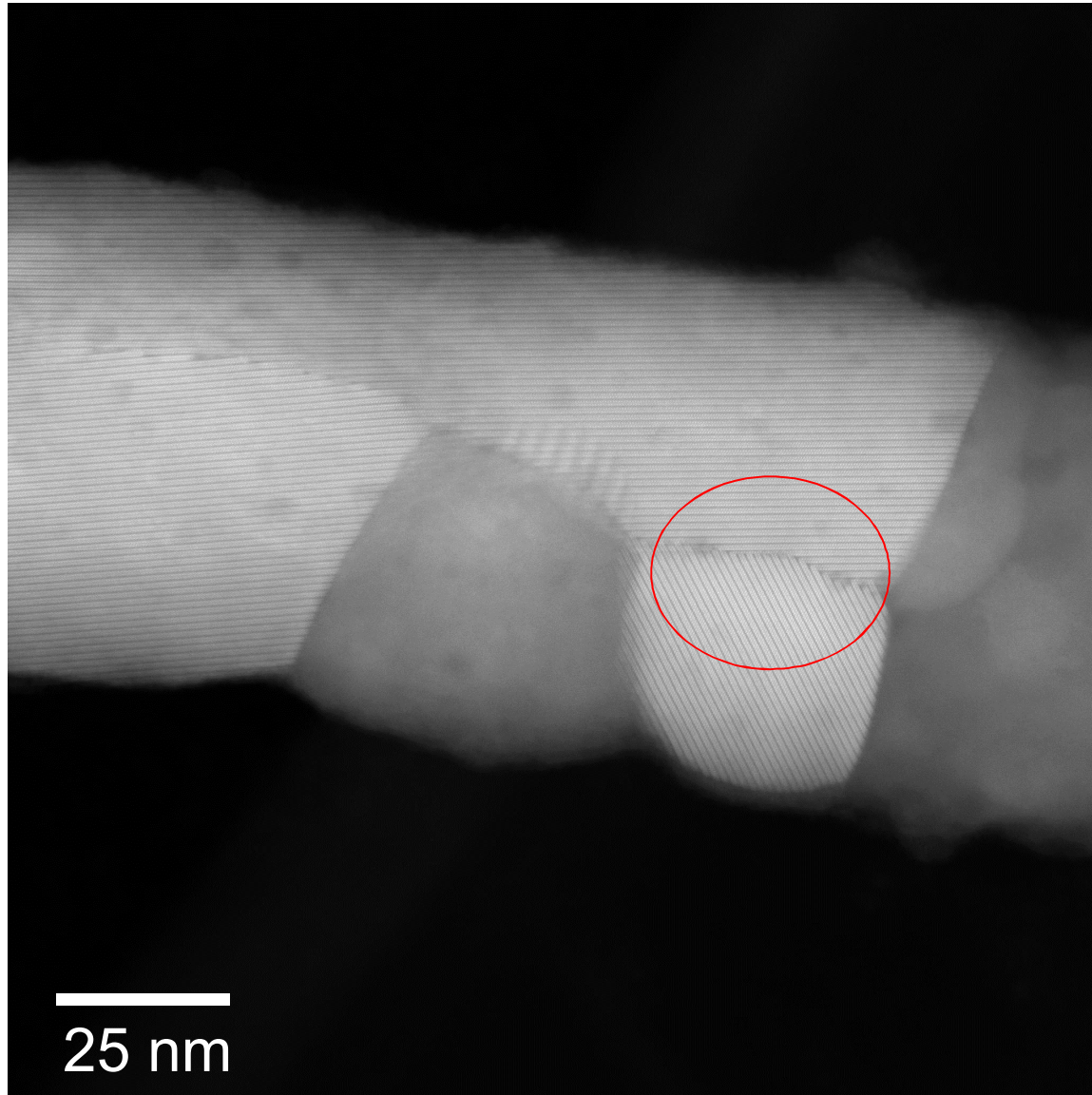


Medlin and Snyder,
JOM (2013), in press.

Medlin and Yang,
Journal of Electronic
Materials, (2012)

Bi_2Te_3 $\langle 2-1-1 \ 0 \rangle // \langle -2 \ 1 \ 1 \ 0 \rangle$ 63.78° Boundary

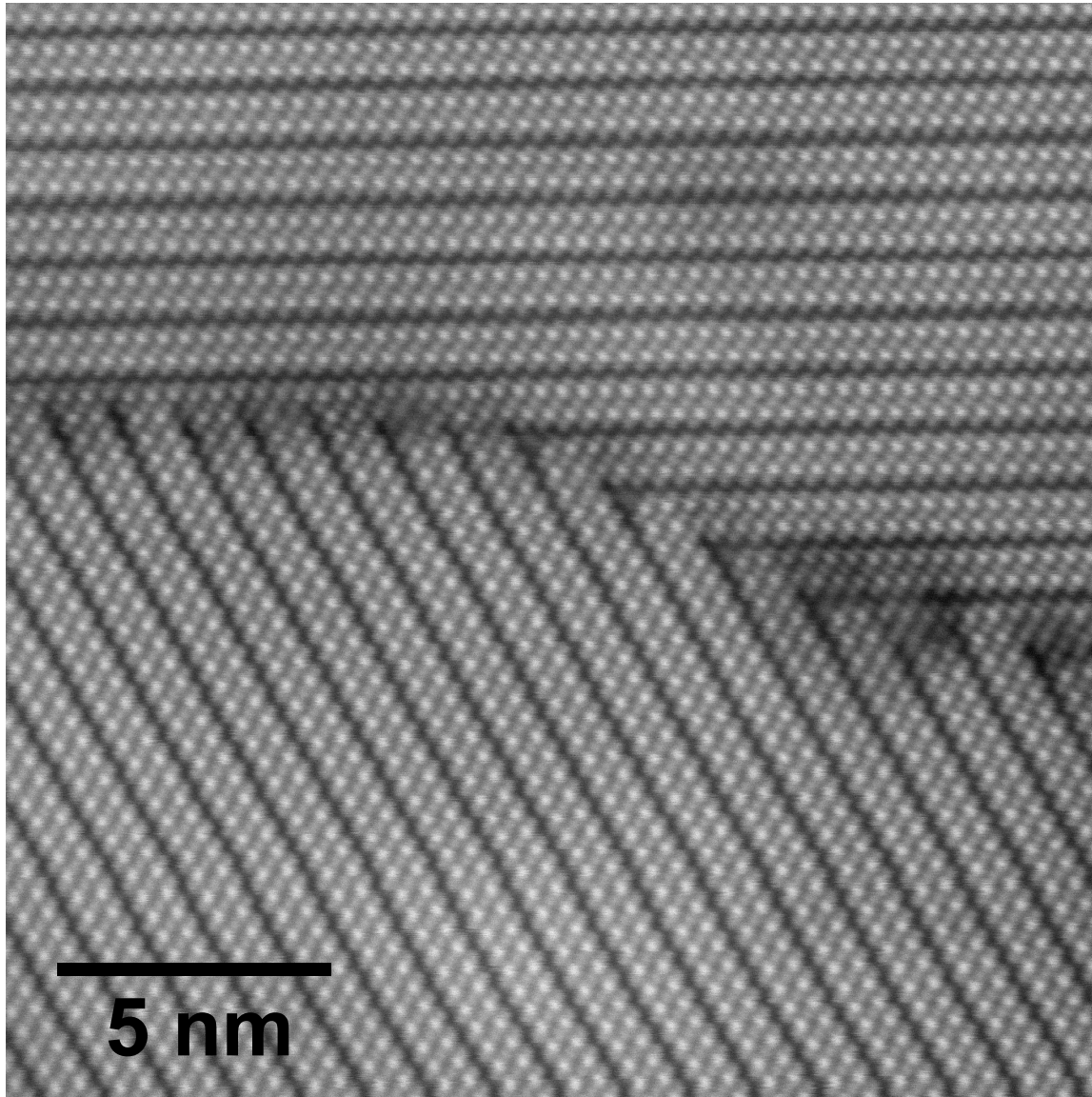
Electrodeposited
 Bi_2Te_3 nanowire
Annealed 300°C



LLNL-Titan
HAADF-STEM
300 keV

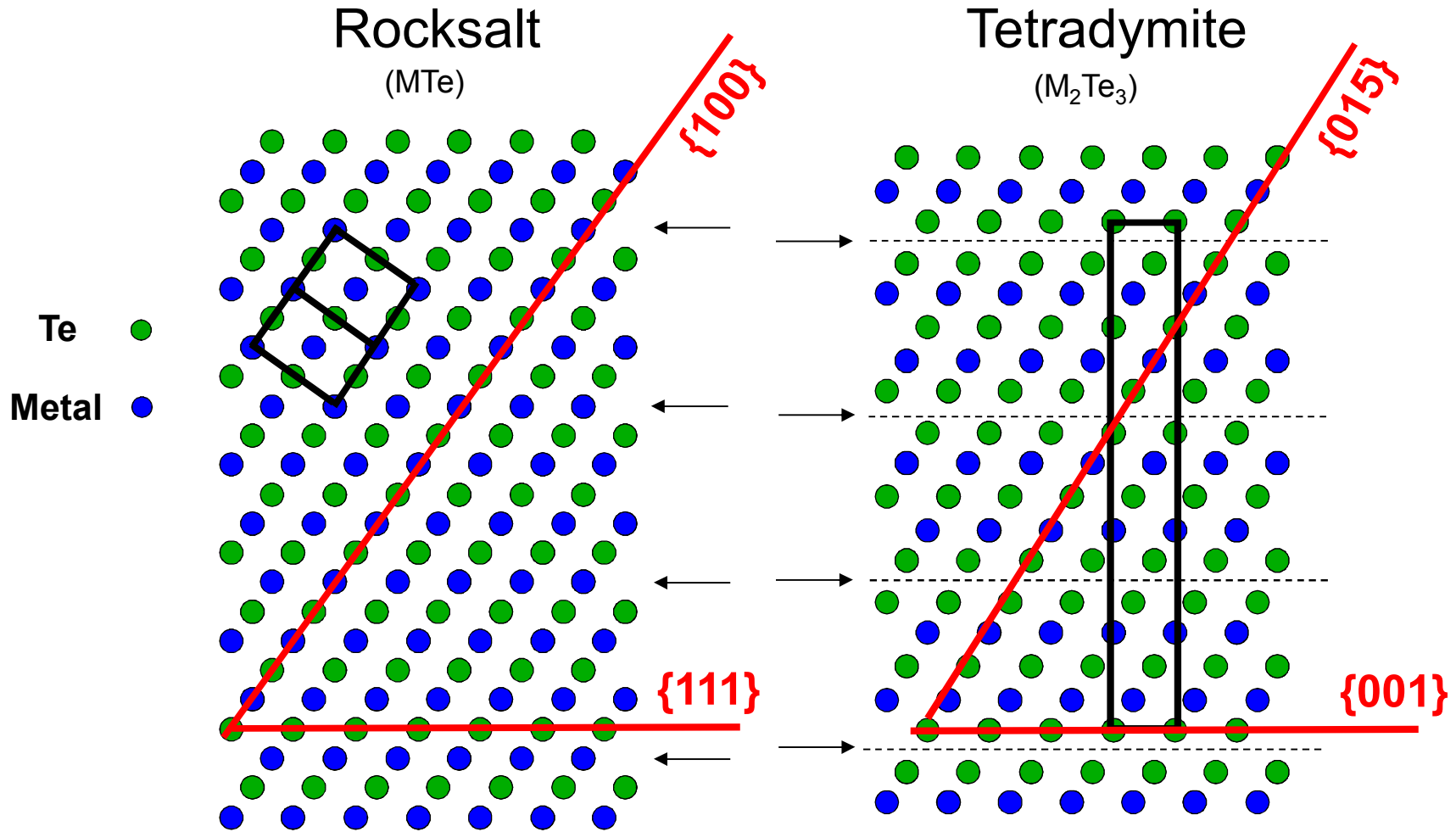
Bi_2Te_3 $\langle 2-1-1 \ 0 \rangle // \langle -2 \ 1 \ 1 \ 0 \rangle$ 63.78° Boundary

Electrodeposited
 Bi_2Te_3 nanowire
Annealed 300°C



LLNL-Titan
HAADF-STEM
300 keV

Structure of Bi_2Te_3 (tetradymite type) is closely related to rocksalt



Bi₂Te₃ <2-1-1 0>//<-2 1 1 0> 63.78° Boundary

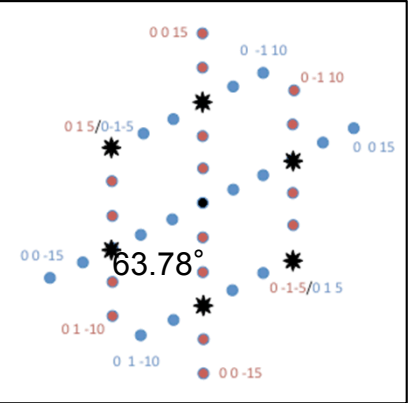
{015} planes are aligned across boundary

{015}

{015}

5 nm

Power Spectrum



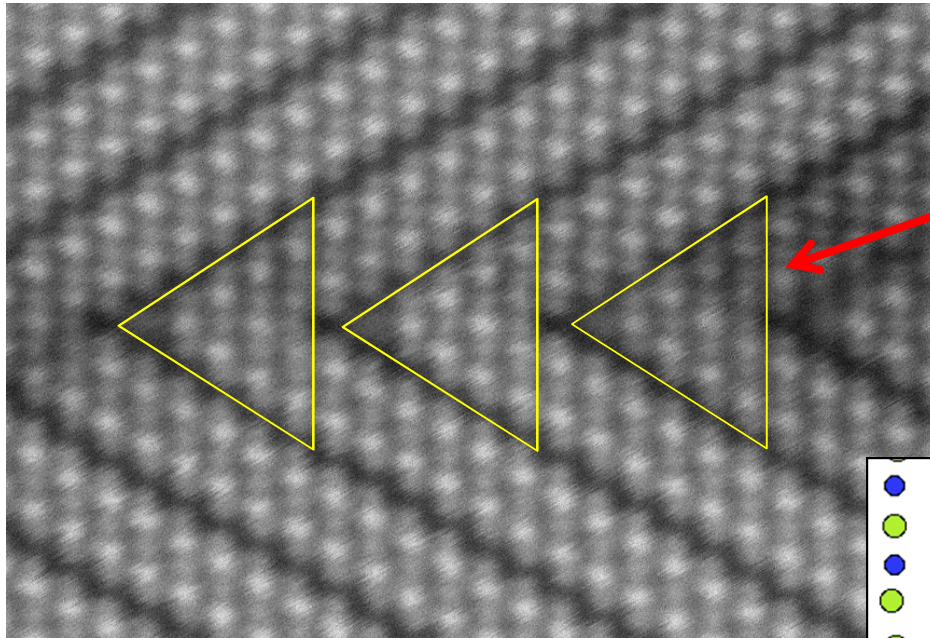
Electrodeposited
Bi₂Te₃ nanowire
Annealed 300° C

**LLNL-Titan
HAADF-STEM
300 keV**

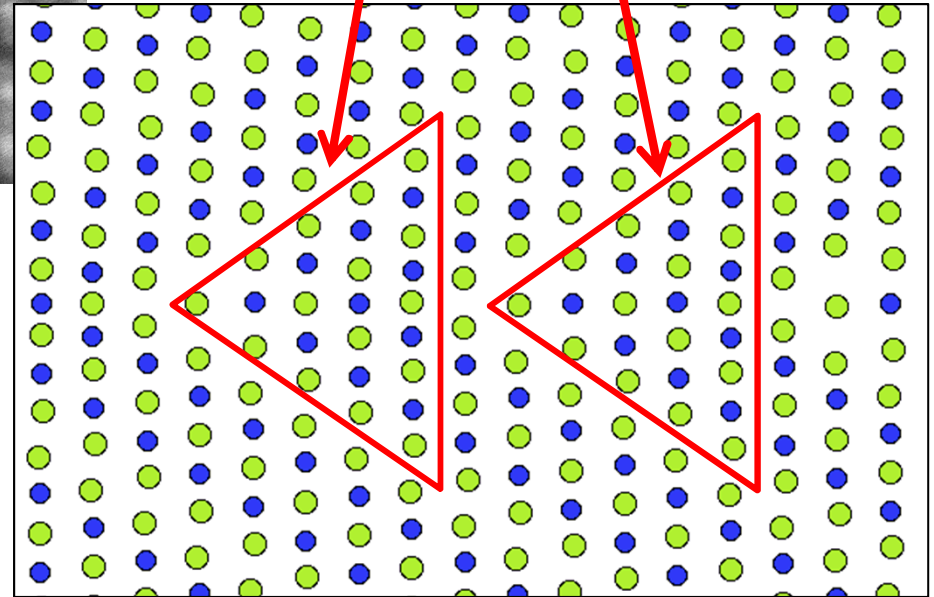


Symmetrical Interface Configuration

(0,-1,1,13) interface inclination



***Rocksalt coordinated
grain boundary units***

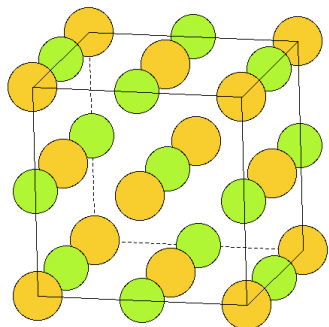


Each triangular unit:
10 Bi 15 Te

2:3 ratio of Bi and Te maintained at interface

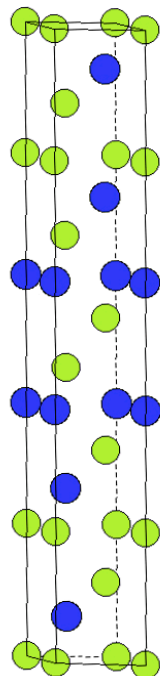
Heterophase Rocksalt/Tetradymite Telluride Interfaces

Rock-Salt (PbTe, AgSbTe₂)



Fm-3m

Tetradymite (Bi₂Te₃, Sb₂Te₃)



R-3m

What happens at interface?
How do transformations occur?
Misfit accommodation?

-Interest in forming thermoelectric nanocomposites of rock-salt and tetradymite tellurides:

- Possibility for well ordered interfaces.
- Transformations provide bulk route to synthesis.

Ikeda, et al., *Chem Mater.* 2007

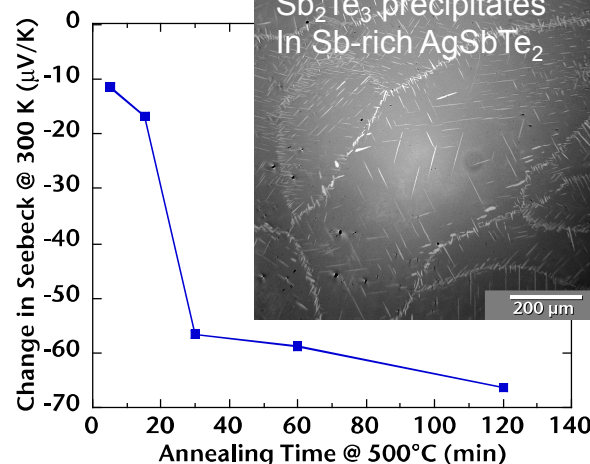
Snyder and Toberer, *Nature Materials* 2008

-AgSbTe₂:

- Constituent of TAGS (GeTe)_x(AgSbTe₂)_{1-x} and LAST (PbTe)_x(AgSbTe₂)_{1-x} zT ~ 1.8

-High performance TE material: zT > 1.2

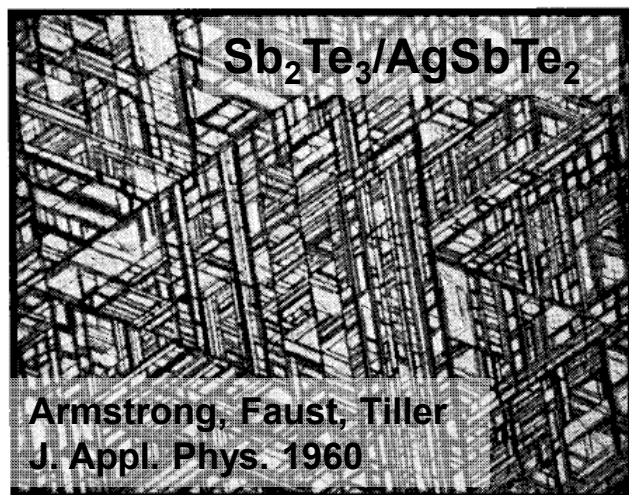
-Degradation of Seebeck coefficient with Sb₂Te₃ precipitation



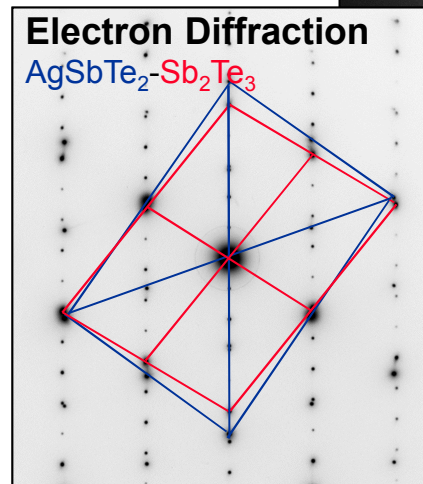
Sharma, Sugar, Medlin *J. Appl. Phys.* 2010

Crystallographic alignment between rocksalt and tetradymite phases

Widmanstätten plates

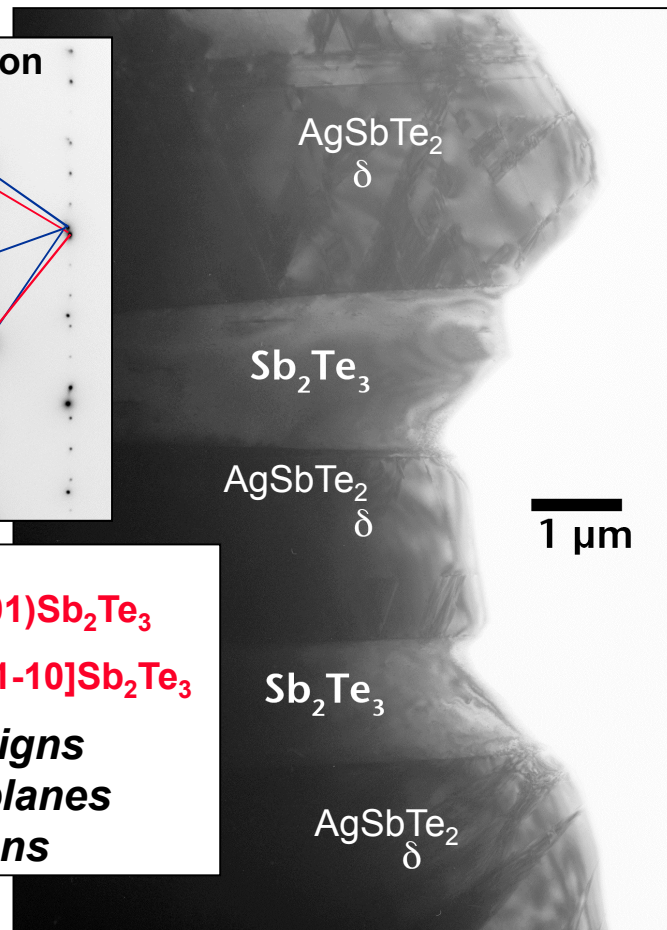


TEM Sb₂Te₃/AgSbTe₂



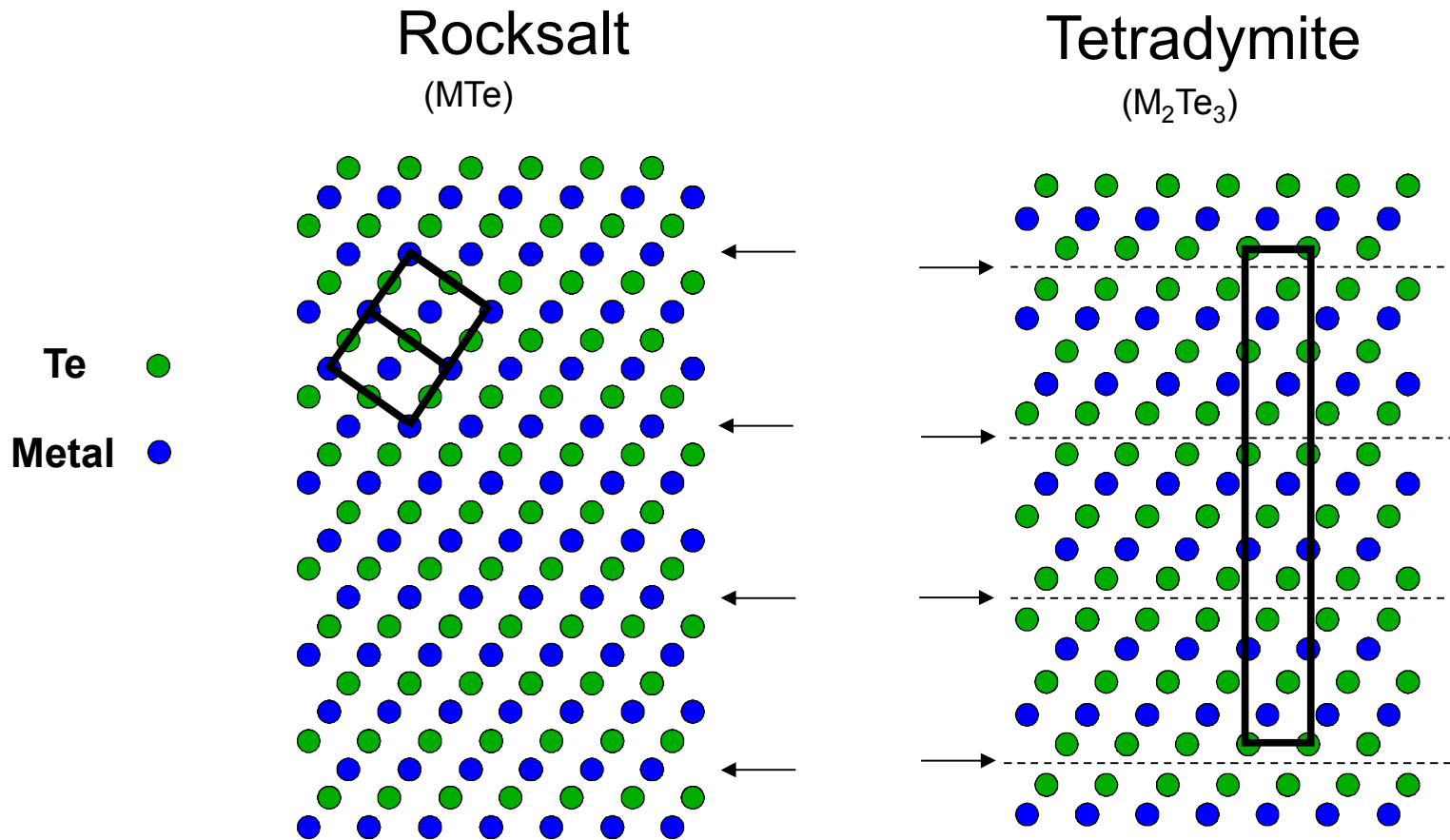
(111)AgSbTe₂ // (0001)Sb₂Te₃
[-101]AgSbTe₂ // [2-1-10]Sb₂Te₃

***Orientation aligns
close-packed planes
and directions***



Medlin and Sugar,
Scripta Mat 2010

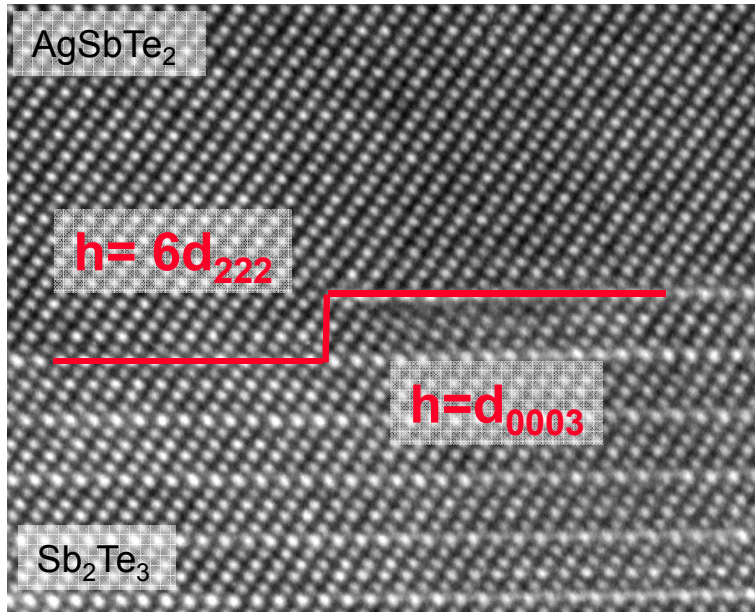
How to convert between rocksalt and tetradymite structures?



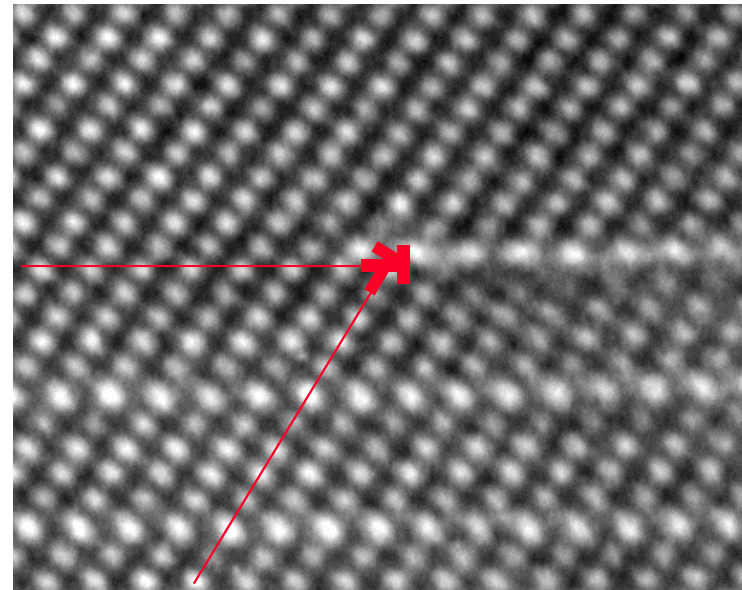
- Remove metal plane every 6 layers
- Shear blocks by $\frac{1}{3}\langle 10-10 \rangle$ (or $\frac{1}{6}\langle 112 \rangle$ relative to cubic coordinates)

Transformation can be accomplished through a ledge mechanism

HRTEM : Step at $\text{AgSbTe}_2/\text{Sb}_2\text{Te}_3$ Interface



JEOL 4000EX HRTEM



Defect has both *step* and *dislocation* character.

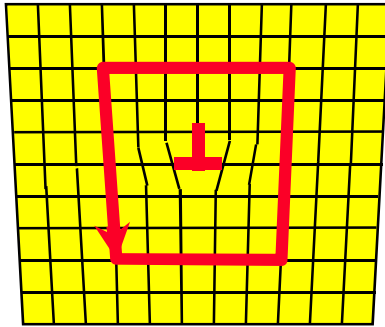
- Interfacial “Disconnection” (e.g. Hirth and Pond, Acta Mat 1996).
- Geometric properties of disconnections control mass flux and structural rearrangements of phase transformations.

Step joins 6 {222} planes in AgSbTe_2 with 5 {000 15} planes in Sb_2Te_3

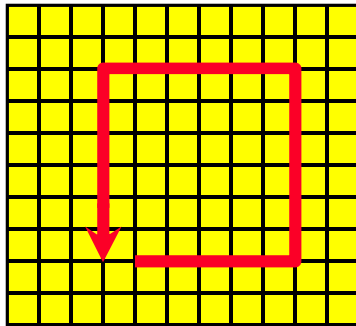
Complex dislocation configuration.

Defining the topological properties of line defects requires a reference frame

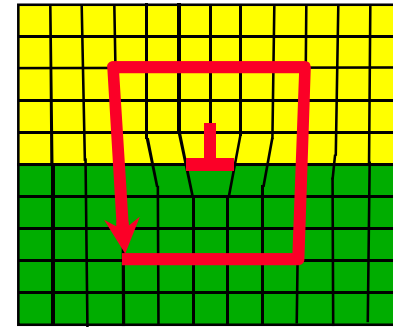
Bulk Lattice Dislocation.



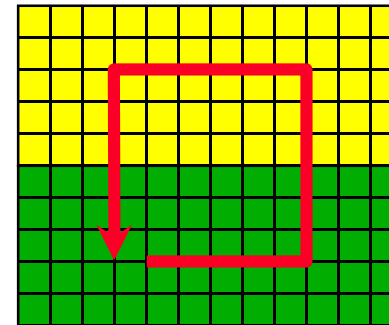
Reference Frame:
Perfect Crystal



Heteroepitaxial Misfit Dislocation.



Reference Frame:
Coherently Strained Interface



Circuit analysis to quantify defect character

Burgers vector:

$$\mathbf{b} = -(\mathbf{C}_\lambda + \mathbf{P}\mathbf{C}_\mu)$$

Upper crystal circuit

Lower crystal circuit

Crystal coordinate transformation

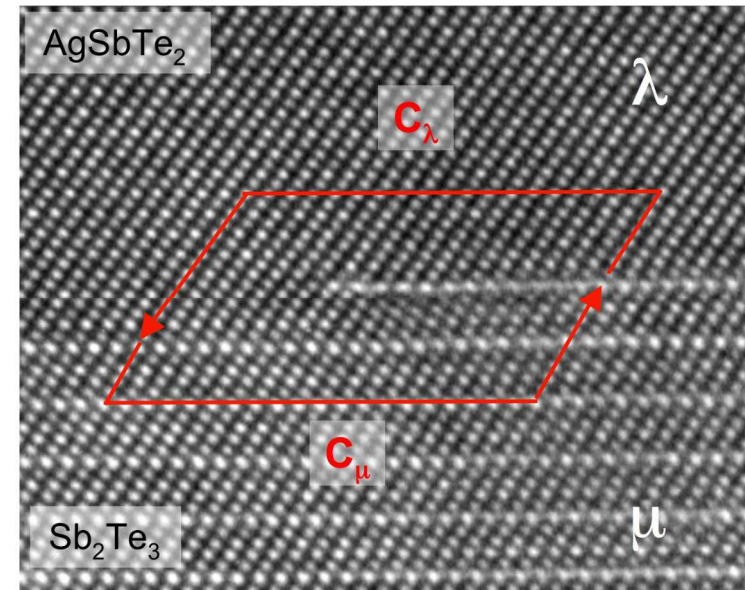
Referenced to Coherent Frame:

Strain to bring μ and λ into coherency

$$\mathbf{P} = \mathbf{L} \mathbf{A} \mathbf{M} = \begin{pmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{c_{hex}}{a_{cub} \sqrt{3}} \\ 0 & \frac{1}{2} & \frac{c_{hex}}{a_{cub} \sqrt{3}} \\ \frac{-1}{2} & 0 & \frac{c_{hex}}{a_{cub} \sqrt{3}} \end{pmatrix}$$

Converts from orthonormal to λ crystal coordinates

Converts from μ crystal coordinates to orthonormal coordinates



Misfit: 0.79%

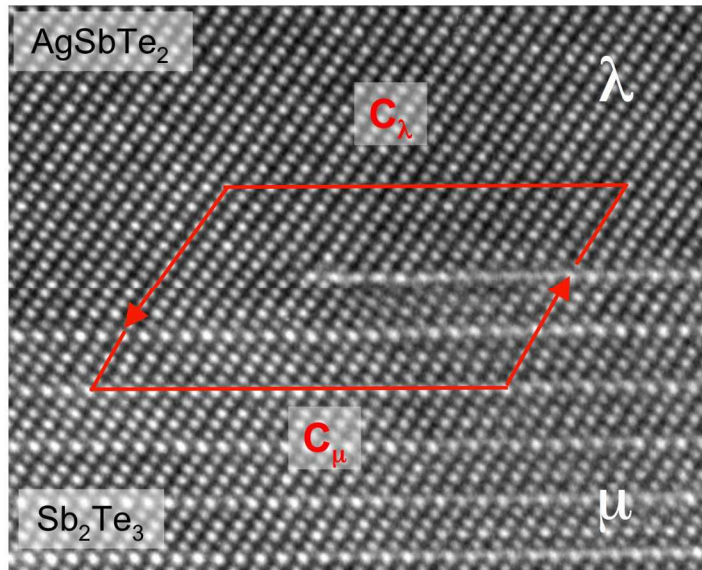
$$r = \frac{1}{\sqrt{2}} \frac{a_{cub}}{a_{hex}} = 1.0079$$

Sb₂Te₃: a=4.264 Å
c=30.458 Å

AgSbTe₂: a=6.078 Å

Role of defect in precipitate growth:

Burgers vector:



Upper crystal circuit

Lower crystal circuit

$$\mathbf{b} = -(\mathbf{C}_\lambda + \mathbf{P}\mathbf{C}_\mu)$$

Coordinate Transformation
From Tetradymite to
Rock-salt reference frame

Resolve $\mathbf{b}$ into components
normal and parallel to interface

$$\mathbf{b}_n = (a_{cub} - c_{hex} / 3\sqrt{3})[111]$$

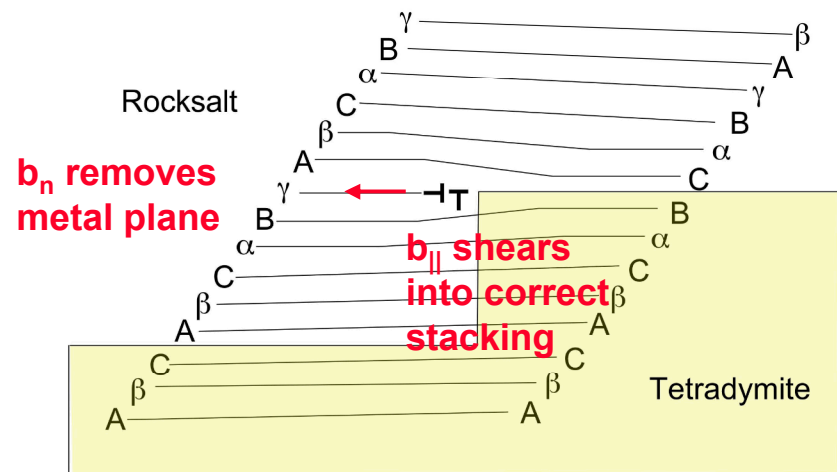
•mismatch of step heights.

$$|\mathbf{b}_n| = 0.3747\text{\AA}$$

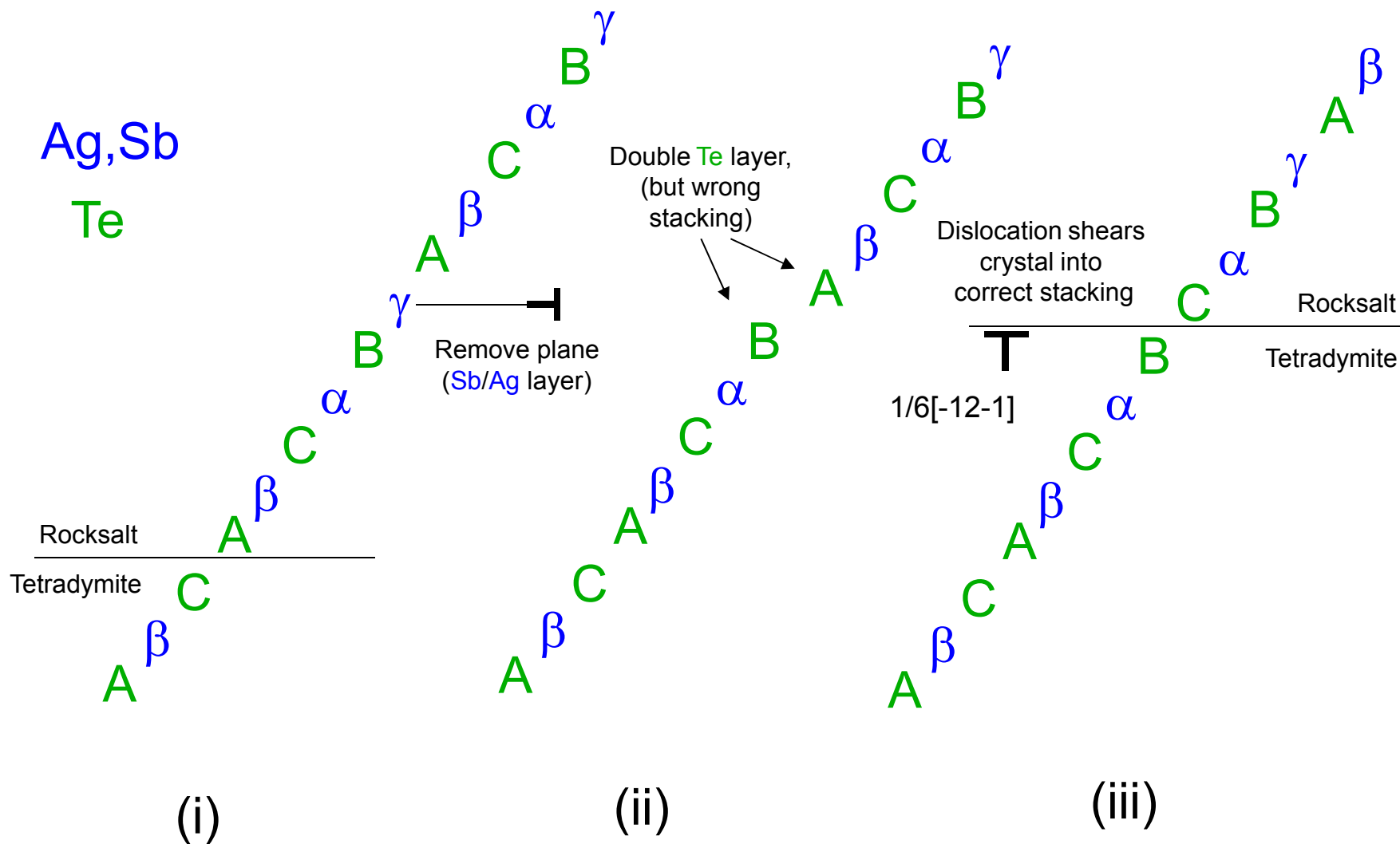
$$\mathbf{b}_\parallel = \frac{a_{cub}}{6}[\bar{1}2\bar{1}]$$

•Analogous to
Shockley partial
Dislocation

$$|\mathbf{b}_\parallel| = 2.48\text{\AA}$$

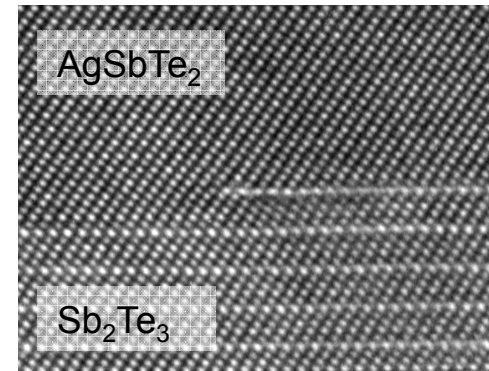
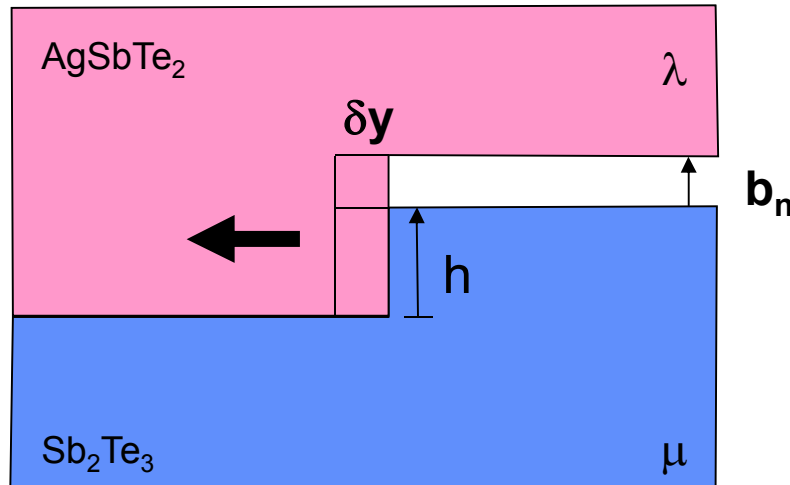


Schematic of Transformation Sequence



Defect properties give local mass flux required for transformation

Partition flux for defect motion into step and dislocation components



$$\frac{\Delta N_i}{L \delta y} = \underbrace{(\chi_i^\lambda - \chi_i^\mu)h}_{\text{step}} + \underbrace{\chi_i^\lambda b_n}_{\text{dislocation}}$$

Hirth & Pond, Acta Mat 1996

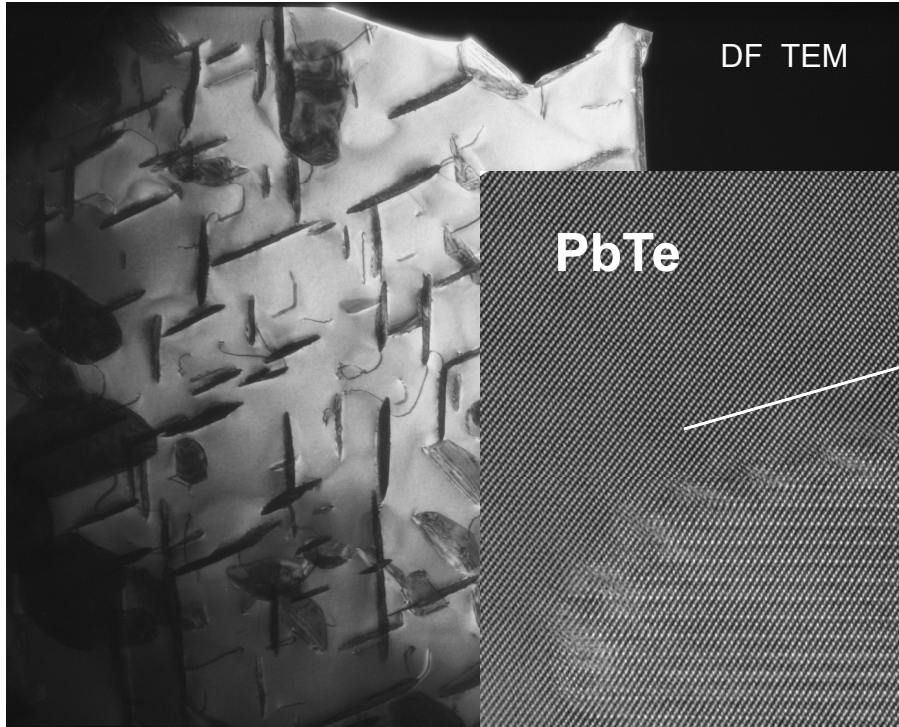
**Reject Ag and Incorporate Sb
in ratio of 3:1**

**Tellurium:
Step and Dislocation fluxes cancel.
No long-range Te transport required.**

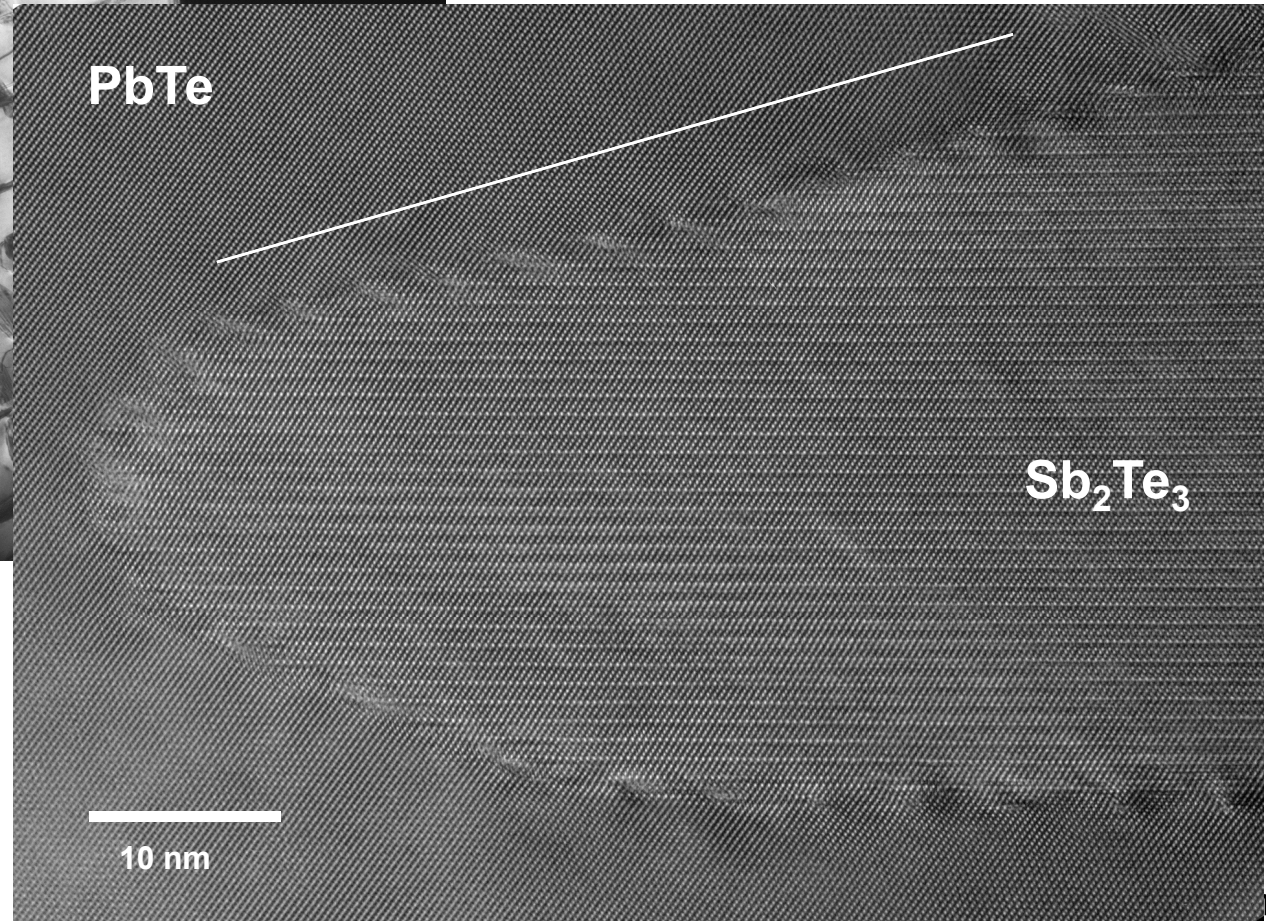
Species	Step flux (atoms/Å ²)	Dislocation flux (atom/Å ²)	Total flux (atom/Å ²)
Ag	$\frac{2 c_{hex}}{3 a_{cub}^3}$ +0.09043	$\frac{2}{a_{cub}^3} (\sqrt{3} a_{cub} - c_{hex} / 3)$ +0.00334	$\frac{2\sqrt{3}}{a_{cub}^2}$ +0.09377
Sb	$\frac{2 c_{hex}}{3 a_{cub}^3} - \frac{8\sqrt{3}}{3 a_{cub}^2}$ -0.03459	$\frac{2}{a_{cub}^3} (\sqrt{3} a_{cub} - c_{hex} / 3)$ +0.00334	$-\frac{2\sqrt{3}}{3 a_{cub}^2}$ -0.03126
Te	$-\frac{4}{a_{cub}^3} (\sqrt{3} a_{cub} - c_{hex} / 3)$ -0.00668	$+\frac{4}{a_{cub}^3} (\sqrt{3} a_{cub} - c_{hex} / 3)$ +0.00668	0

A system with larger misfit: $\text{PbTe}/\text{Sb}_2\text{Te}_3$

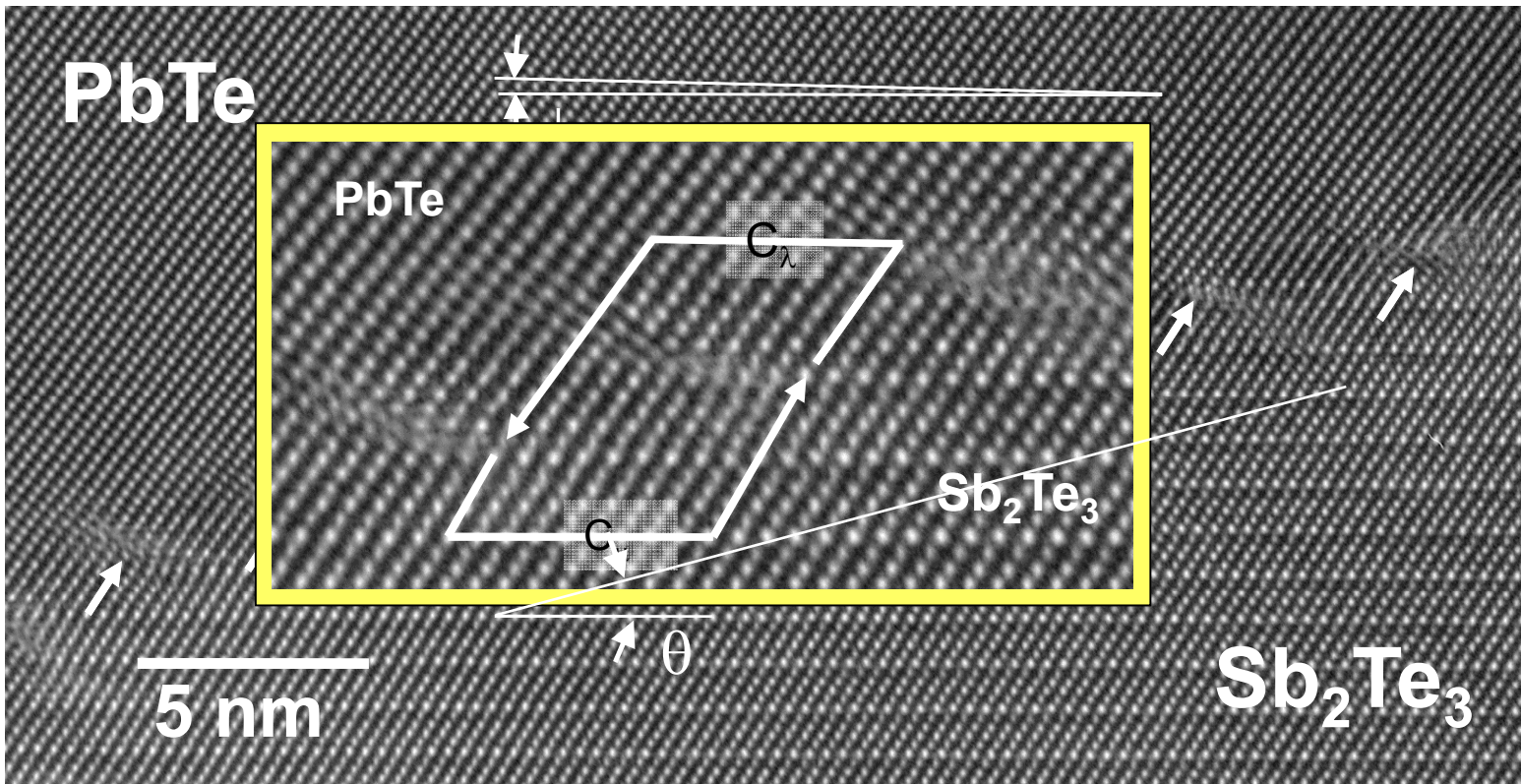
Sb_2Te_3 Precipitates in PbTe



$\text{AgSbTe}_2(111)/\text{Sb}_2\text{Te}_3(0001)$
Misfit: +0.79%



Inclined Section of interface Composed of Disconnections



Circuit Analysis:

Defects identical to the “6/5” disconnections observed in AgSbTe₂/Sb₂Te₃

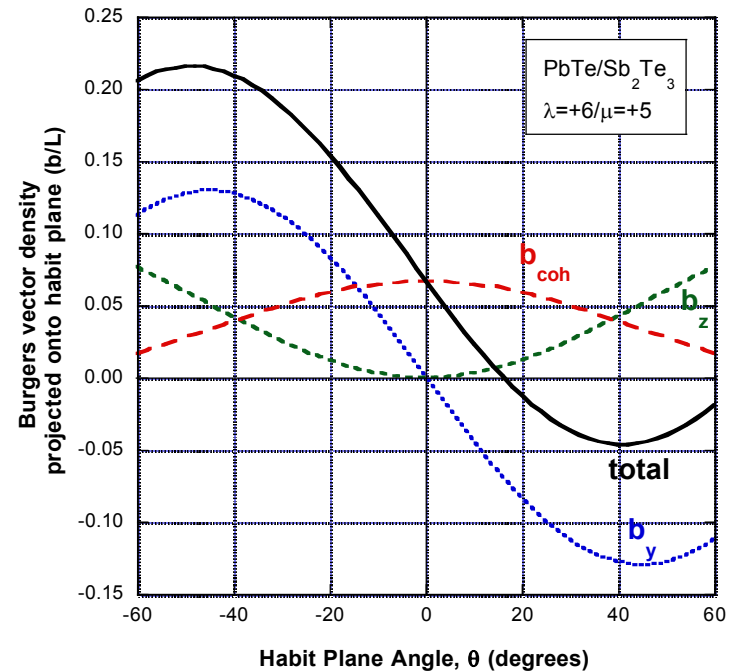
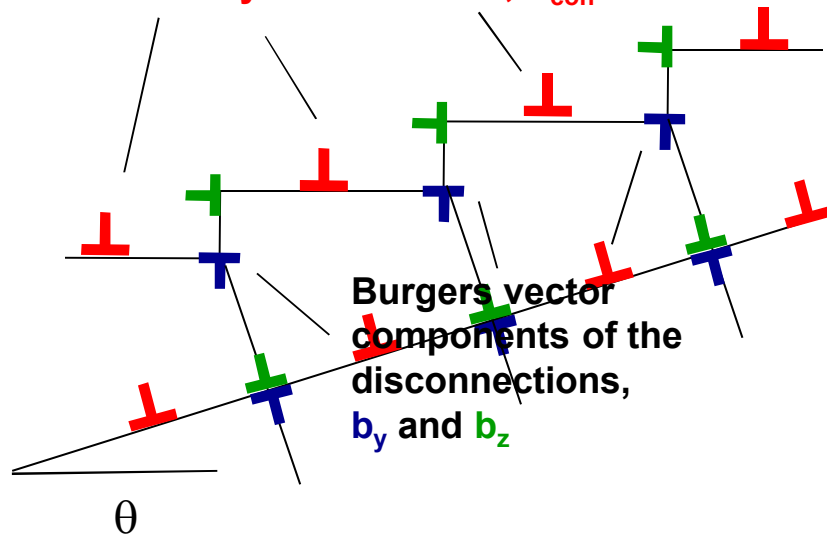
Interface Geometry:

Inclination: $\theta = 14.8^\circ$ Lattice rotation: $\phi = 1.1^\circ$ to 1.4°

Interplay between Misfit Accommodation and Interface Inclination

Project components on inclined interface plane

Adjust spacing to cancel ($\epsilon_{yy} = 0$)
as "coherency" dislocations, b_{coh}



$$-\epsilon = (b_y \tan \theta + b_z \tan^2 \theta) h^{-1} \quad \rightarrow \quad \theta = 16.2^\circ$$

Pond, Celotto, Hirth, Acta Mater. 2003

Out of plane **b** components produce small rigid body crystal rotation,

$$\phi = 2 \sin^{-1} [(b_z \cos \theta - b_y \sin \theta - \epsilon h \cos \theta) \sin \theta / 2h] \quad \rightarrow \quad \phi = 1.7^\circ$$

Disconnection spacing accommodates the (111)/(0001) coherency strain.

Conclusions

Three examples discussed here for Bi_2Te_3 :

$-\frac{1}{3}\langle 2 \ -1 \ -1 \ 0 \rangle$ dislocations

- core termination at $\text{Te}^{(1)}\text{-Te}^{(1)}$ layer (stoichiometric defect core)
- dissociated core structure.
 - likely influence of weak bonding between $\text{Te}(1)\text{-Te}(1)$ planes

-(0001) Basal twin:

- interface termination at $\text{Te}^{(1)}\text{-Te}^{(1)}$ layer
- preference for this termination constrains step configurations.
- Possibly a general effect for grain boundary inclinations vicinal to (0001)

$-\langle 2 \ -1 \ -1 \ 0 \rangle // -\langle 2 \ 1 \ 1 \ 0 \rangle$ 63.78° boundary:

- Alignment of low index {015} Planes
- Local rocksalt coordination with structural units retaining Bi_2Te_3 stoichiometry.

Conclusions, continued

- **Mechanism for tetradymite plate growth by motion of interfacial disconnections:**

- Defect plays two roles:**

- removes metal plane producing Te double-layer.
 - Shears layers into correct stacking.

- Defect spacing consistent with accommodation of misfit strain.**

- Systematic departure from (111)/(0001) habit plane

- Motion of defects unlikely to be independent;**

- instead must be coupled through strain interaction.*

Steps toward establishing set of elementary "building blocks" for a general picture of interfacial structure in chalcogenide thermoelectrics

Important to understanding interfacial formation and stability and, ultimately, interfacial transport properties in nanostructured bulk thermoelectrics.

Acknowledgements

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LBNL/NCEM

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California Institute of Technology

N.A. Heinz, T. Ikeda, G.J. Snyder

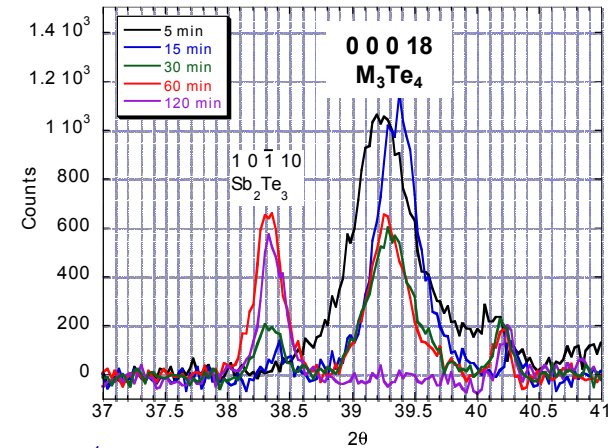
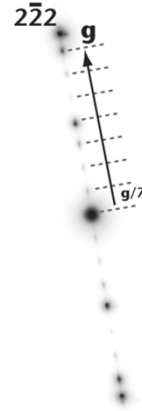
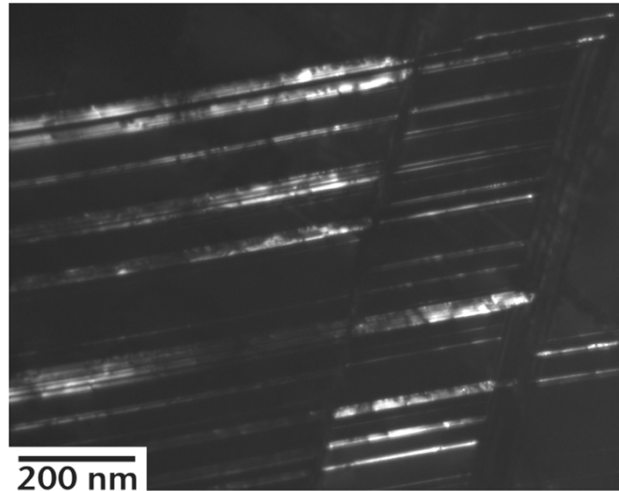
Special thanks to:

- LLNL: John Bradley, for use for LLNL's Titan 80/300 instrument
- LBNL: User program, National Center for Electron Microscopy
- UCD: Z. Zhang and E. Lavernia, for assistance with bulk Bi₂Te₃ processing

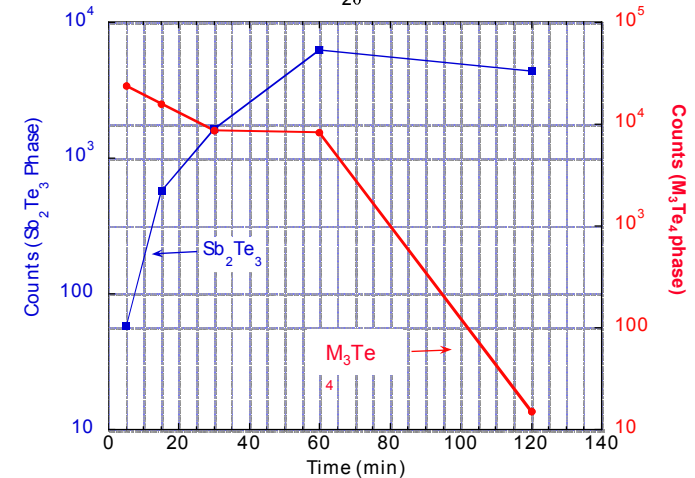
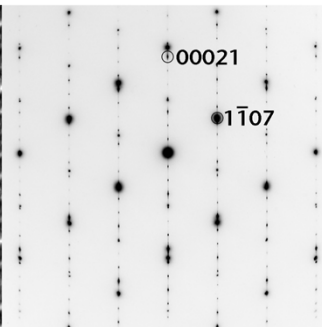
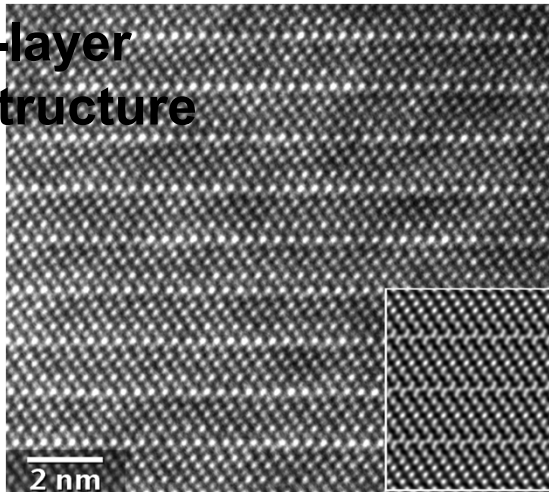
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

- EXTRA

Initial Stages of Precipitation: Transition Phase: $(\text{Ag,Sb})_3\text{Te}_4$



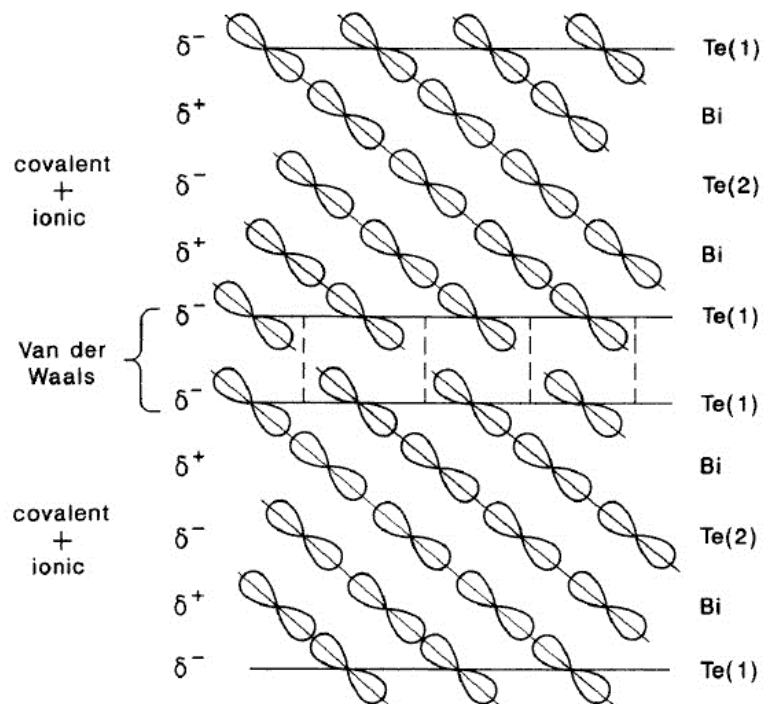
7-layer
Structure



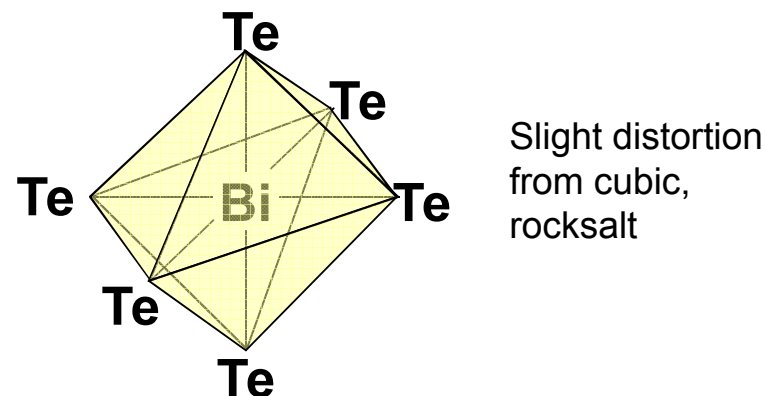
Metal rich intermediate phase

Bonding in Bi_2Te_3

**Perfect crystal:
Linear chains of $\text{pp}\sigma$ bonds**



**Octahedral coordination within
5-layer packets**



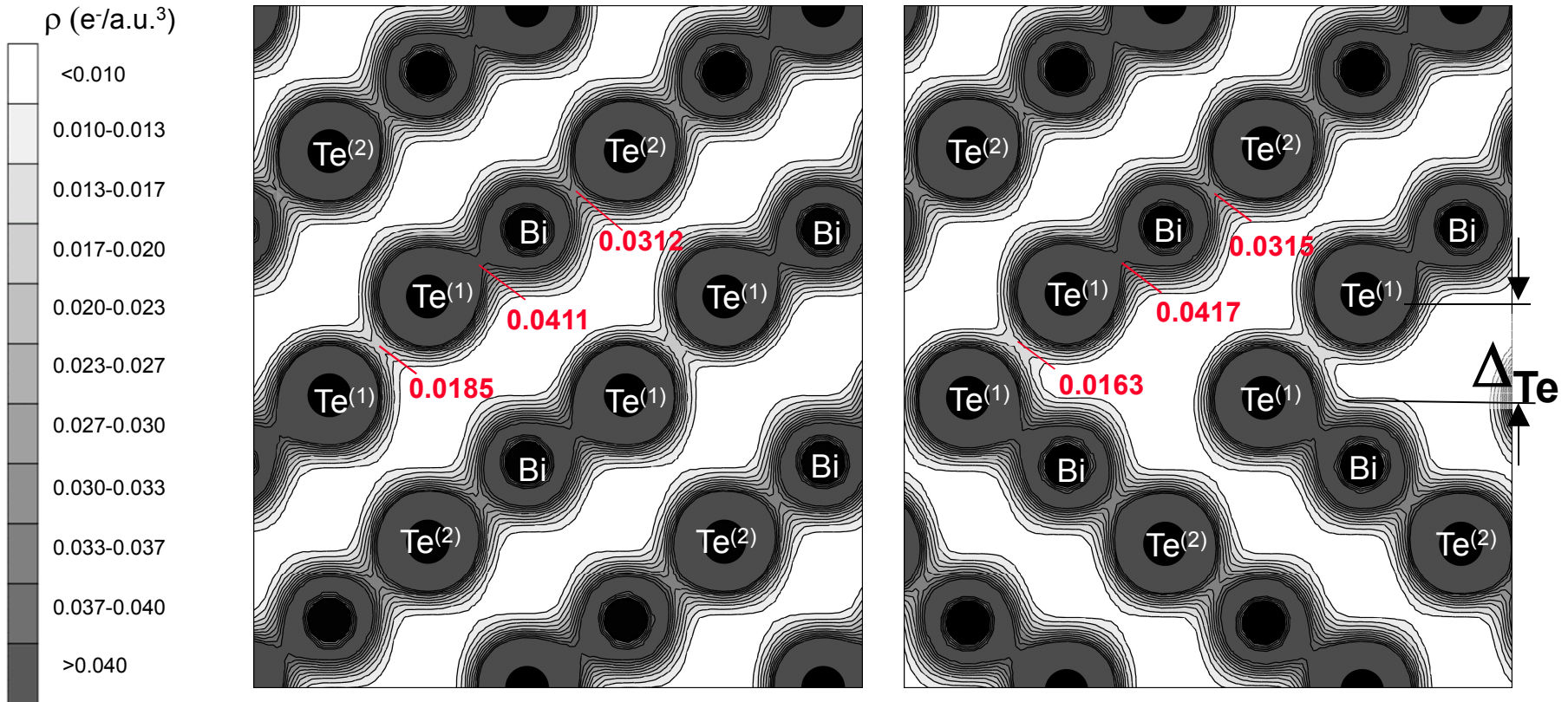
**Twin at Bi or $\text{Te}^{(2)}$ layers would
distort linear $\text{pp}\sigma$ chains.**

Mishra, Satpathy, Jepson J. Phys. Cond. Matter (1997)
Pecher and Toussaint, Physics Letters (1989)

Calculations predict expansion at interface

Bi_2Te_3 -Perfect Crystal

$\text{Te}^{(1)}\text{-Te}^{(1)}$ Twin

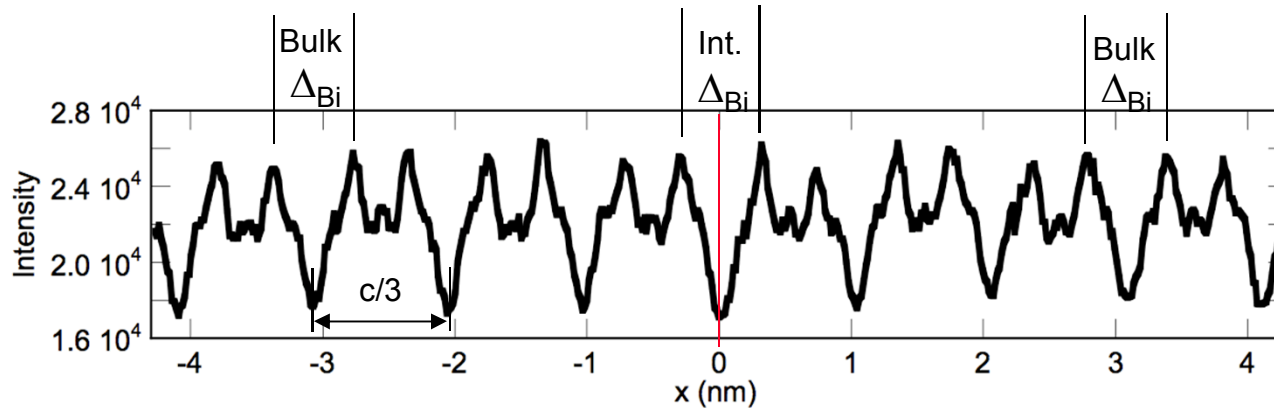


Charge density between $\text{Te}^{(1)}\text{-Te}^{(1)}$ atoms is lower at twin.
Calculations predict expansion normal to interface:

$$\Delta_{\text{Te,interface}} - \Delta_{\text{Te,bulk}} = +0.12\text{\AA}$$

Experimental measurements confirm expansion

Peak positions measured from intensity line profiles



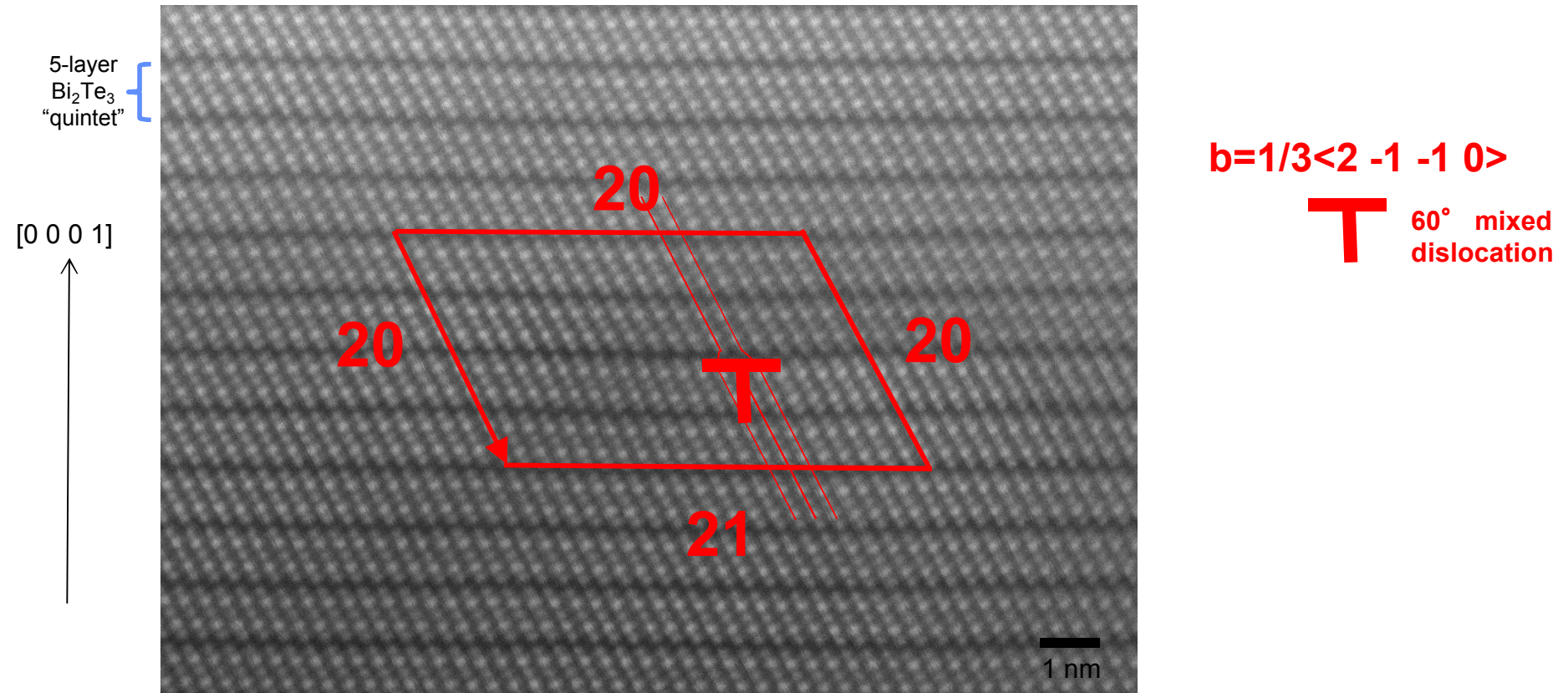
60 line profiles,
integrated over 8Å
width
4 independent images

Peak positions refined by
fitting to sum of Gaussians:

$$I(x) = A_0 + \sum_{i=1}^5 A_i e^{\left[\frac{-(x-x_{0,i})^2}{2\sigma_i^2} \right]}$$

	$\Delta_{\text{int}} - \Delta_{\text{bulk}}$	
	Theory	Exp
Te ⁽¹⁾	+0.120 Å	+0.12 ± 0.04 Å
Bi	+0.116 Å	+0.13 ± 0.03 Å

Dislocation Core structure: termination at $\text{Te}^{(1)}\text{-Te}^{(1)}$ layer, dissociation

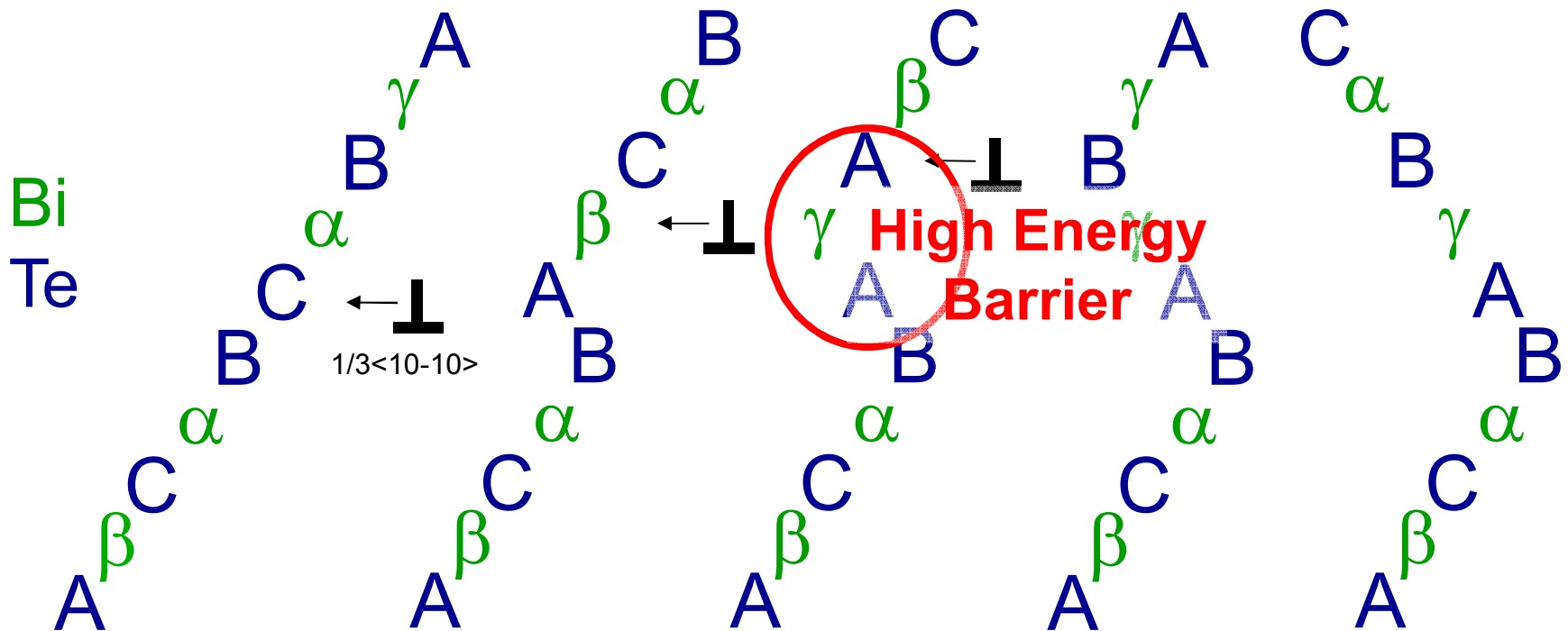


LLNL-Titan
HAADF-STEM
300 keV

$\langle 2\ -1\ -1\ 0 \rangle$ projection

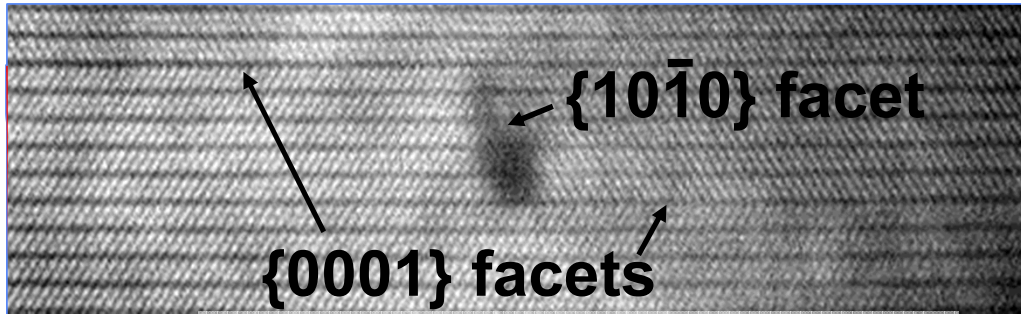
How do twins form in Bi_2Te_3 ?

Sequential motion of twinning dislocations?



- High energy barrier for Bi-terminated interface
→ independent motion of twinning dislocations unlikely.
- Alternative: Coordinated defect motion.
Groupings of *unlike* twinning dislocations

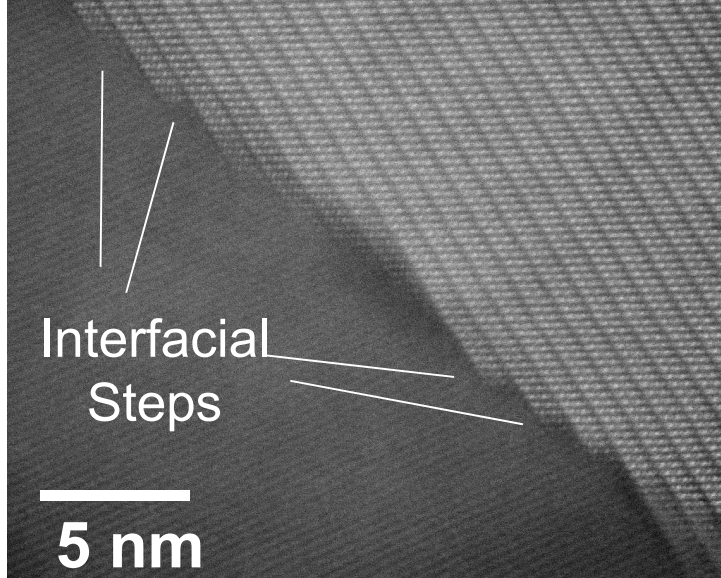
Steps in the Bi_2Te_3 Twin Boundary



5 nm

Steps of integral 5-plane

Bi_2Te_3 Quintets:
Perhaps a general feature?

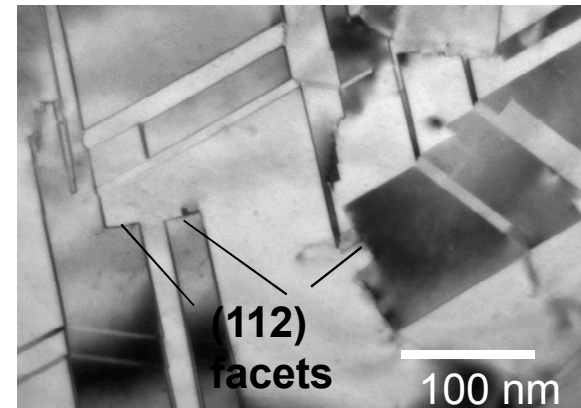


LLNL-Titan
HAADF-STEM 300 keV

NBT20/21mar11/18.15.52

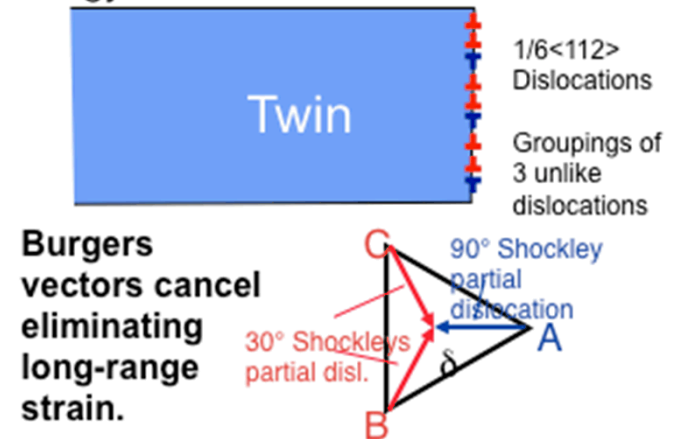
Morphology analogous to annealing and growth twins in FCC materials.

Example: Twins in Electrodeposited Ni

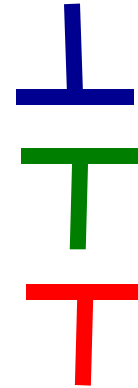
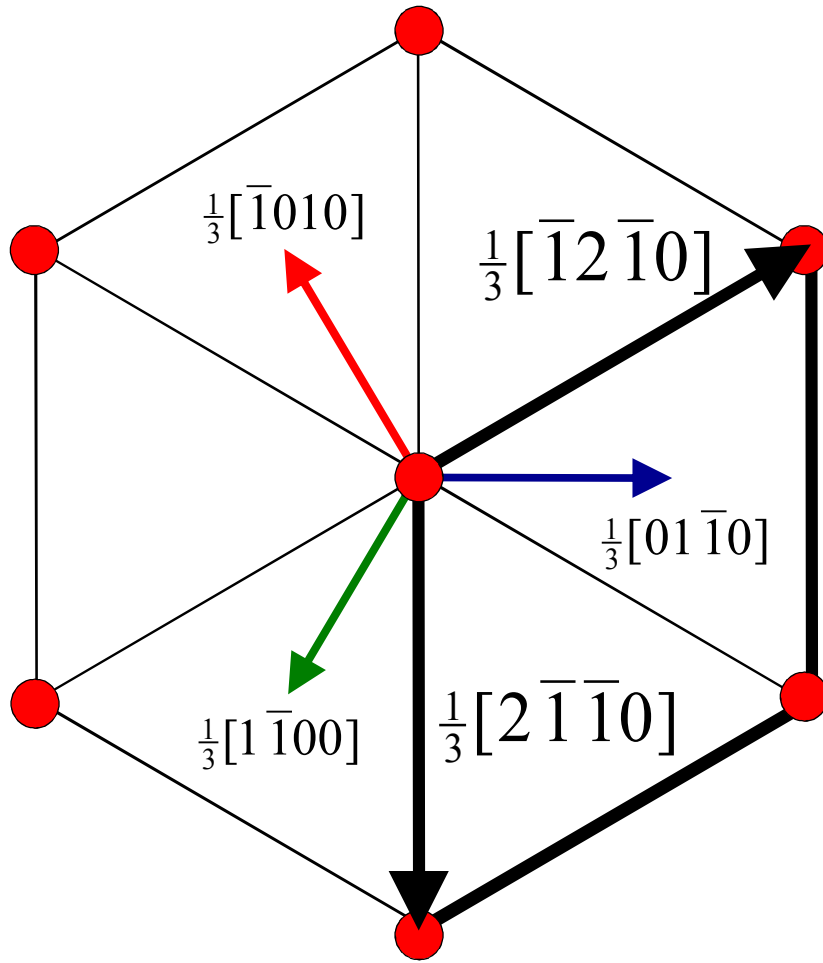


Lucadamo, Medlin, Talin, Yang, Kelly, Phil Mag 2005

Morphology Related to Dislocation Structure

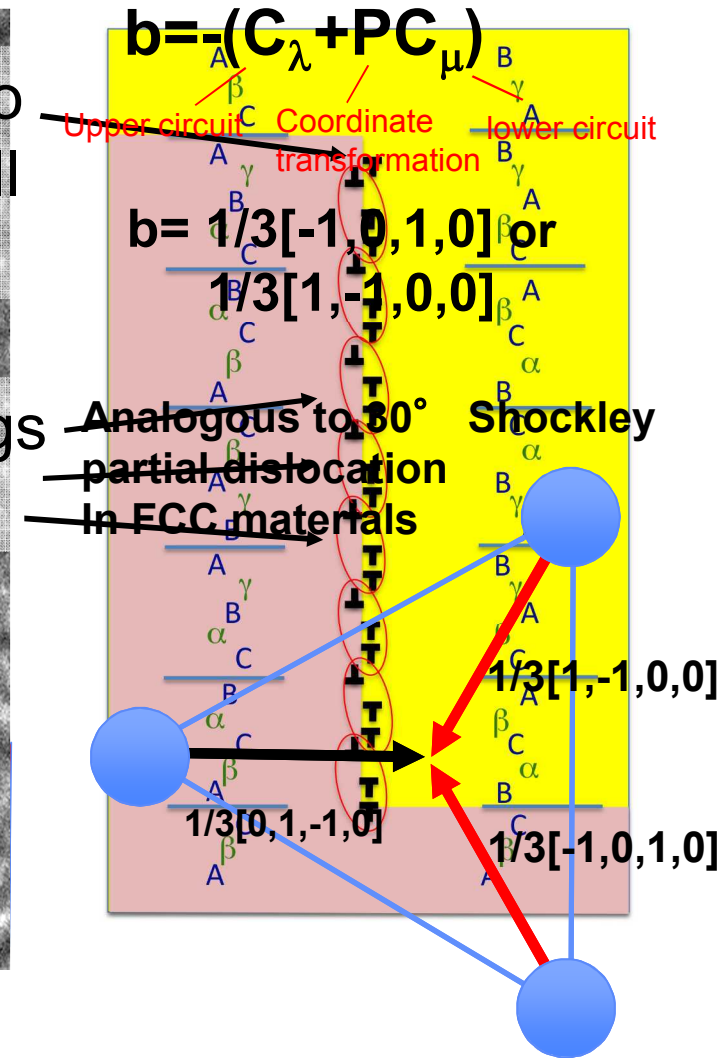
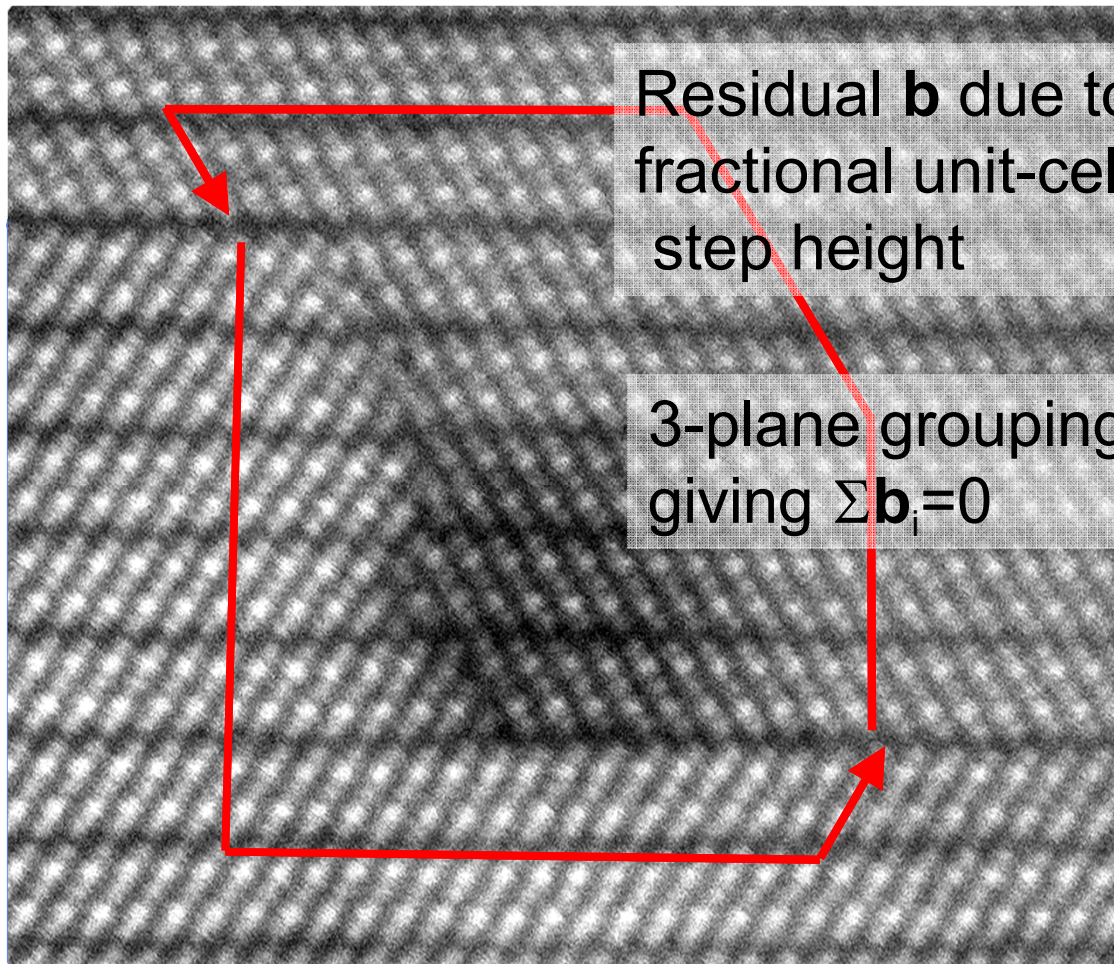


Groupings of 3 allowed twinning dislocations in Bi_2Te_3 structure

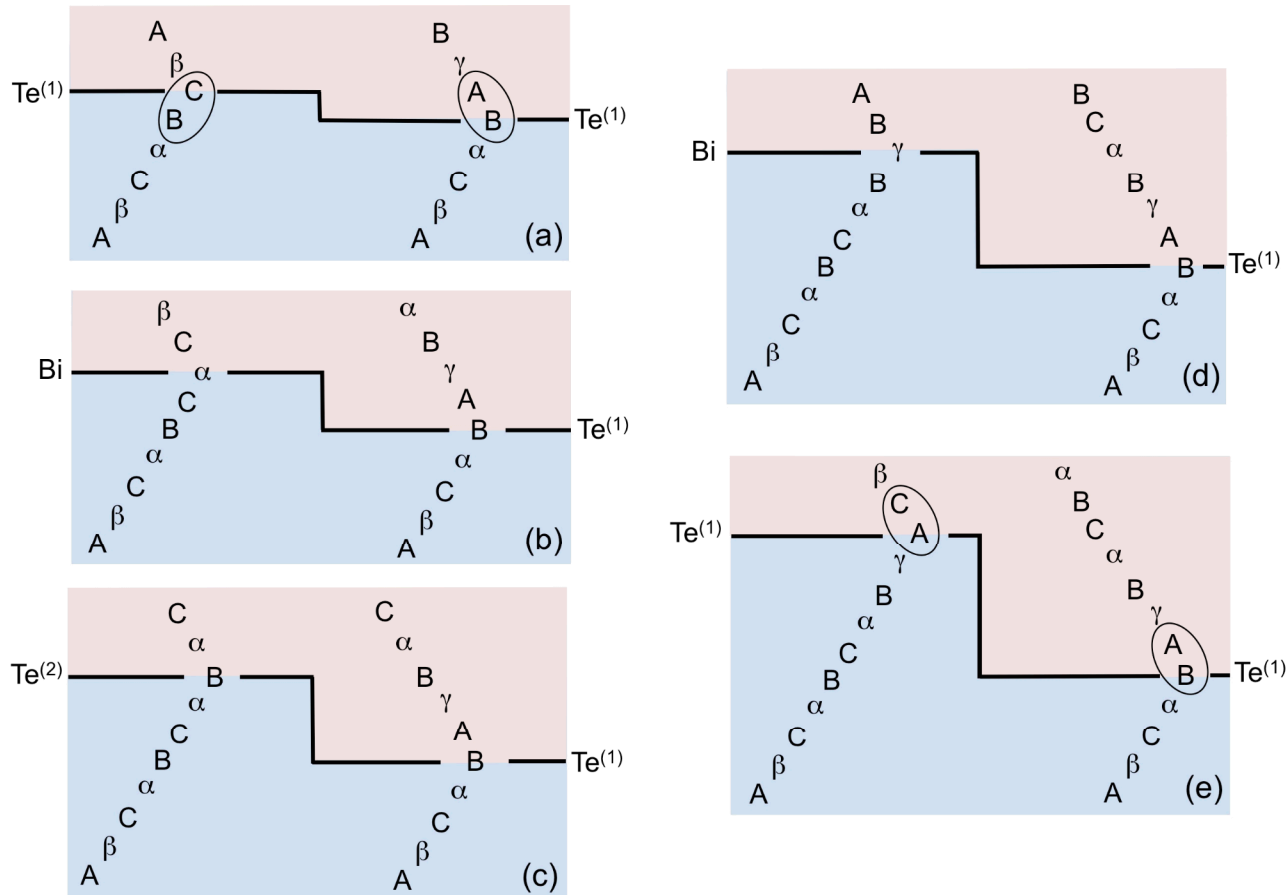


Zero Net Burgers Vector

What is the dislocation content of the step?



Consideration of other possible (0001) twin defects



Consideration of other possible (0001) twin defects

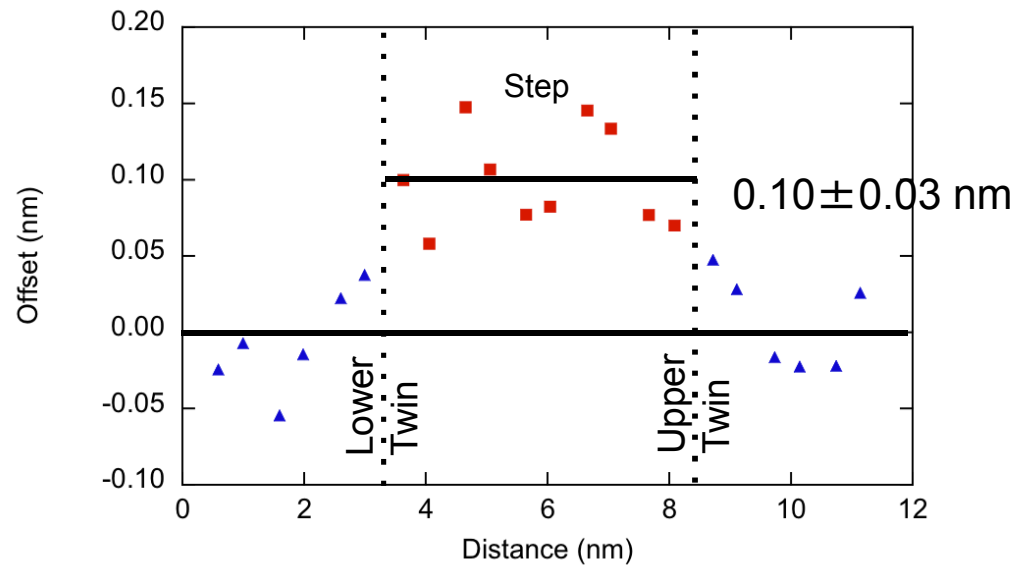
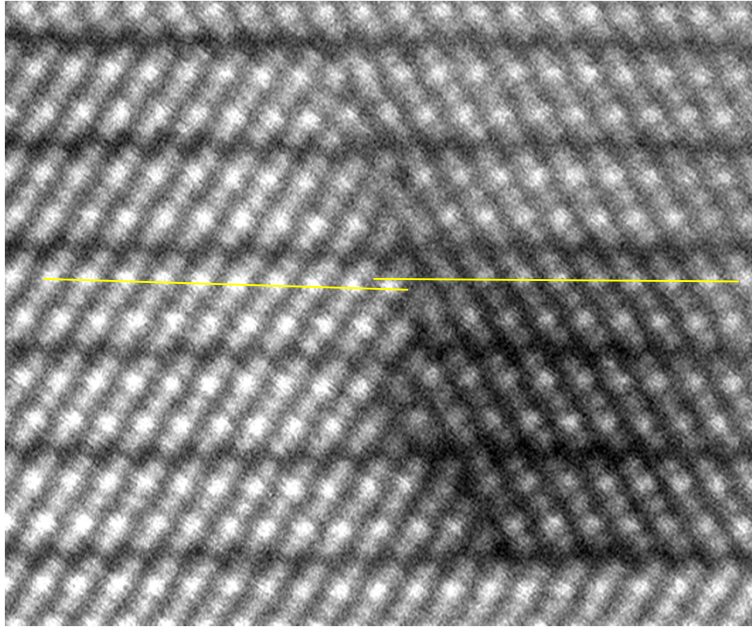
Step Height, h	Terminating Planes on Either Side of Step	Equivalency of Adjacent Twin Terraces	Burgers Vector, b
1	Te ⁽¹⁾ /Te ⁽¹⁾	Equivalent (inverted)	$\frac{1}{3}\langle 10\bar{1}0 \rangle$
	Bi/Te ⁽¹⁾	Nonequivalent	
	Te ⁽²⁾ /Bi	Nonequivalent	
2	Te ⁽¹⁾ /Bi	Nonequivalent	$\frac{1}{3}\langle 10\bar{1}0 \rangle$
	Te ⁽²⁾ /Te ⁽¹⁾	Nonequivalent	
	Bi/Bi	Equivalent (inverted)	
3	Te ⁽¹⁾ /Te ⁽²⁾	Nonequivalent	0
	Bi/Bi	Equivalent (inverted)	
	Bi/Te ⁽¹⁾	Nonequivalent	
4	Te ⁽¹⁾ /Bi	Nonequivalent	$\frac{1}{3}\langle 10\bar{1}0 \rangle$
	Bi/Te ⁽²⁾	Nonequivalent	
	Te ⁽¹⁾ /Te ⁽¹⁾	Equivalent (inverted)	
5	Same	Equivalent	$\frac{1}{3}\langle 10\bar{1}0 \rangle$
10	Same	Equivalent	$\frac{1}{3}\langle 10\bar{1}0 \rangle$
15	Same	Equivalent	0

Low Energy: Te⁽¹⁾/Te⁽¹⁾ termination.

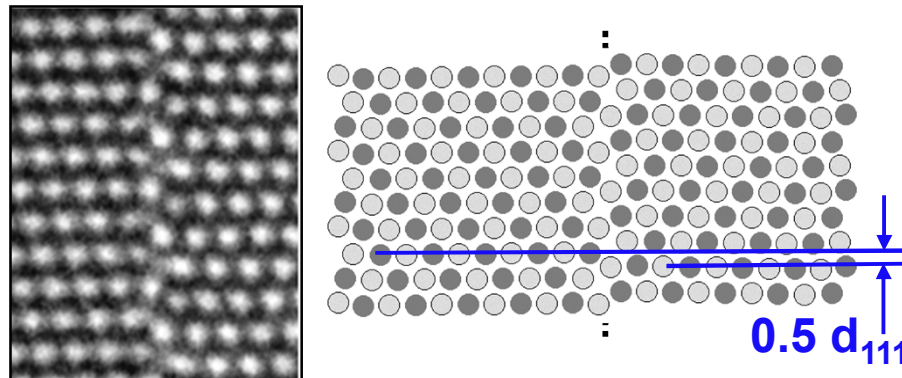
Intermediate energy:

Termination at either Te site: Te⁽¹⁾ and Te⁽²⁾

(0001) Planes are offset at step:



Offset similar to FCC {112} Twins
Example: Gold

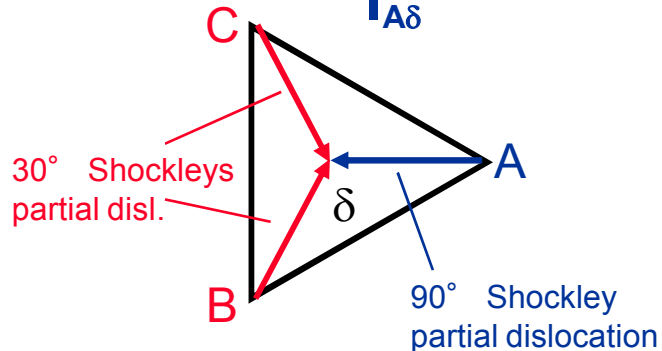
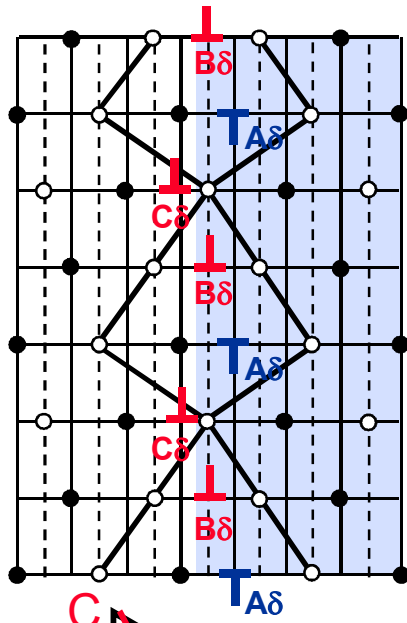


Marquis, Hamilton, Medlin, Léonard, Phys. Rev. Lett. (2004)

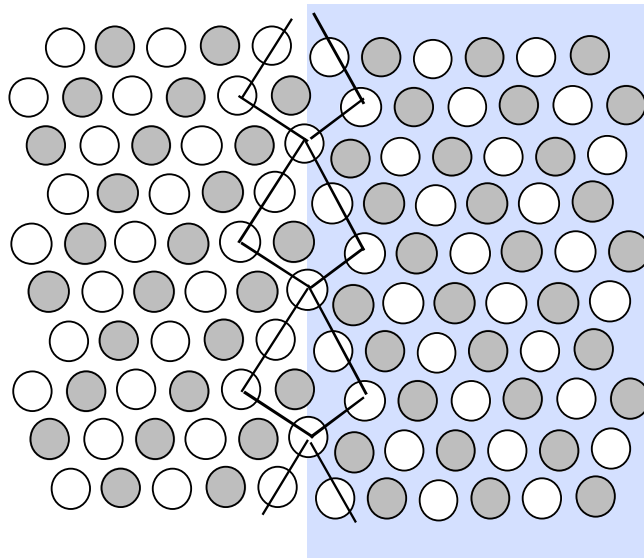
Grouping of 3 twinning dislocations is analogous to FCC {112} twin facets

Example: Aluminum {112} Twin Structure:

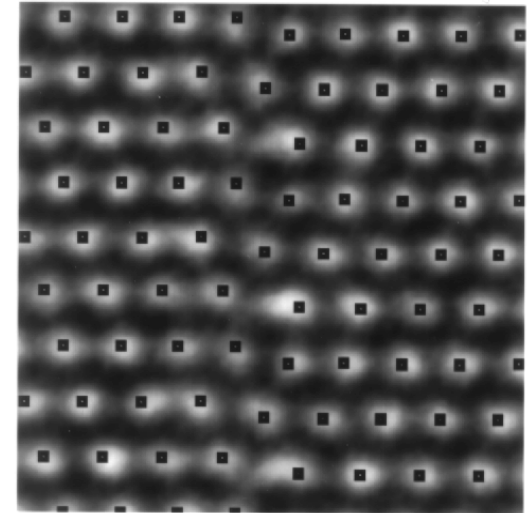
Boundary dislocation arrangement



Relaxed Structure
(Aluminum-Voter & Chen EAM)



HRTEM

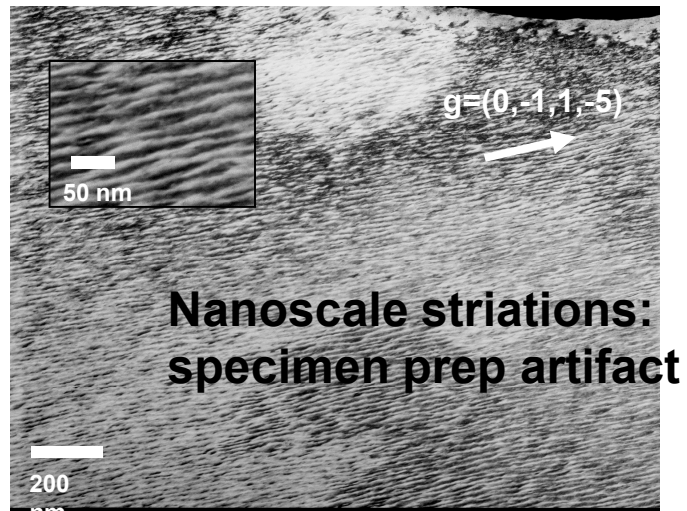


-D.L. Medlin, M.J. Mills, W.M. Stobbs, M.S. Daw, F. Cosandey MRS 295 (1993).
-D.L. Medlin, S.M. Foiles, G.H. Campbell, C.B. Carter, Materials Science Forum (1999).

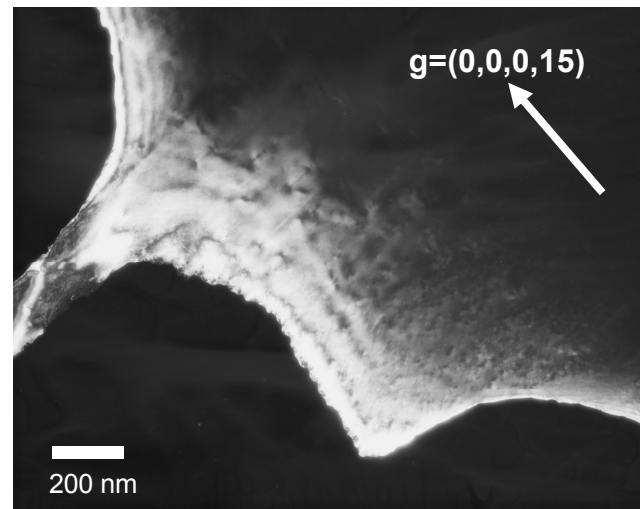
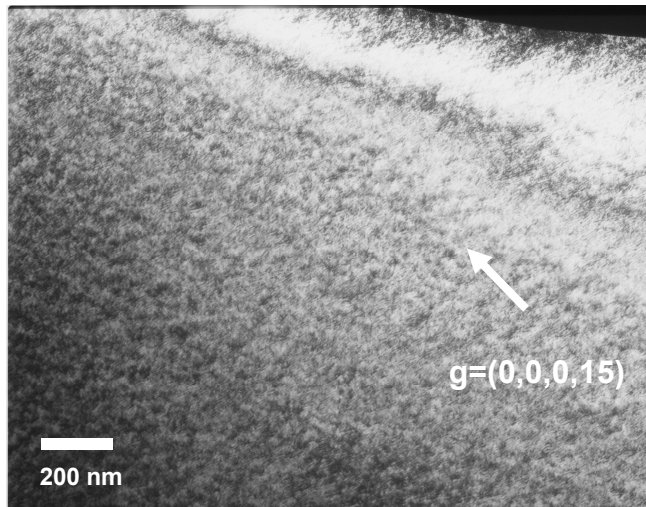
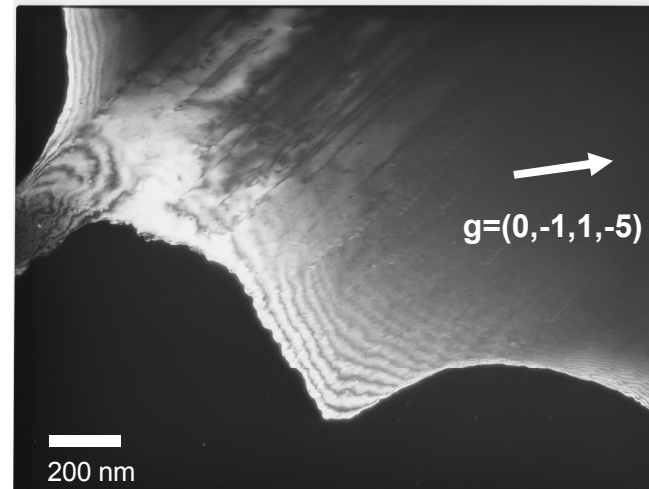
***Facile migration of {112} facets by
coordinated motion of 3-layer
groupings of 90° and 30°
1/6<112> dislocations***

Aggressive ion-milling produces nanoscale artifacts in Bi_2Te_3

Ion Milled (Gatan DualMill 5 kV Ar⁺)



Electrochemical Polish



Can avoid artifacts using low-voltage, low-angle ion milling with cryo-cooling