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Deformation by Dislocations, Twinning, and Phase Transformations in Multi-Principal Component FCC Solid Solutions

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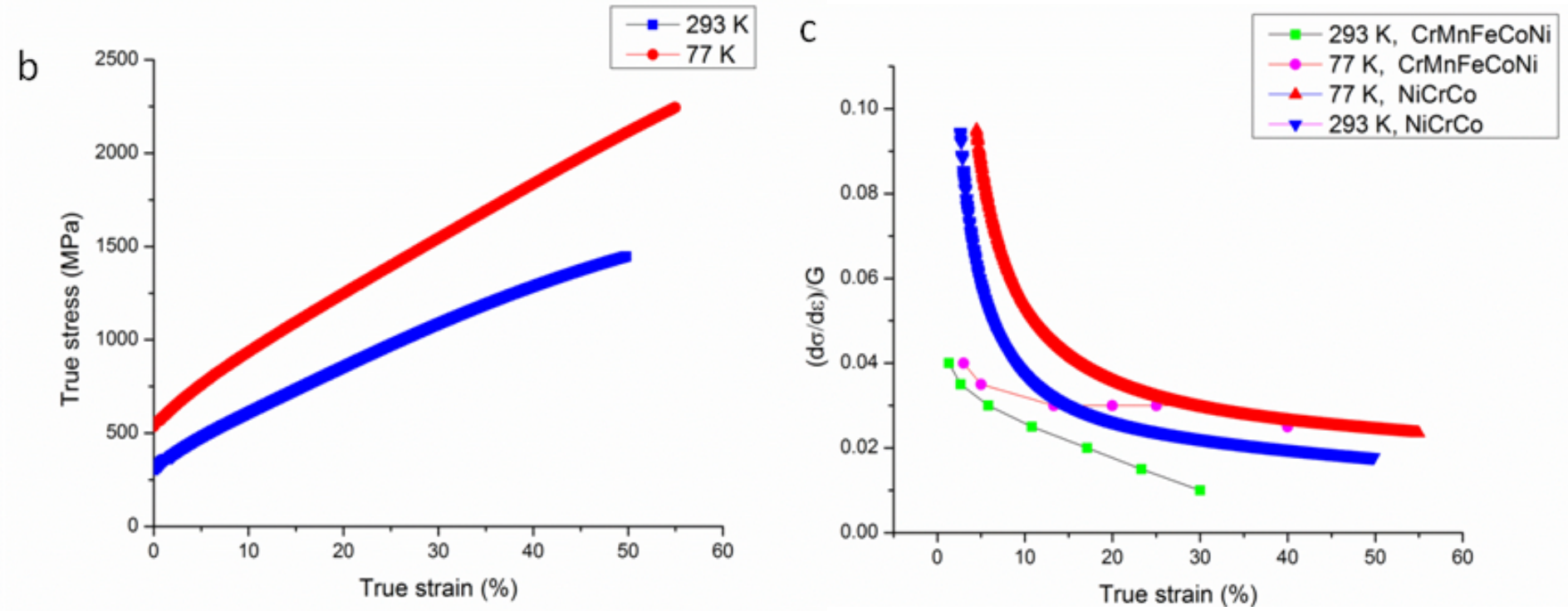
SPP on HEAs and CCAs
Karlsruhe 2019

Outline

- FCC based “high entropy” alloys (NiCoCr and Cantor)
- Deformation substructure evolution by dislocation plasticity and twinning and relation to work hardening
- FCC -> HCP phase (ε martensite) transformation and its effects on deformation
- Cold-rolling, recrystallization and prospects for achieving extraordinary strength / ductility combinations
- Summary

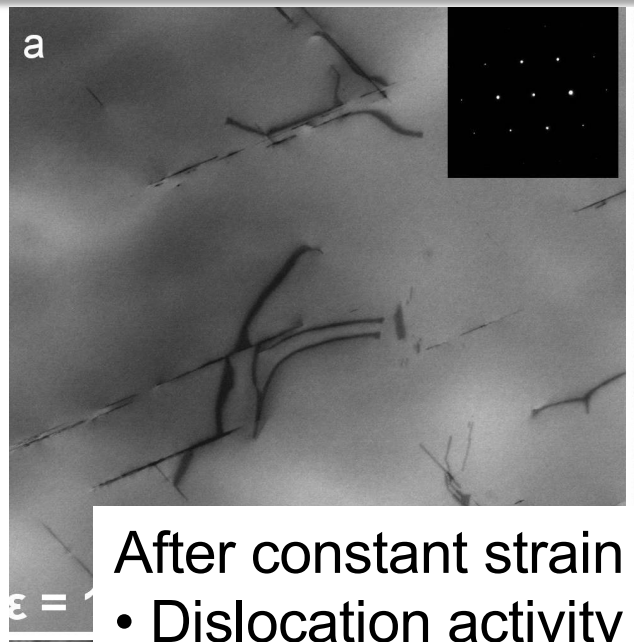
Tensile Testing of Equiatomic Ni-Co-Cr vs. Cantor Alloy

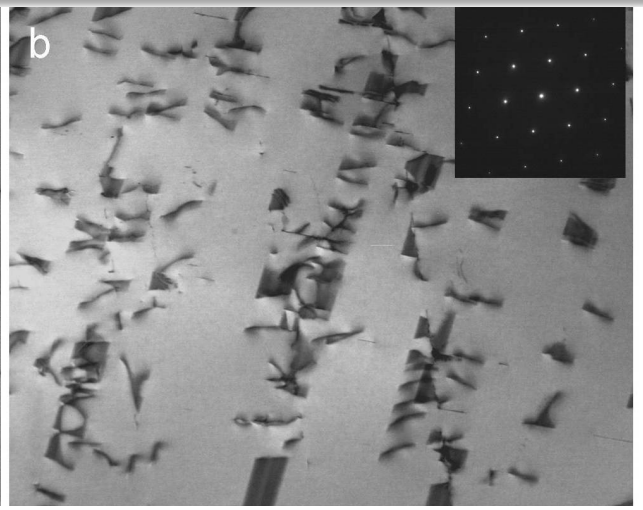


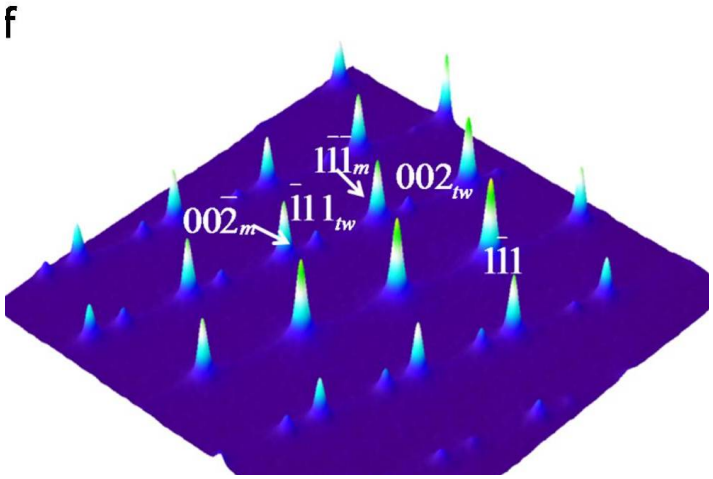
- Mean grain size 15 microns
- High strength and exceptionally large hardening rates
- Large hardening rates persist at room temperature (compared with CrMnFeCoNi Cantor alloy)

Miao, Slone, Niu, Bei, Ghazisaeidi, Pharr, Mills, Acta Mater, 2017

Substructure Analysis: RT Deformed Ni-Co-Cr

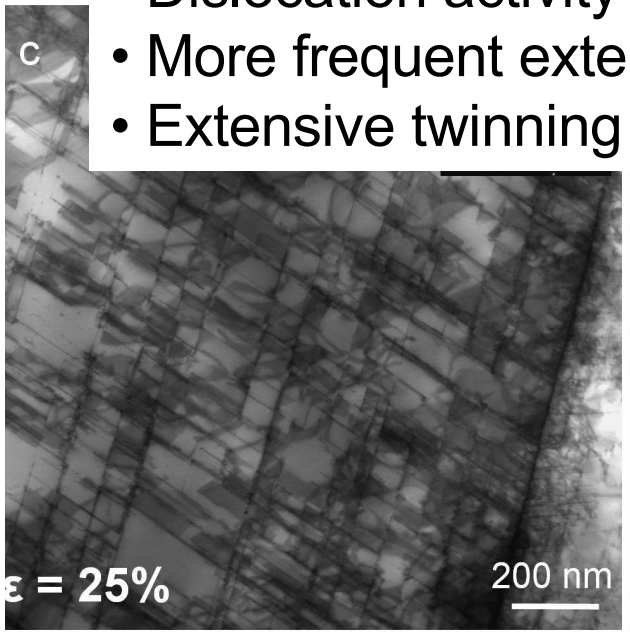


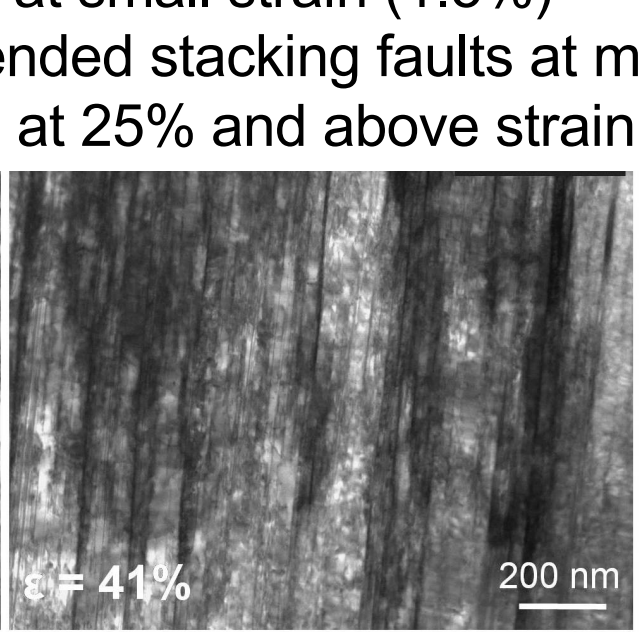


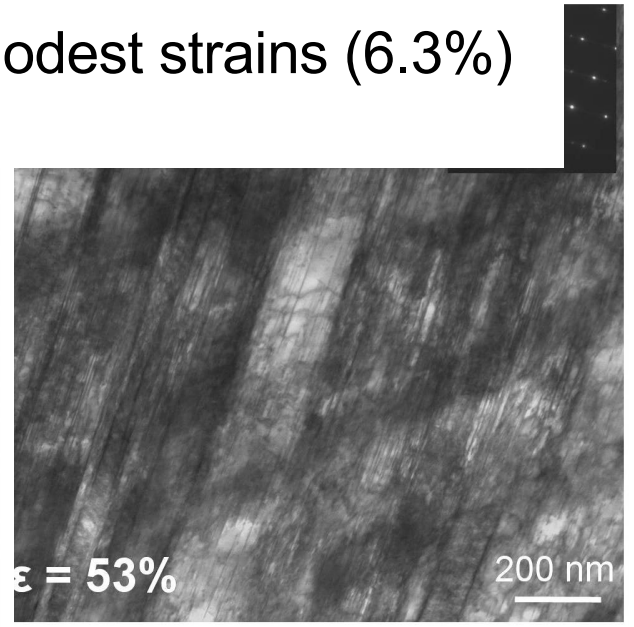


After constant strain rate testing at RT:

- Dislocation activity at small strain (1.5%)
- More frequent extended stacking faults at modest strains (6.3%)
- Extensive twinning at 25% and above strain

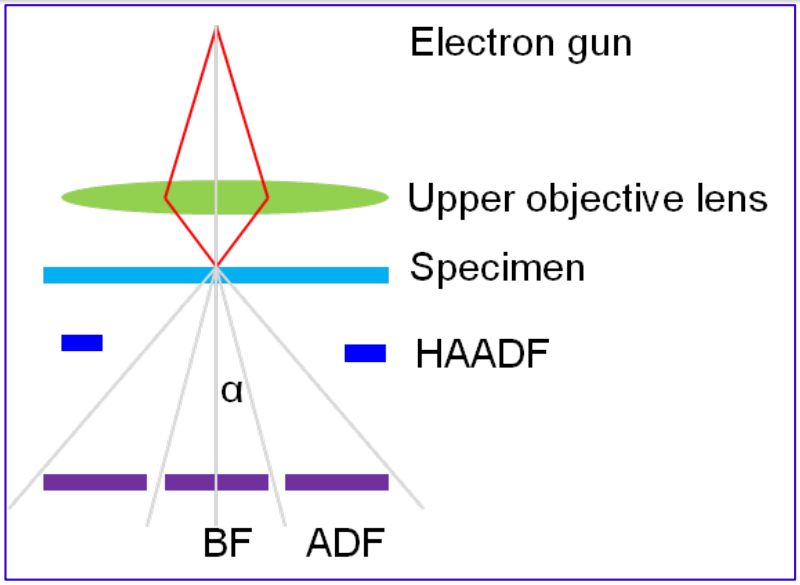


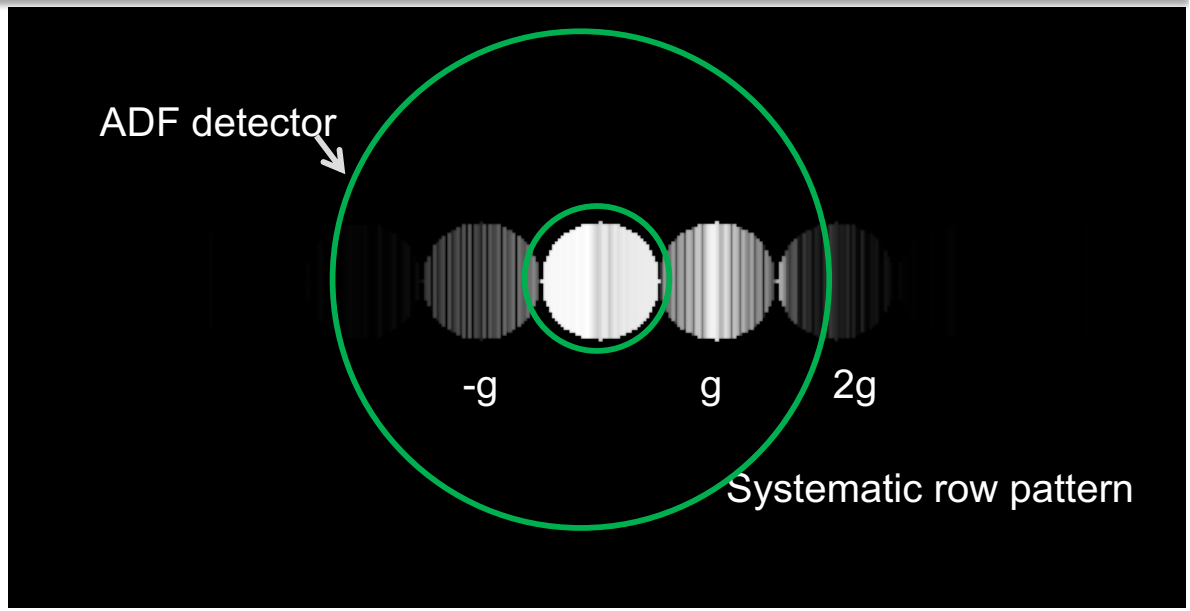




Miao, et al., Acta Mater., 132, 35–48 (2017)

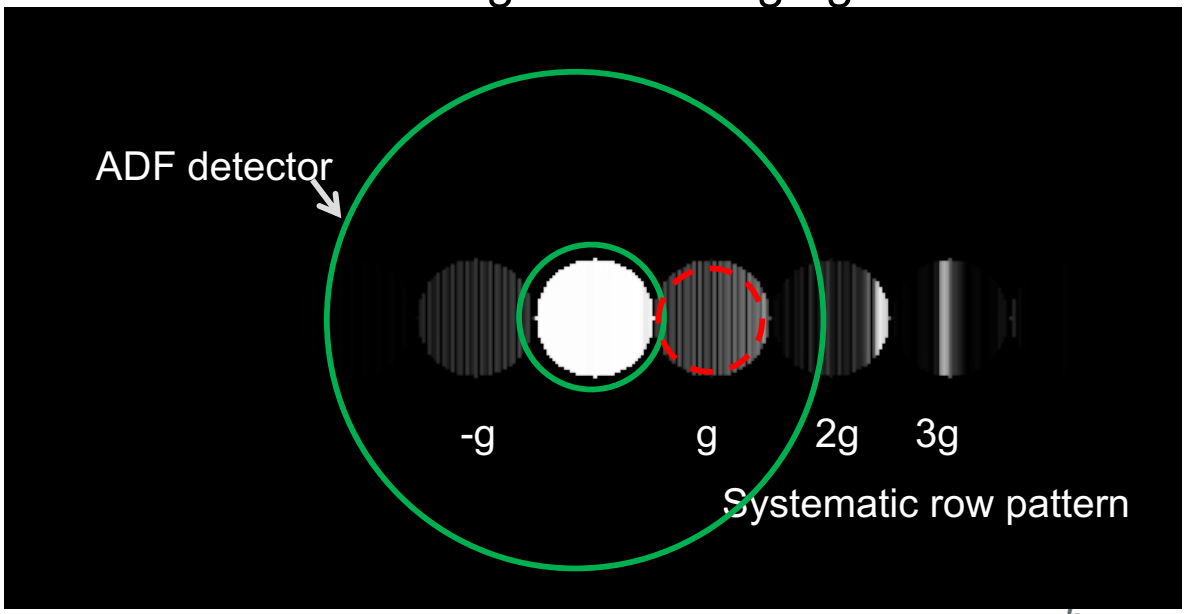
Weak Beam Dark Field (WBDF) STEM Imaging





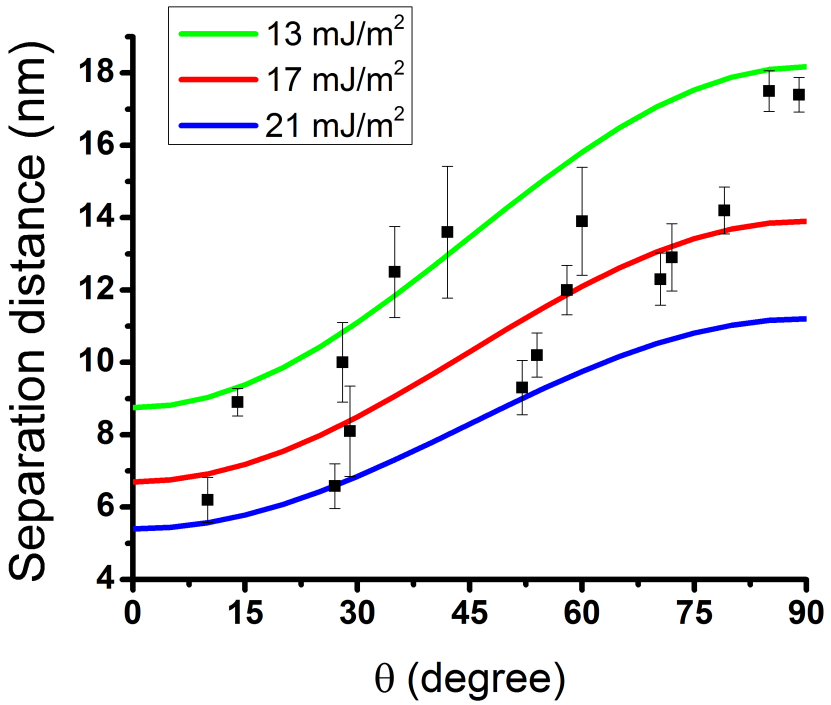
Strong beam imaging

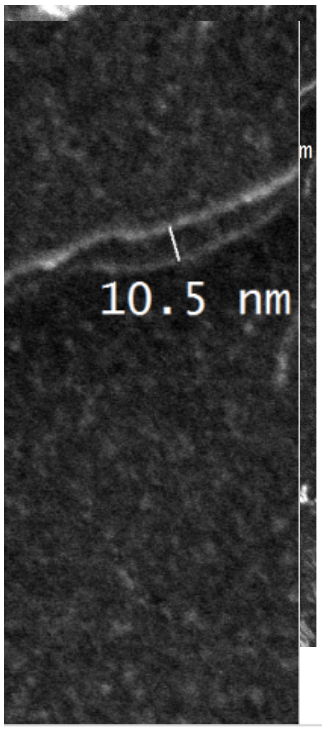
- In weak beam dark field (WBDF) STEM imaging, high order diffraction such as 3g is in Bragg condition.
- In WBDF STEM method, g reflection is used for imaging and objective aperture used to select g reflection, thus avoiding the contribution or interaction from other reflection.



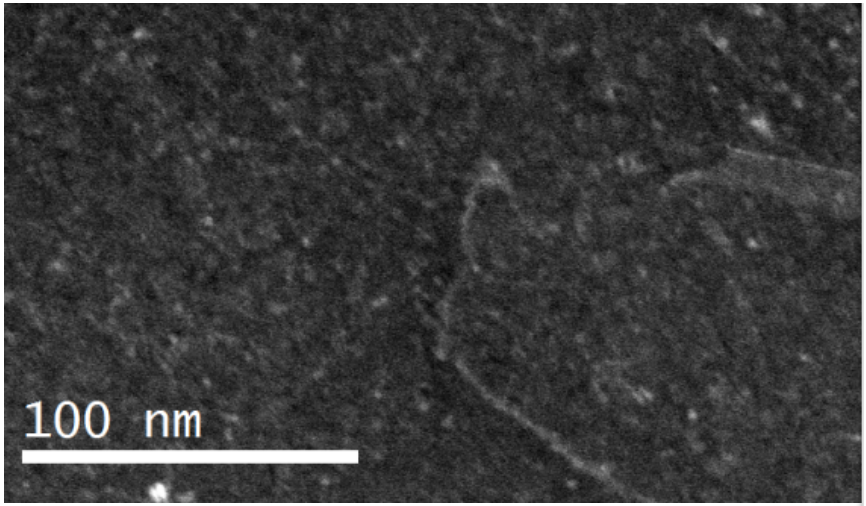
Weak beam dark field imaging

Weak Beam STEM Diffraction Contrast Imaging of Dissociated Dislocations



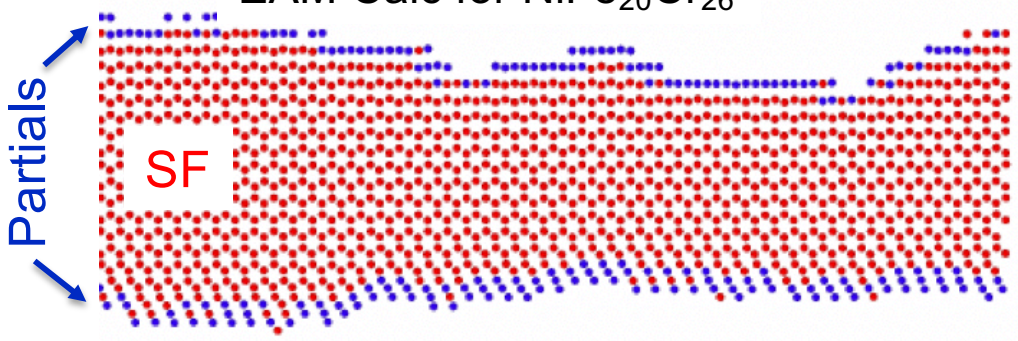


- Variable dissociation distance commonly observed
- SFE measurement possible
- Assume equilibrium conditions (?)



Smith, et al, Acta Mater. 110 (2016) p. 352

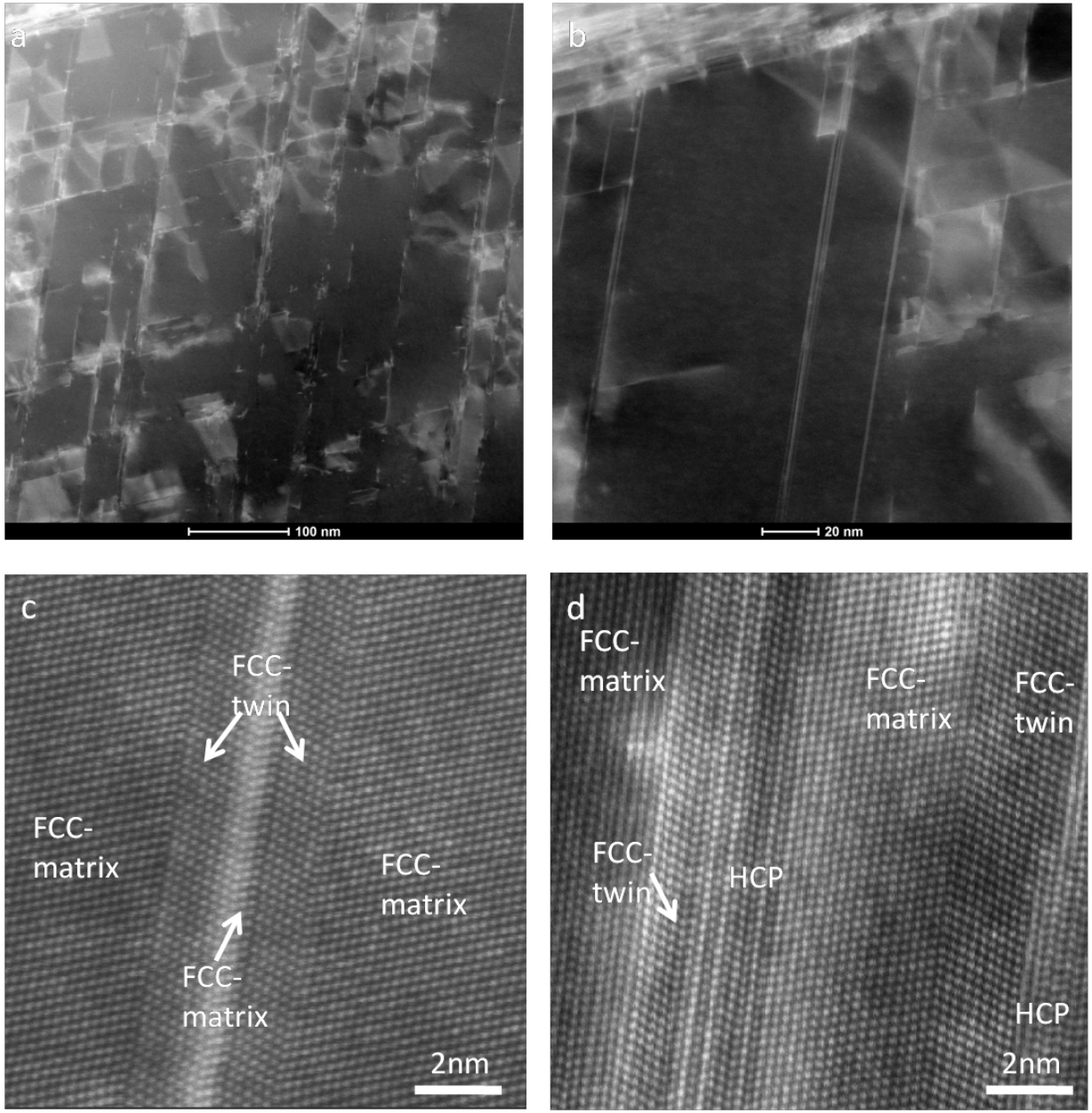
EAM Calc for $NiFe_{20}Cr_{26}$



LAADF STEM along <110> Zone: RT Deformed Ni-Co-Cr

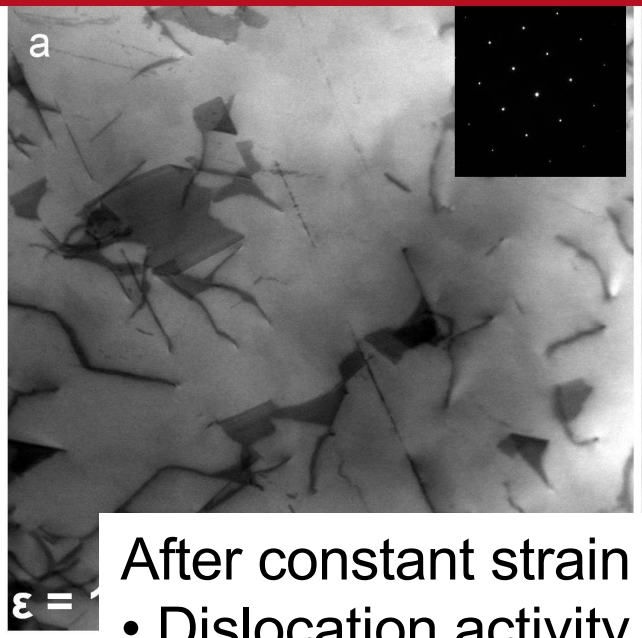
After constant strain rate testing at RT for 25%:

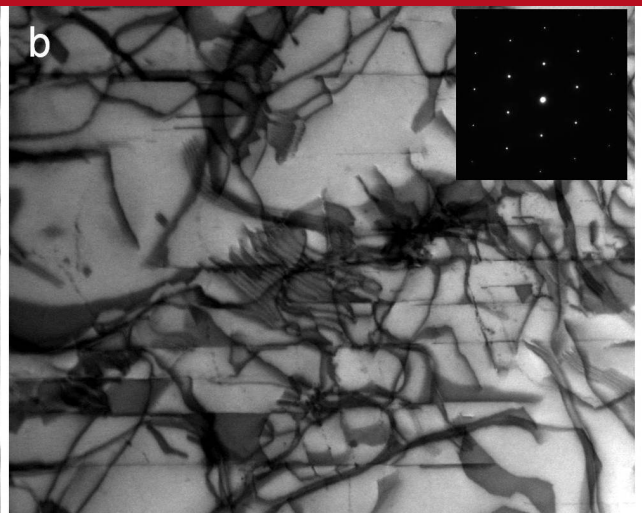
- Fine scale nano-twinning
- Multiple slip/twin systems operative
- Thin laths of HCP structure always in conjunction with nanotwins

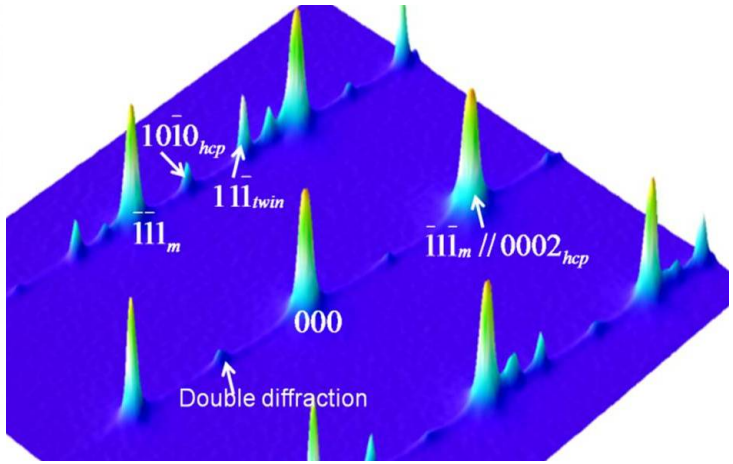


Miao, et al., Acta Mater., 132, 35–48 (2017)

Substructure Analysis: 77K Deformed Ni-Co-Cr

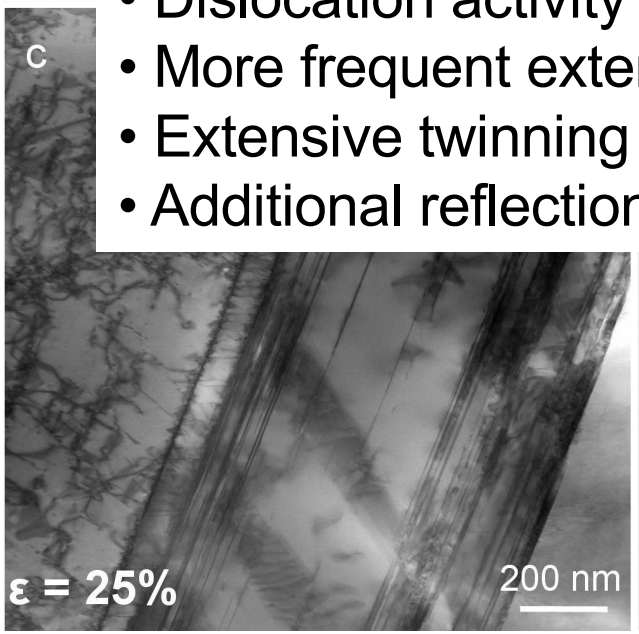


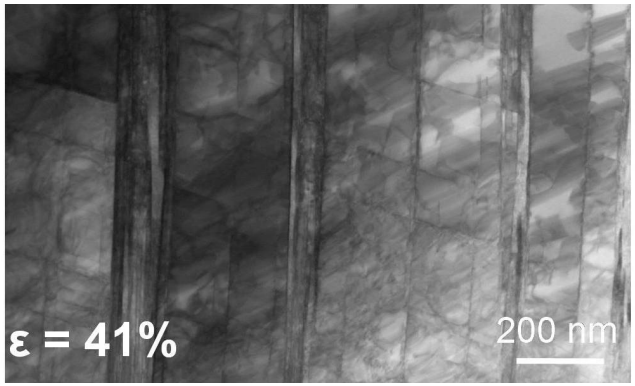


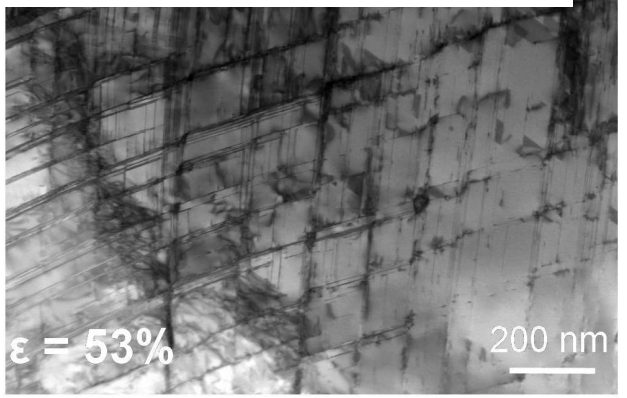


After constant strain rate testing at LN temperature:

- Dislocation activity at small strain (1.5%)
- More frequent extended stacking faults at modest strains (6.3%)
- Extensive twinning at 25% strain and above
- Additional reflections observed in SAD patterns







Miao, et al., Acta Mater., 132, 35–48 (2017)

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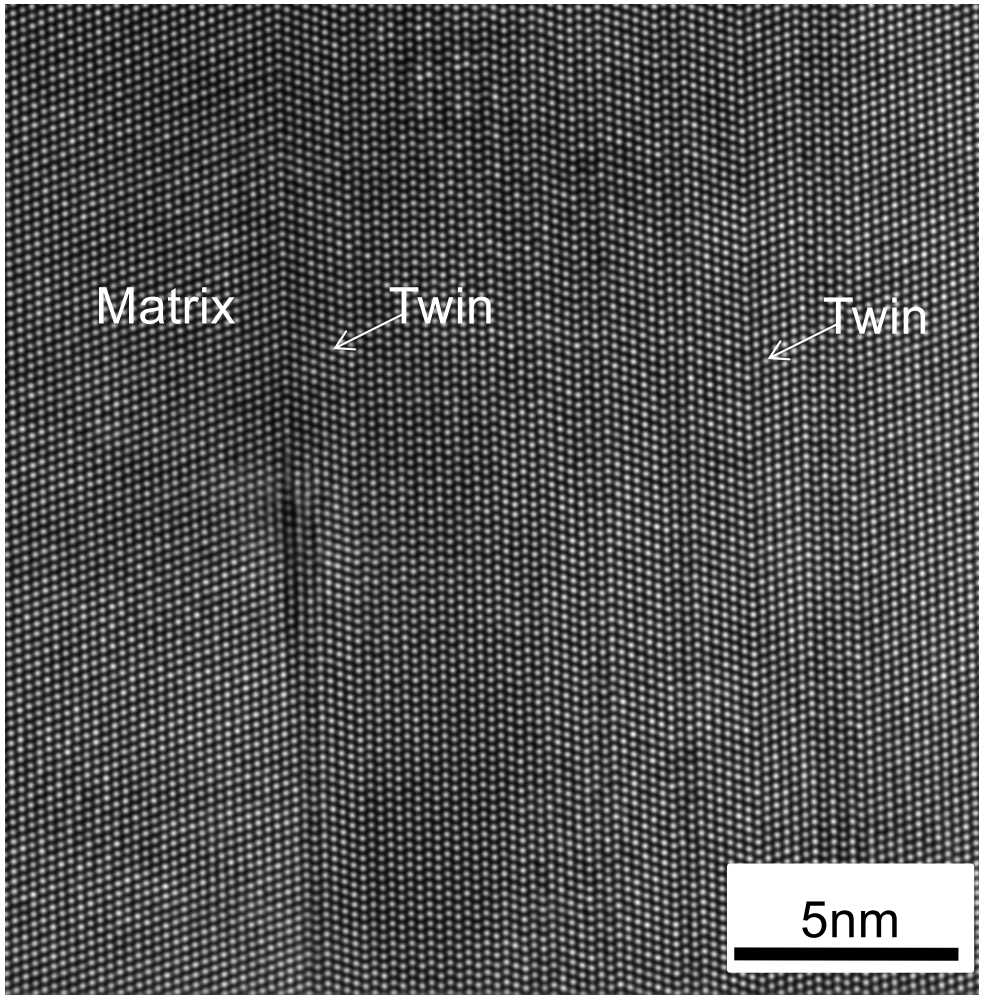
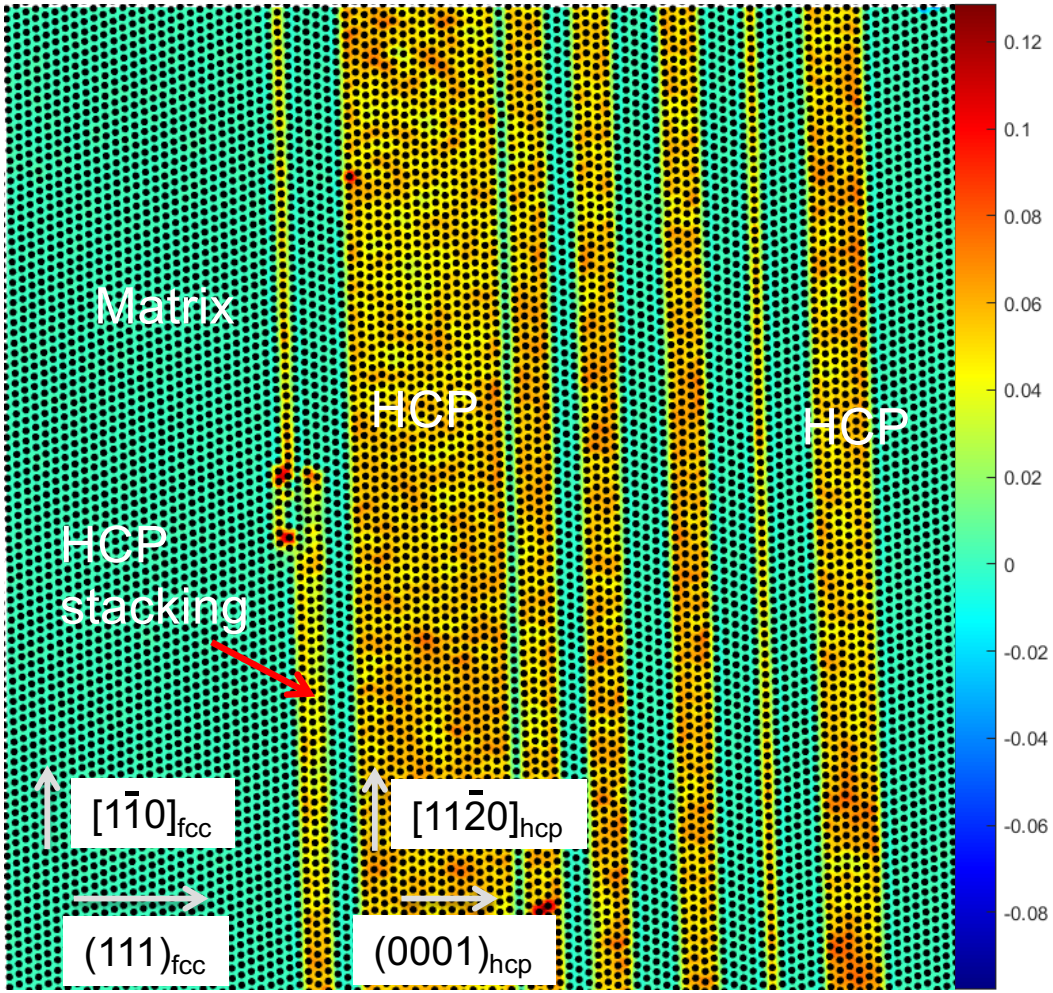
HAADF STEM along <110> Zone: 77K Deformed 29% Ni-Co-Cr

HAADF-STEM



Center of Symmetry Map



Consistent Orientation Relationship:

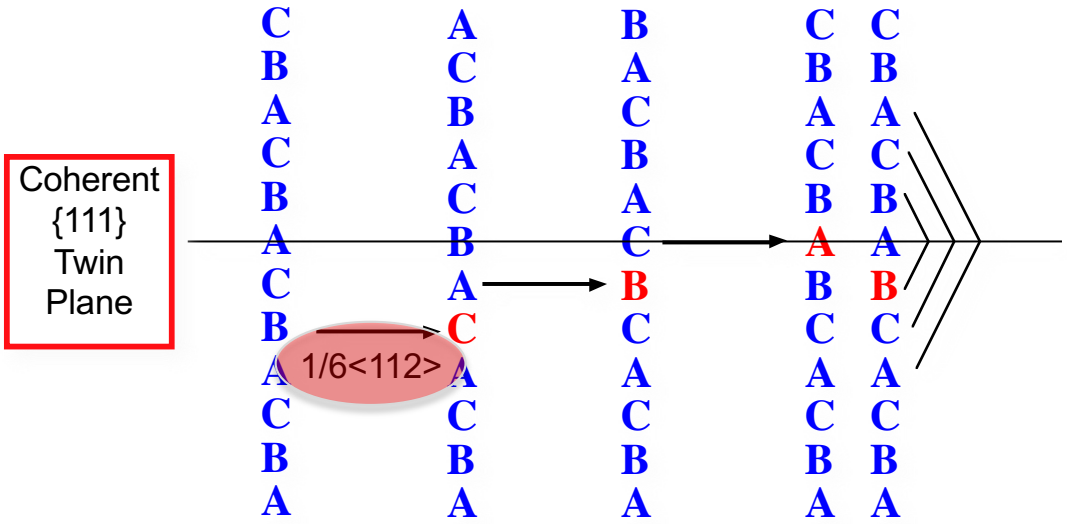
$\{0001\}_{hcp} \parallel \{111\}_{fcc}$ and $<11\bar{2}0>_{hcp} \parallel <110>_{fcc}$

Twin boundaries

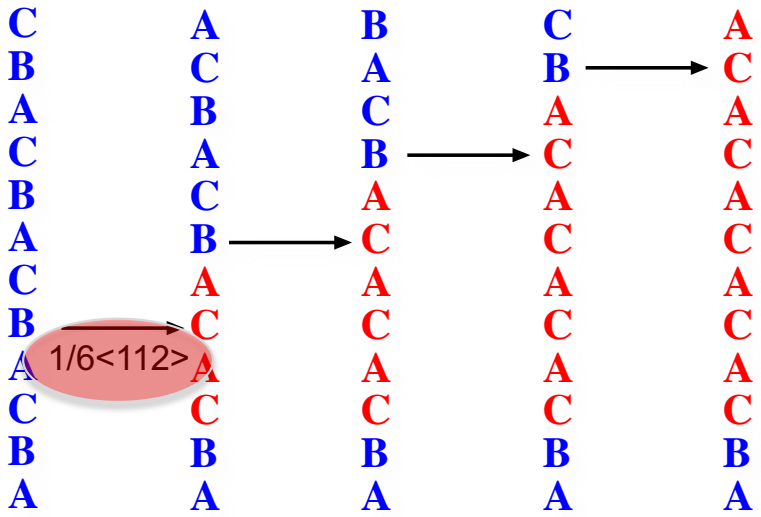
Identical to ε martensite in high Mn TRIP steels (but much smaller vol. fraction)

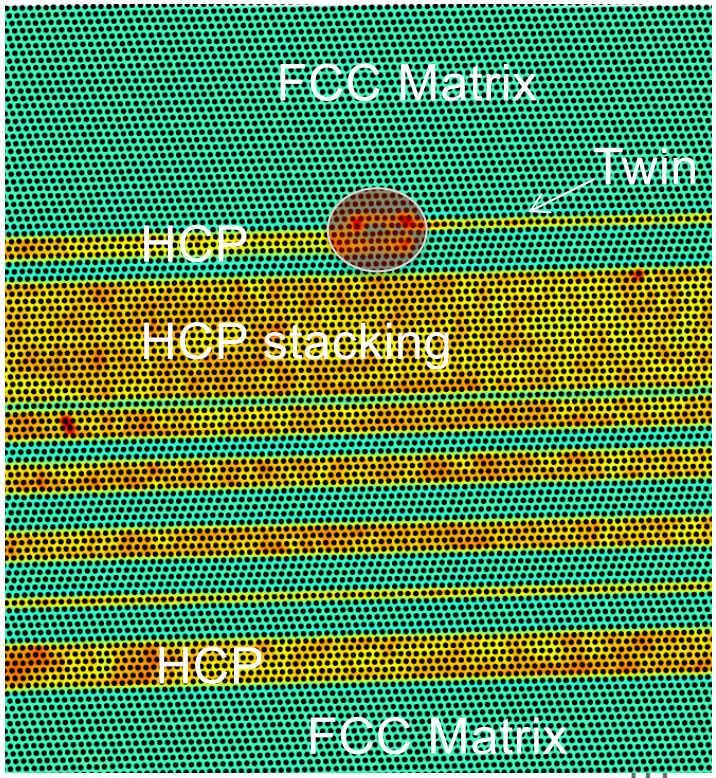
Relationship Between Twinning and HCP Formation

Twins in FCC form by the successive movement of 1/6<112> Shockley partial dislocations on adjacent glide planes:



FCC to HCP *Phase transformation* can also occur by sequential motion of partials on every other {111} plane:





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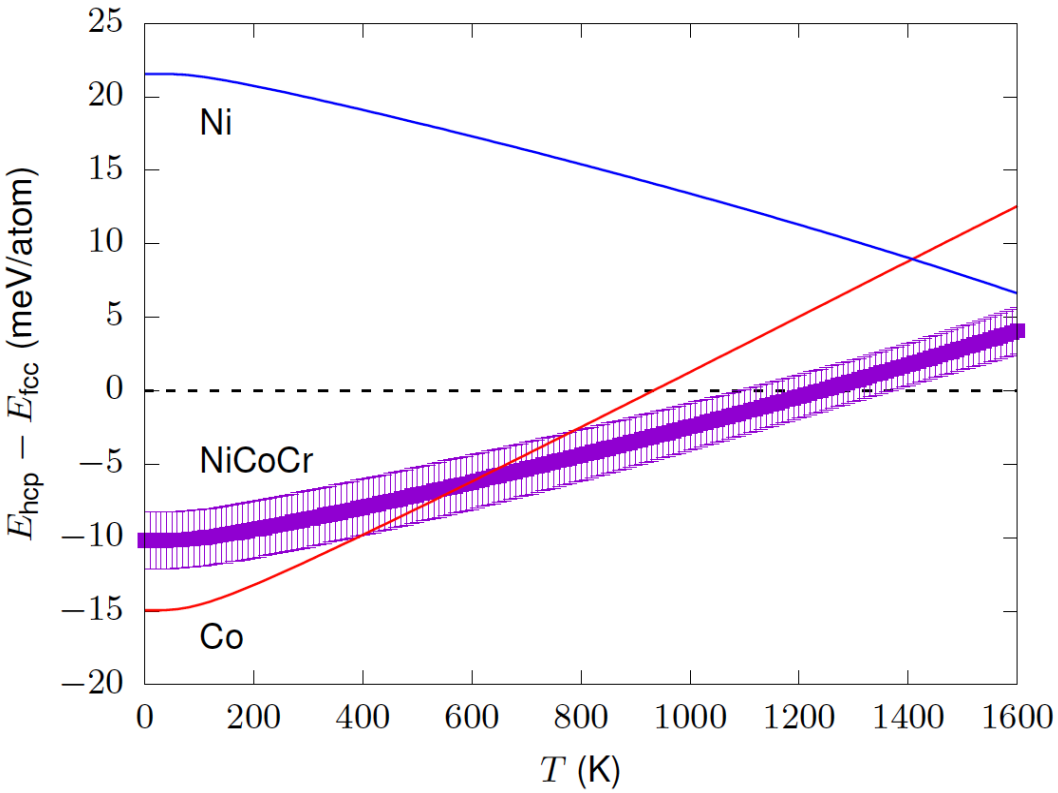
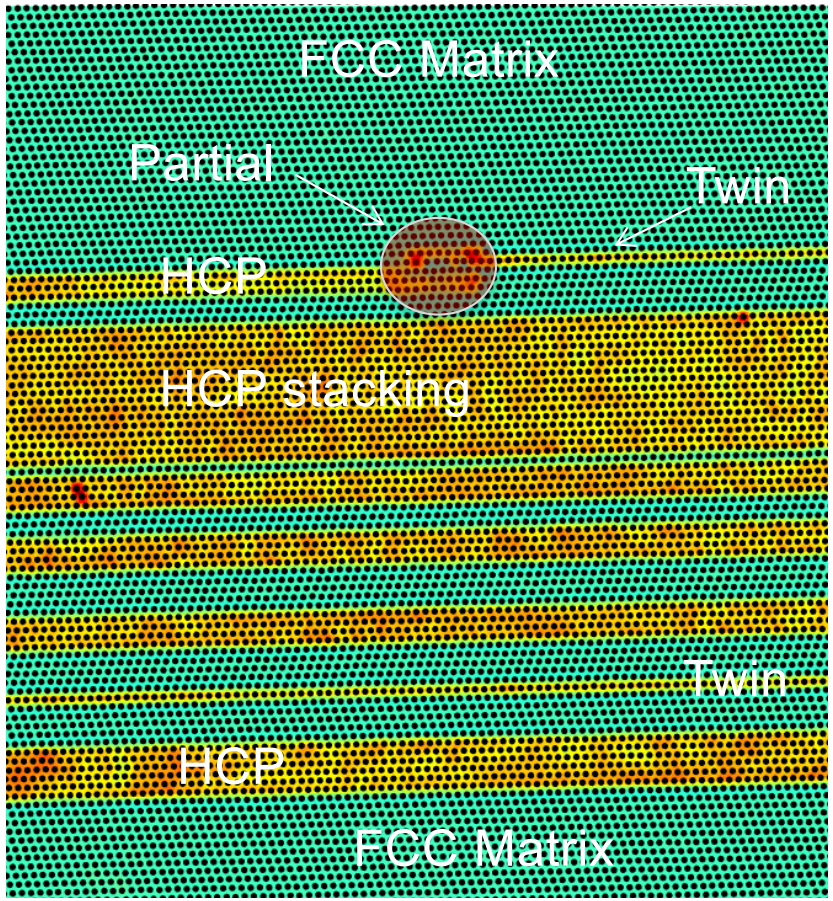
Relative Stability for FCC and HCP for NiCoCr

DFT Calculations



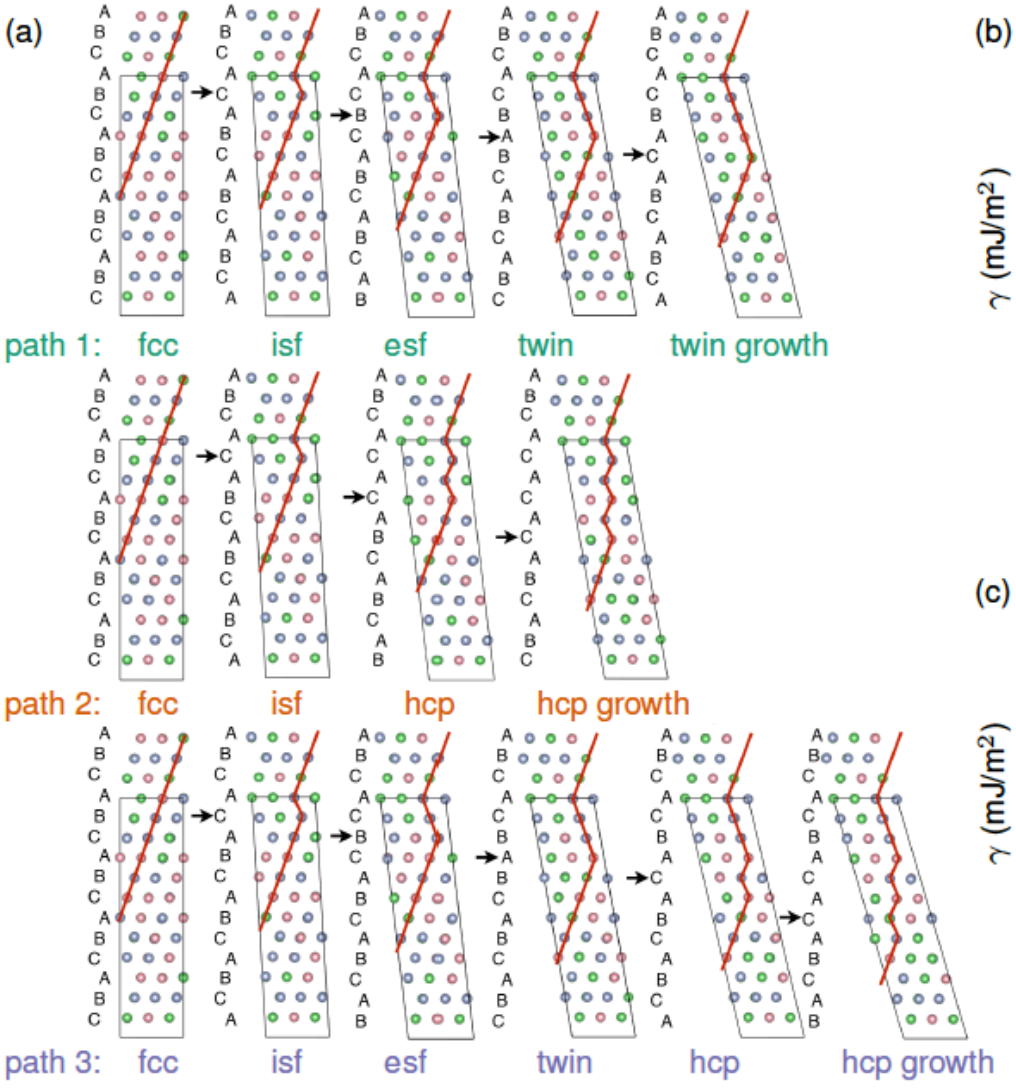
Center of Symmetry Map

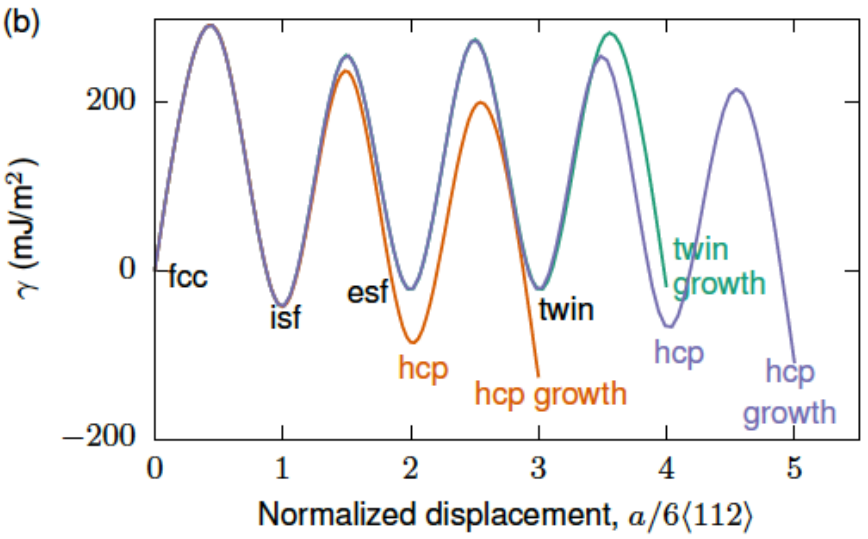


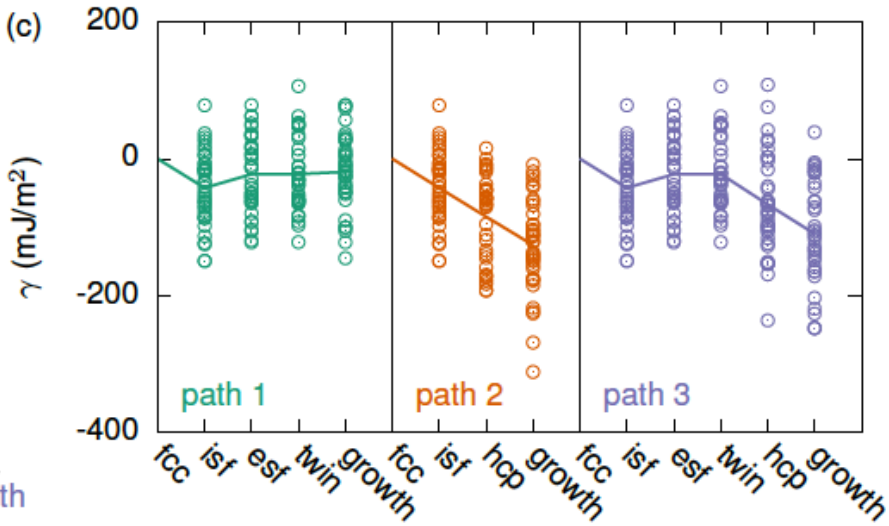
- Quasi-harmonic approximation
- Values for 6 distinct cells with random atomic arrangement
- HCP phase favored relative to FCC phase below approx. 1000°C

Niu, LaRosa, Miao, Mills, Ghazisaeidi, Nature Comm. (2018)

DFT of Planar Fault Energies for Twinning and HCP Formation



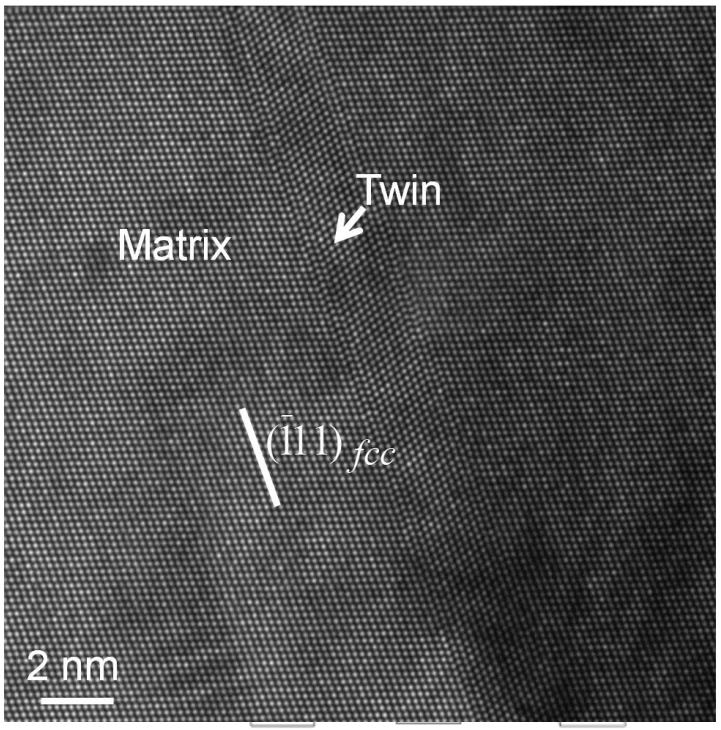


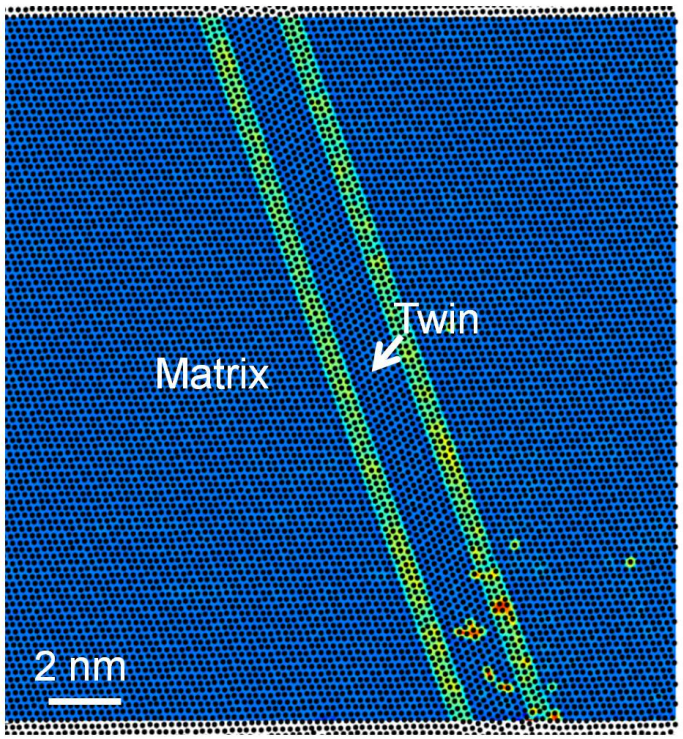


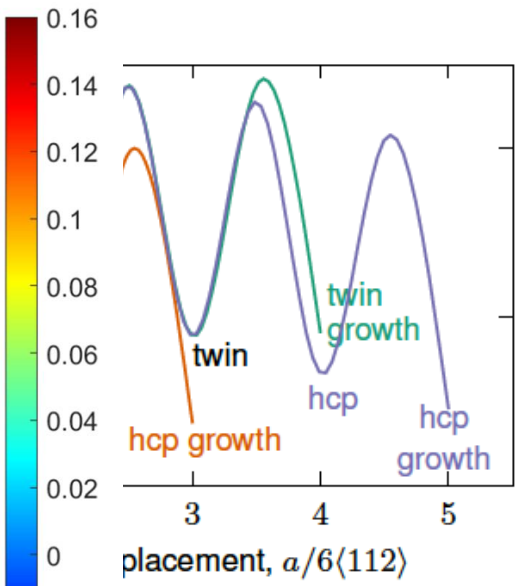
HCP formation energetically favored at SFs and twin boundaries

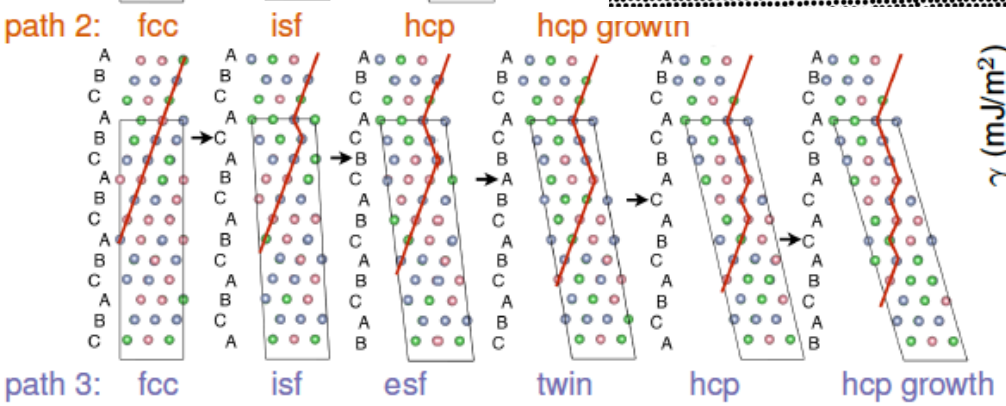
Niu, LaRosa, Miao, Mills, Ghazisaeidi, Nature Comm. (2018)

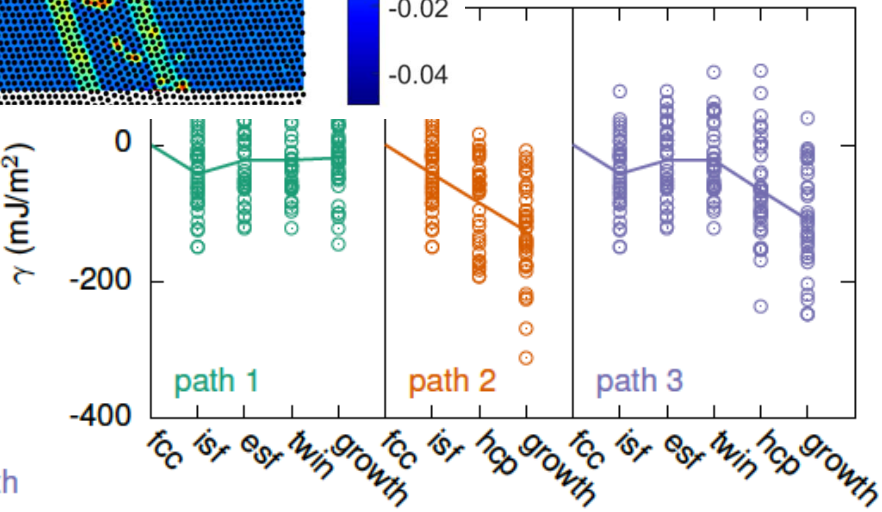
DFT of Planar Fault Energies for Twinning and HCP Formation









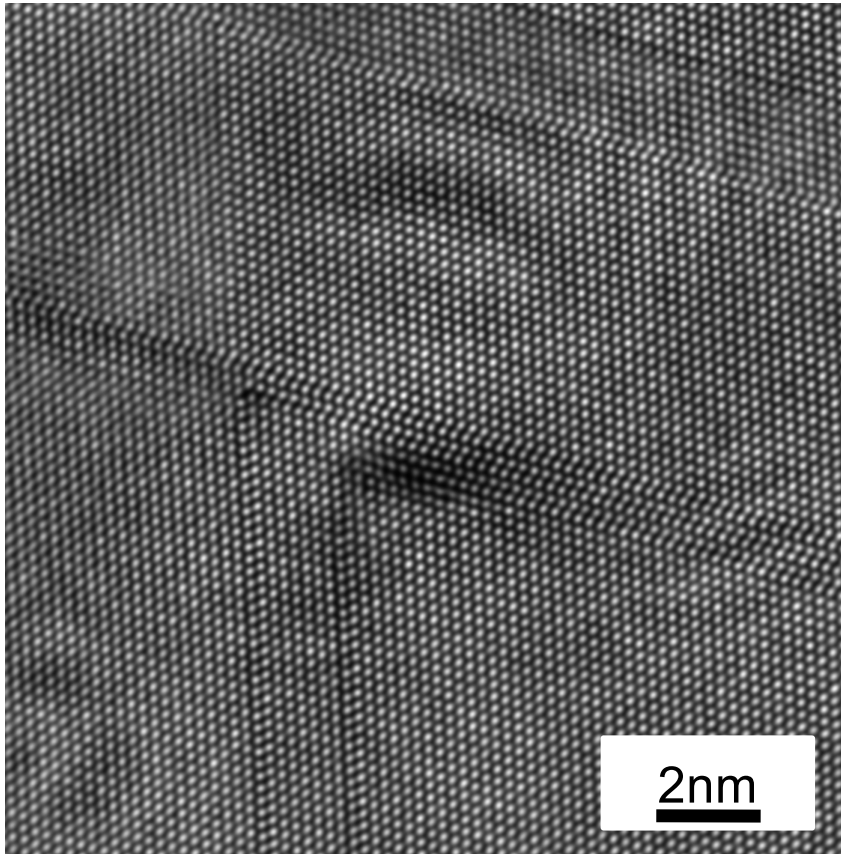


HCP formation energetically favored at SFs and twin boundaries

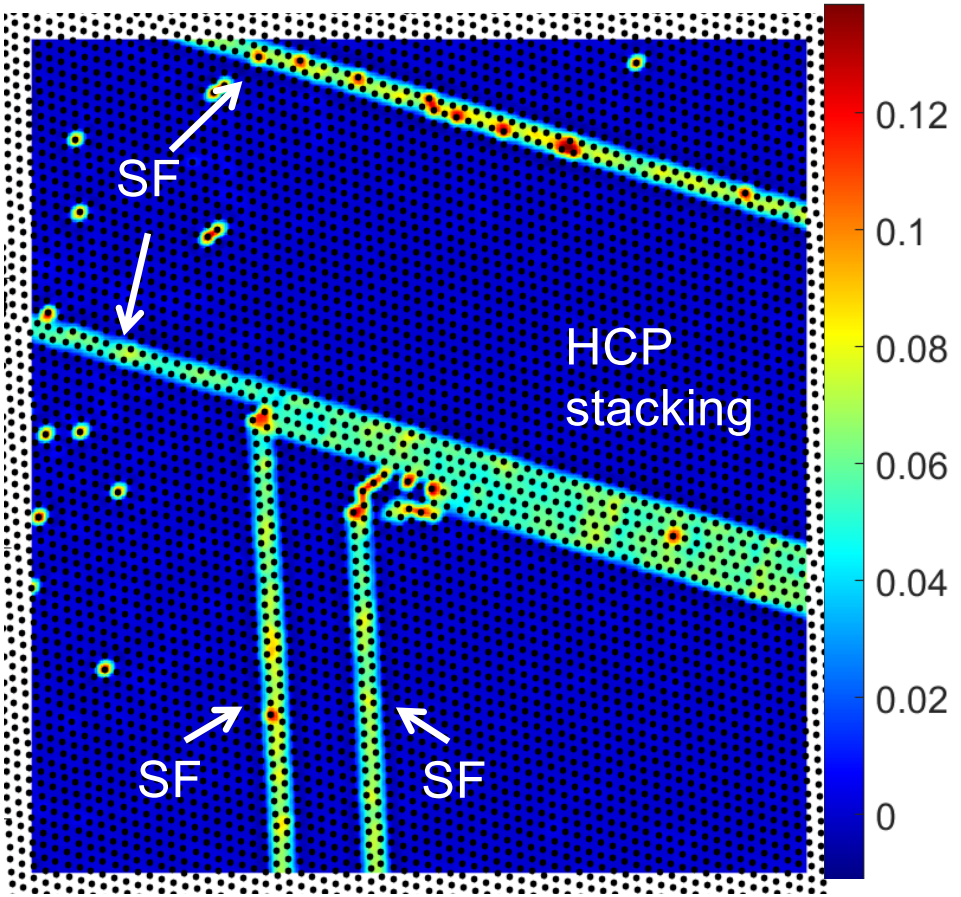
Niu, LaRosa, Miao, Mills, Ghazisaeidi, Nature Comm. (2018)

Source of Partials Creating HCP?

HAADF-STEM



Center of Symmetry Map

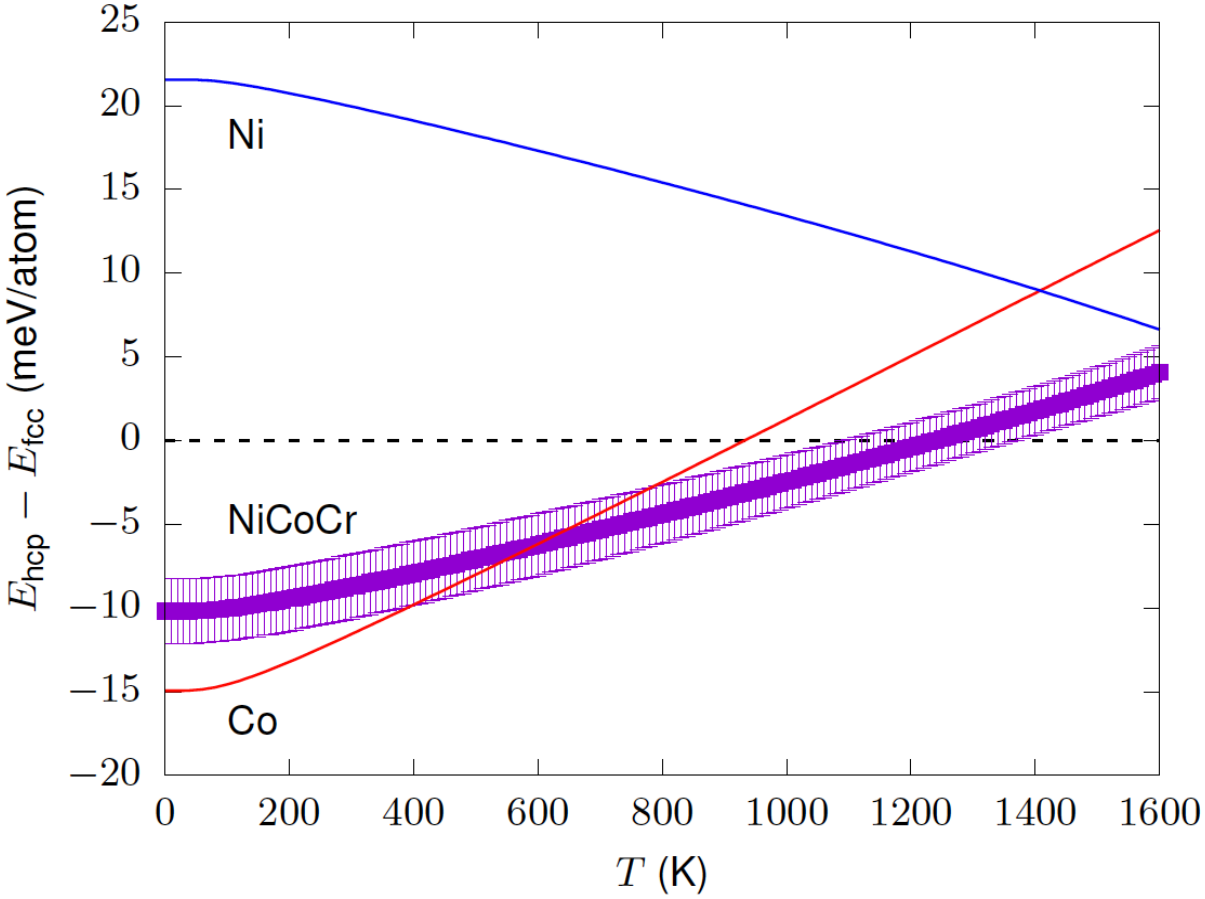


- Fine scale nanotwinning
- Thin HCP laths at stacking faults and twin boundaries
- Cross-slip to conjugate {111} promotes HCP formation

Niu, LaRosa, Miao, Mills, Ghazisaeidi, Nature Comm. (2018)

Atomistic Calculations To "Mimic" DFT

DFT Calculations



Prohibitive to perform DFT for studying dislocation/twin/HCP interactions

DFT indicates that Co could provide a surrogate for NiCoCr:

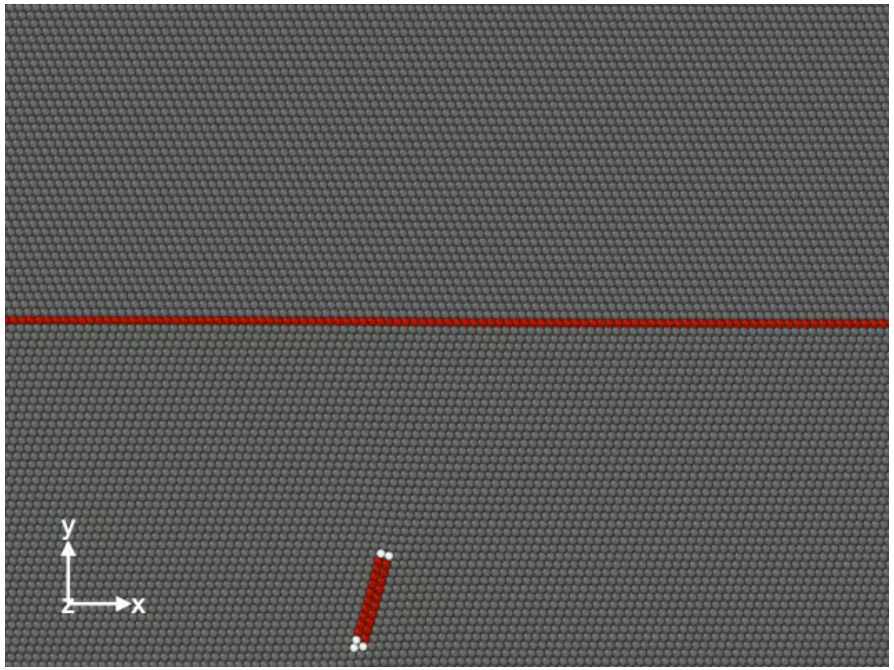
Atomistic simulations with LAMMPS enables large-scale defect calculations

Co potential from P. Purja Pun, Yamakov and Mishin, MSMSE 23, 065006 (2015)

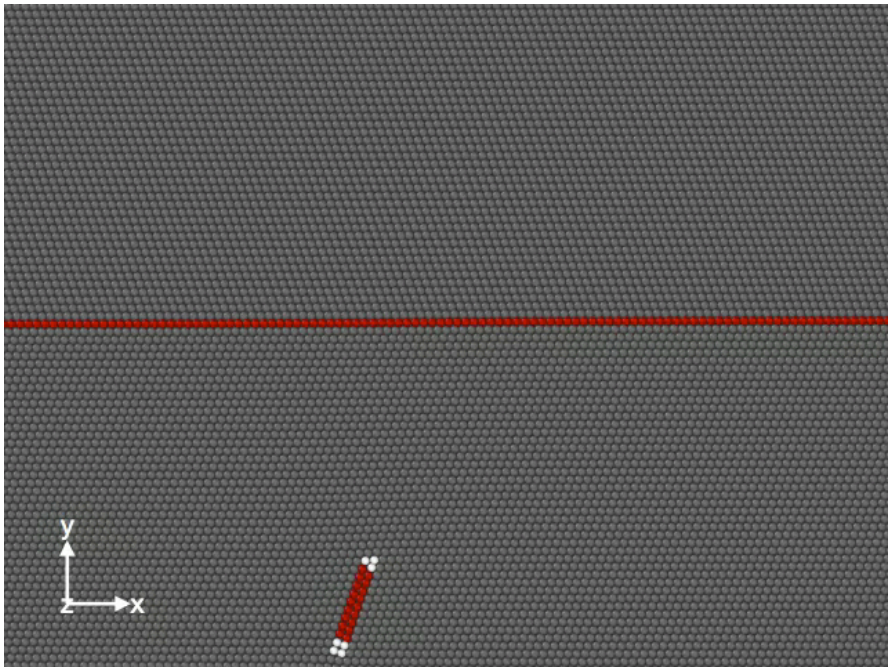
Niu, LaRosa, Miao, Mills, Ghazisaeidi, Nature Comm. (2018)

EAM Calculation of Dislocation/Twin Interaction Using Co Potential

90° partial leading $\gamma_{xy} = -0.067$



30° partial leading $\gamma_{yz} = 0.067$



fcc hcp

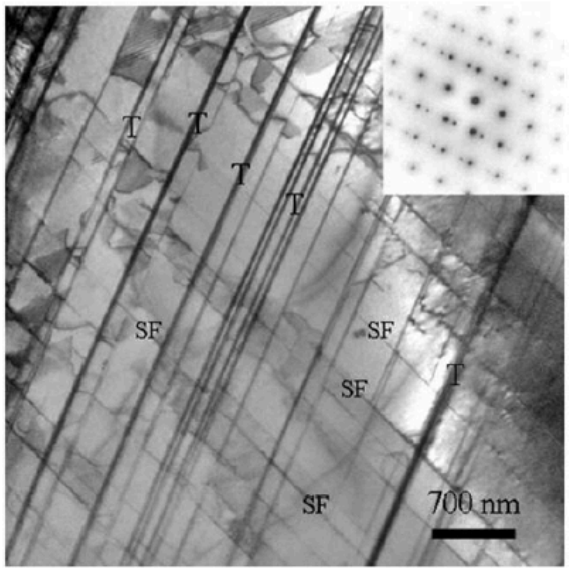
Mechanism for heterogenoeus nucleation of HCP laths at twin boundaries in FCC Co (surrogate for NiCoCr)

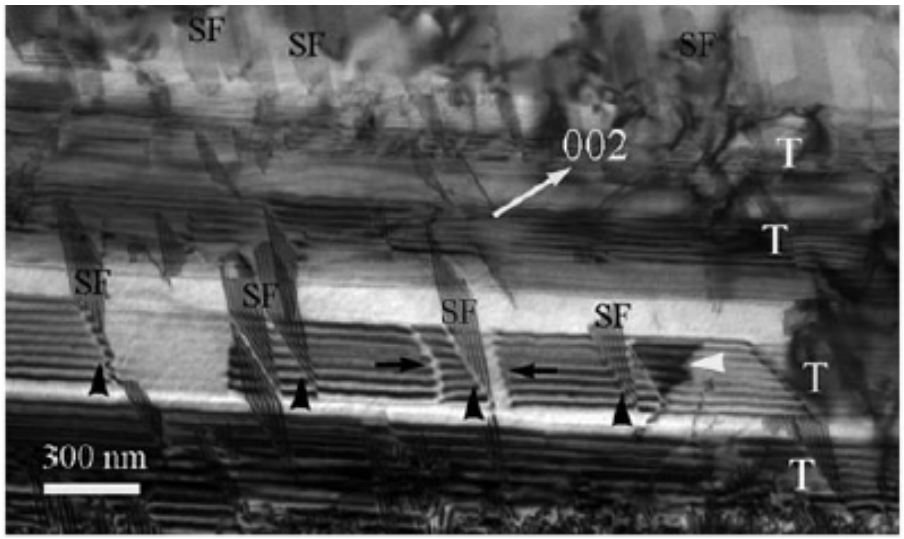
Niu, LaRosa, Miao, Mills, Ghazisaeidi, Nature Comm. (2018)

Analogous Mechanism for Twin Growth

Idrissi, et al, Phil. Mag., 93 (2013)

Fe-28Mn-3.5Si-2.8Al TWIP Steel

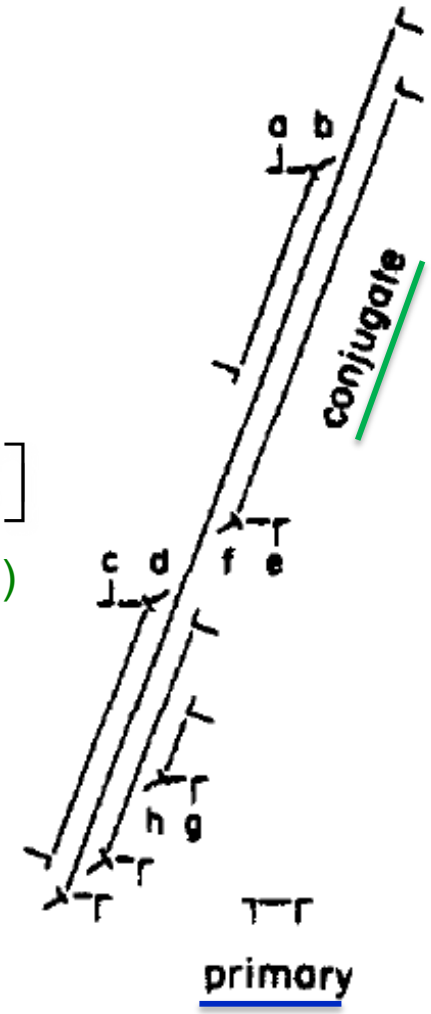




Can occur for interaction of mixe (60°) ½<110> dislocations with pre-existing twins

$$\frac{1}{6}[\bar{1}2\bar{1}] + \frac{1}{6}[\bar{1}\bar{1}0] \Rightarrow \frac{1}{6}[\bar{2}1\bar{1}]$$

on (111) — Stair-rod partial — on (11-1)



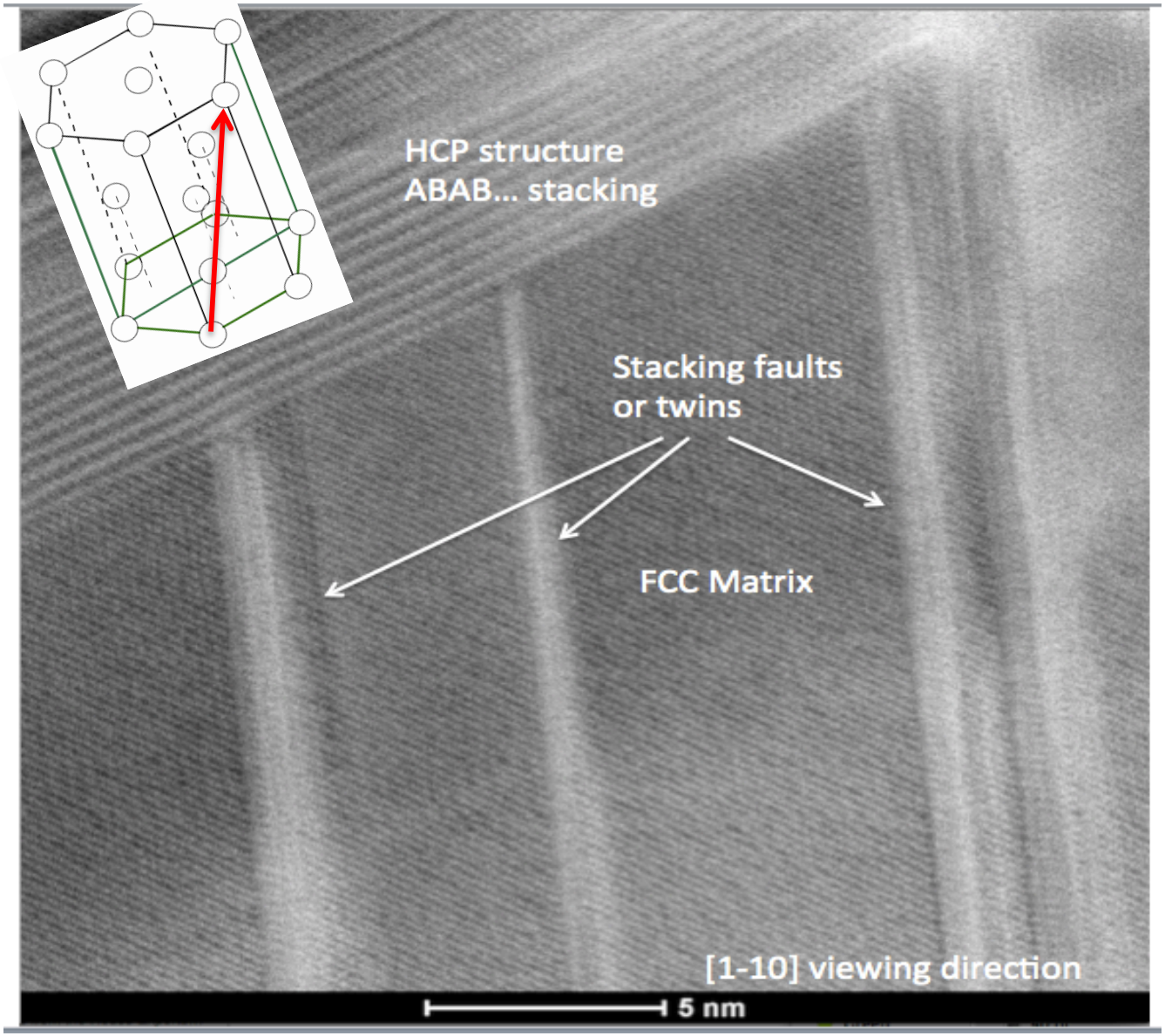
Mori and Fujita, Acta Metall. 28 (1980)

Cu-11%Al FCC Solid Solution

LAADF STEM along <110> Zone: 77K Deformed Ni-Co-Cr

After constant strain rate testing at LN for 53%:

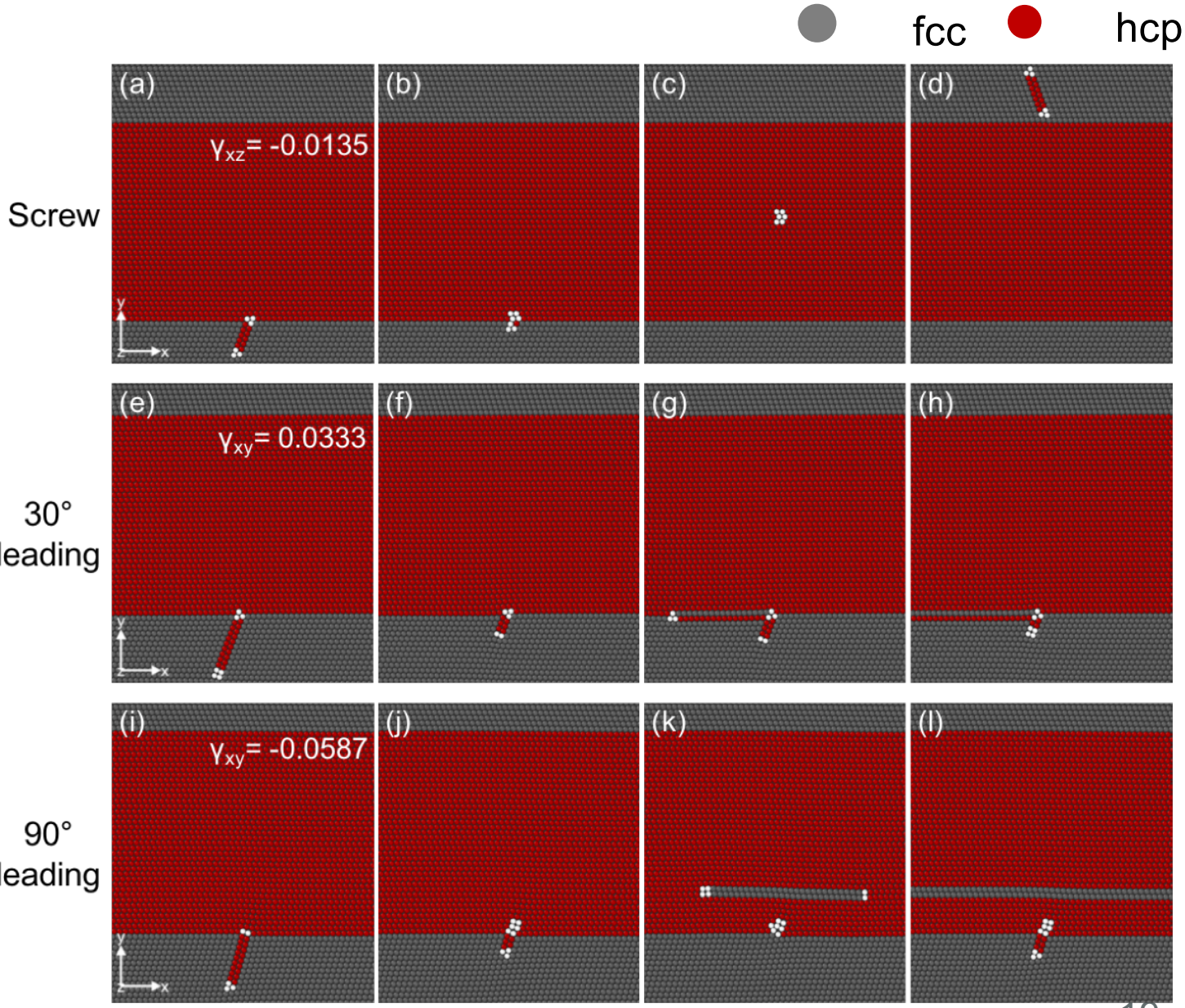
- Fine scale nano-twinning
- Thicker HCP laths act as strong barriers to conjugate slip/twinning
- For slip transmission, need to activate <c> component dislocations or twinning in HCP laths



Miao, et al., Acta Mater., 132, 35–48 (2017)

Dislocation Interaction with HCP/FCC Interface

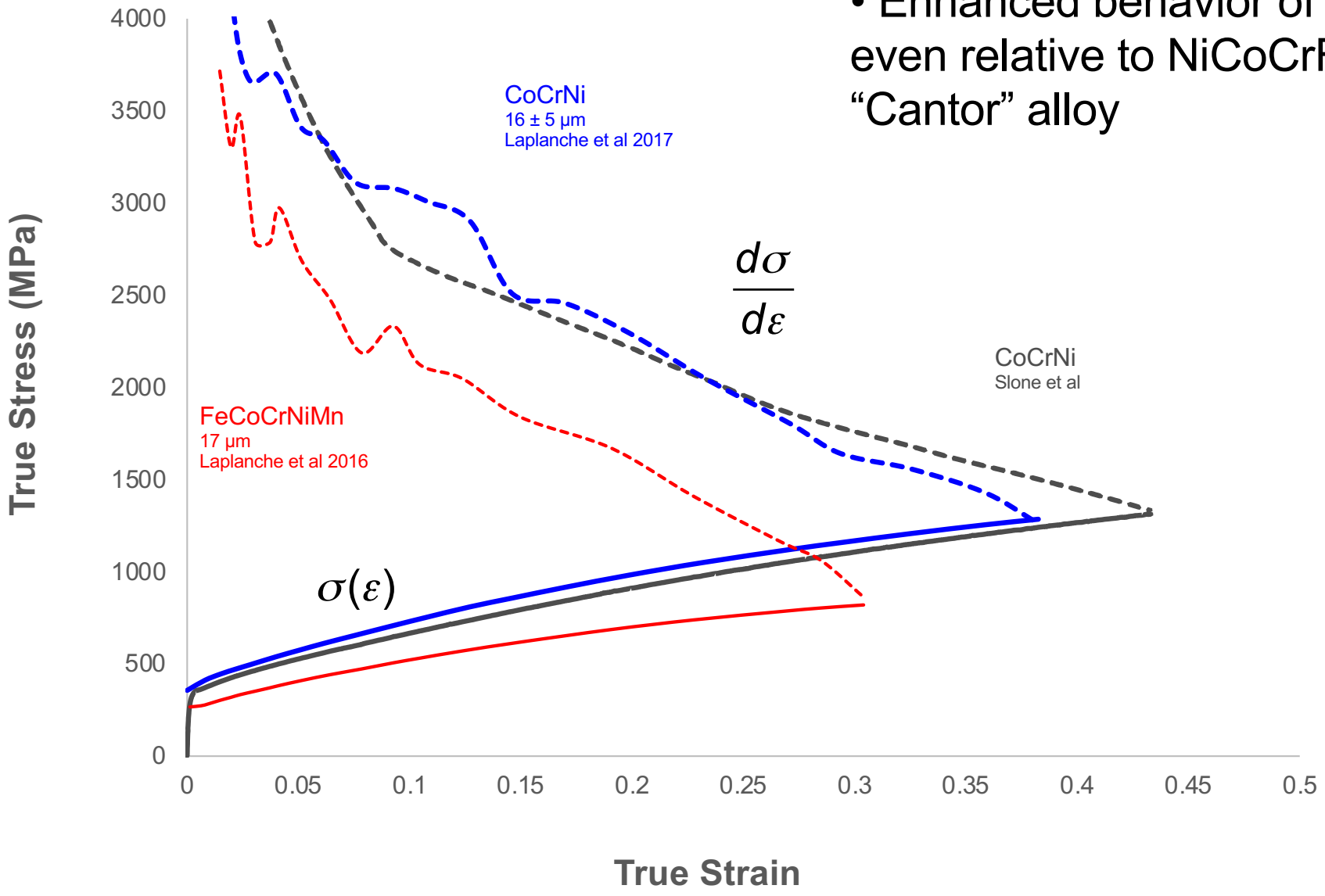
- FCC/HCP interface poses a barrier to dislocation motion: Strengthening
- Dislocations are accommodated within the HCP region: stress concentrations minimized
- HCP regions can grow or "heal" by dislocation motion



Niu, LaRosa, Miao, Mills, Ghazisaeidi, Nature Comm. (2018)

Comparison of Equiatomic FCC Alloys

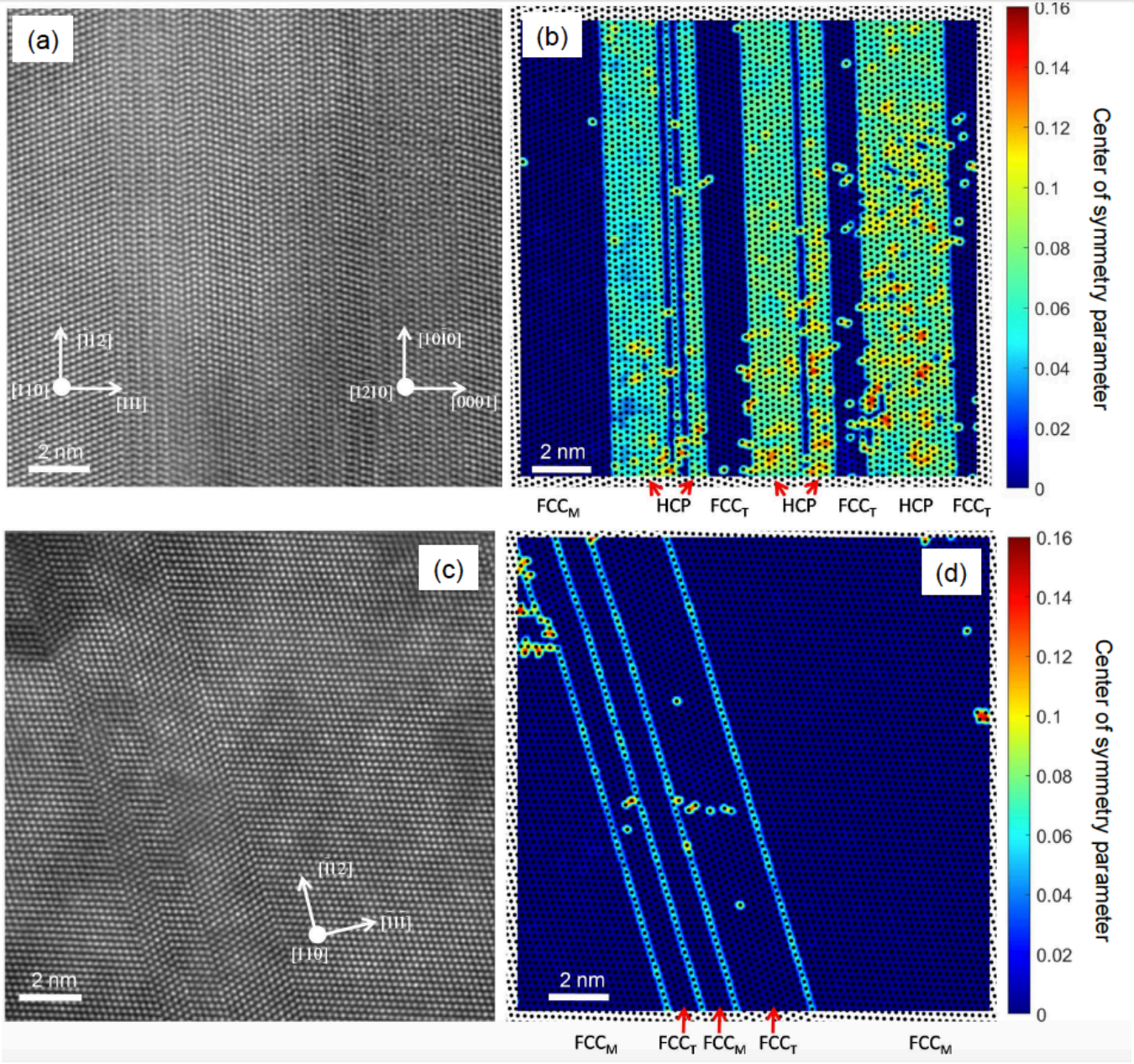
- Enhanced behavior of NiCoCr even relative to NiCoCrFeMn "Cantor" alloy



HCP ε Martensite in FCC HEAs After LN Deformation

NiCoCr

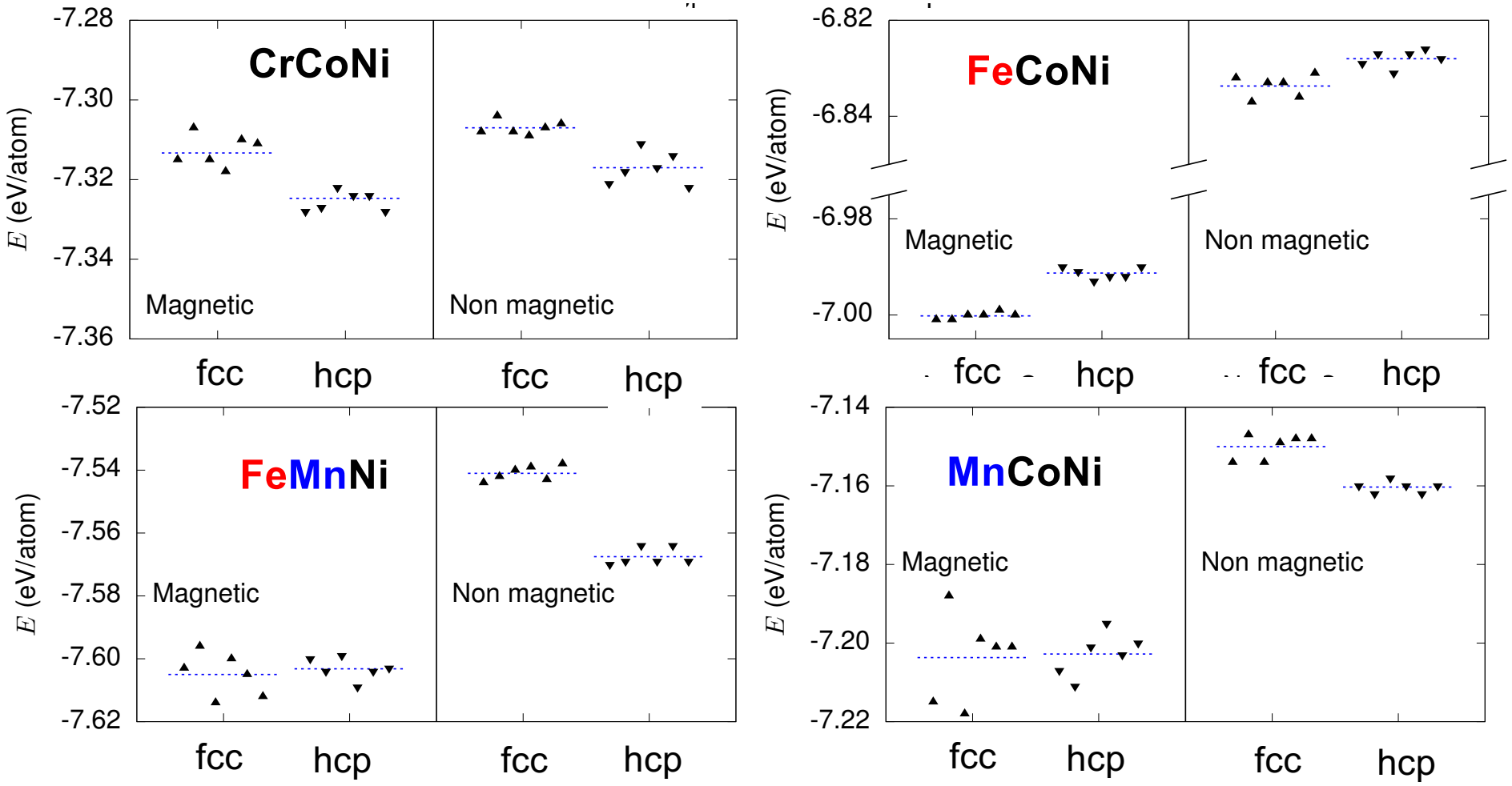
"Cantor" Alloy NiCoCr MnFe



- HCP phase formation at twin boundaries in NiCoCr
- Only twinning observed in Cantor alloy – *HCP phase is absent*
- Related to enhanced properties of NiCoCr ?

Niu, LaRosa, Miao, Mills, Ghazisaeidi, Nature Comm. (2018)

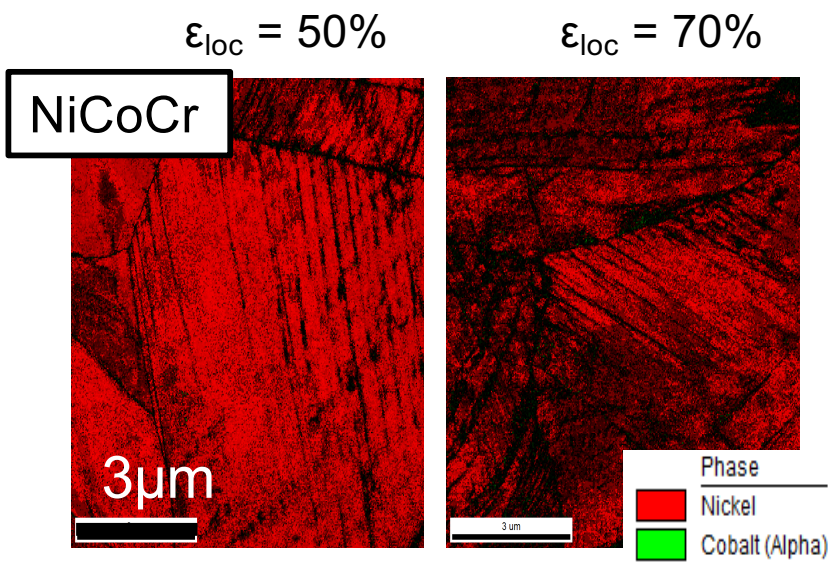
Chemistry/Magnetism on Phase Stability

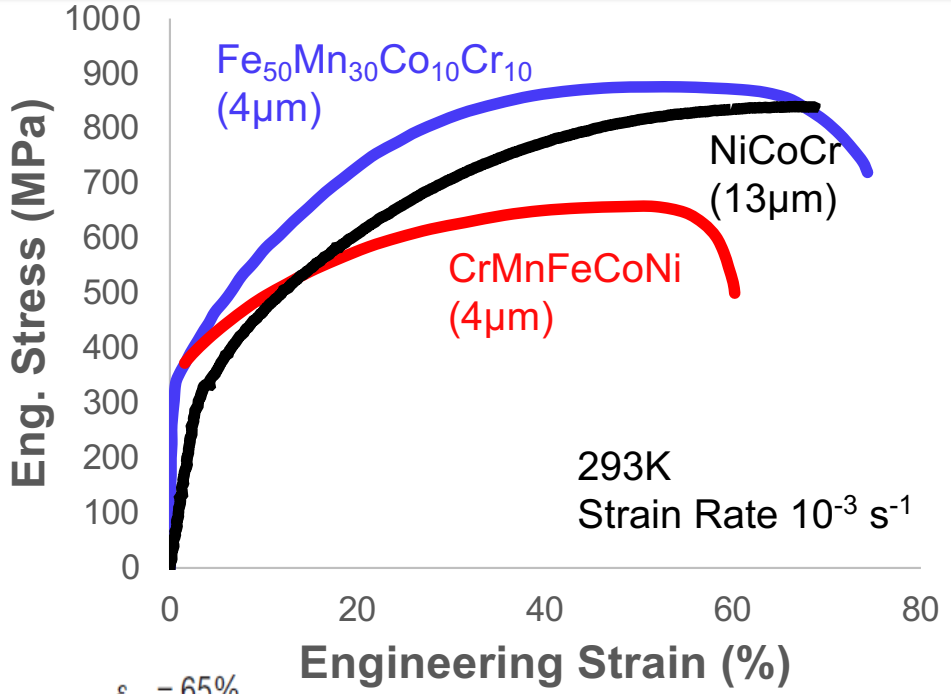


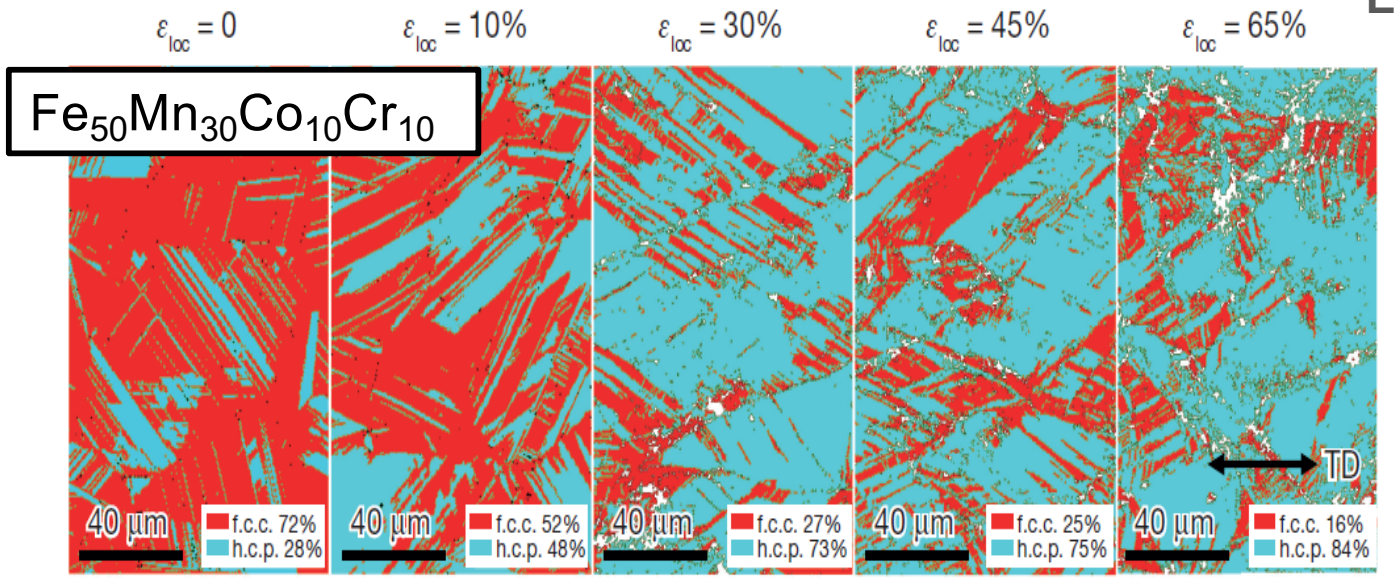
Mn / Fe (with magnetism) eliminates the HCP preference for NiCo-X

Niu, LaRosa, Miao, Mills, Ghazisaeidi, Nature Comm. (2018)

Comparison to Other Dual-Phase CCAs





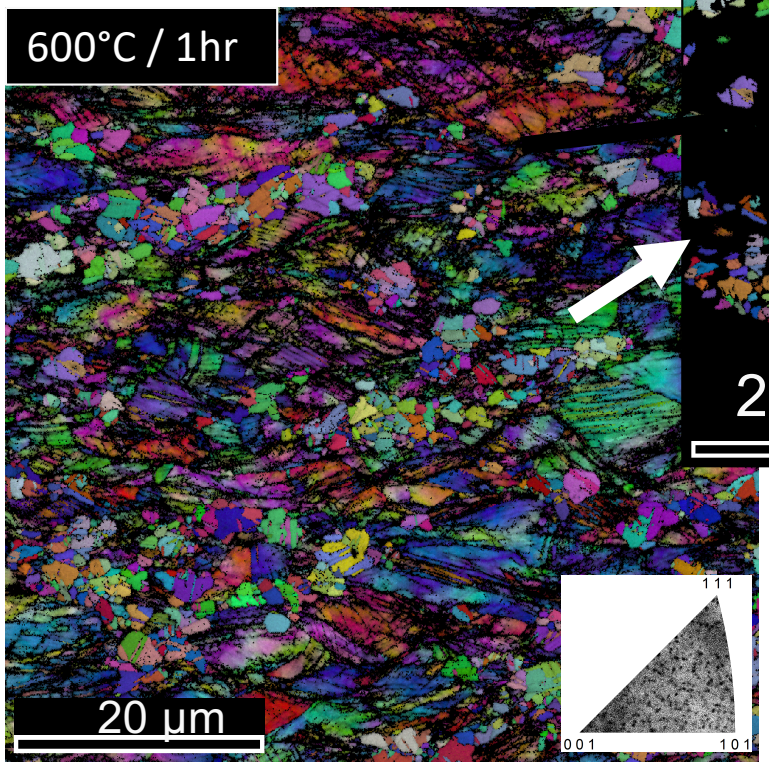


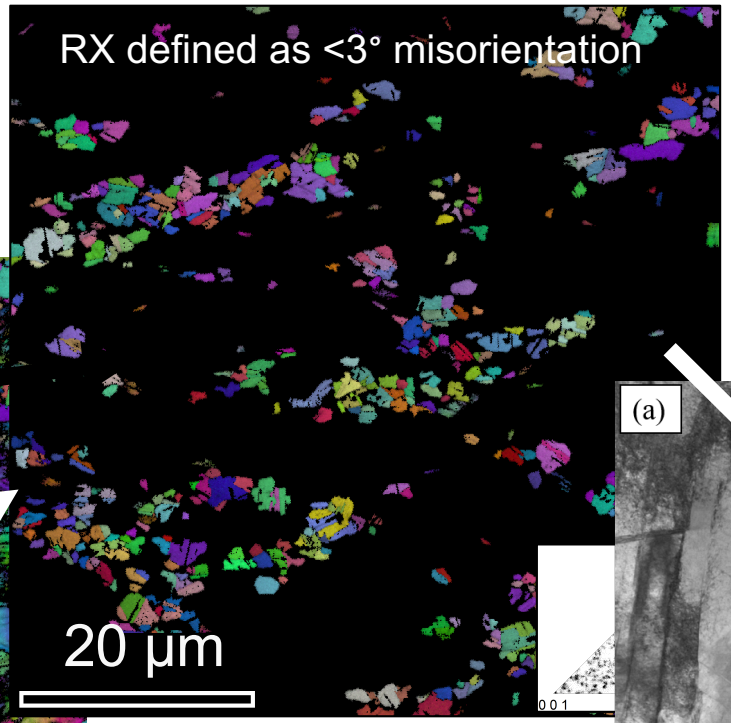
Zhiming Li et al, Nature Letters 2016

- HCP laths = ε martensite
- In contrast to dual phase TRIP steels, volume fraction of HCP remains very small in NiCoCr
- May still be key to extraordinary hardening

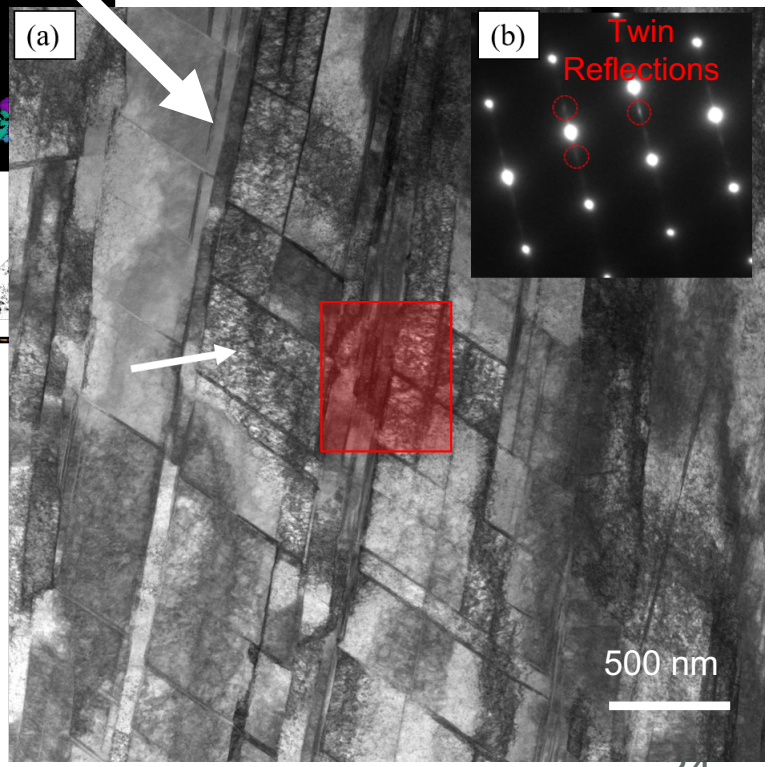
Partially Recrystallized (RX) NiCoCr

70% reduction in thickness, then anneal…





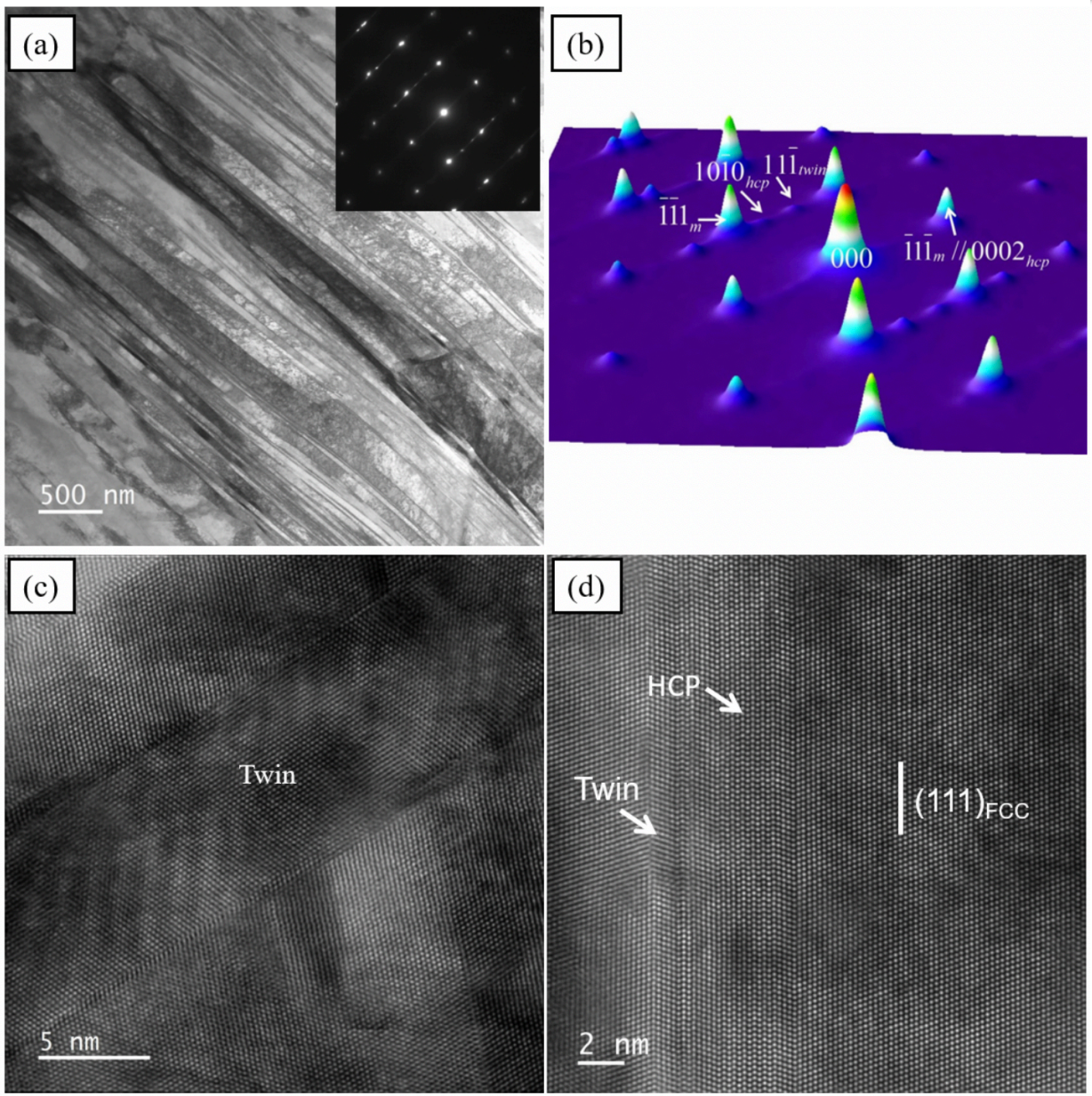
Twin structures and high dislocation density still present in Non-RX grains !



C.E. Slone et al, Acta Mater, 165 (2019)

Partially Recrystallized (RX) NiCoCr

600°C / 1hr



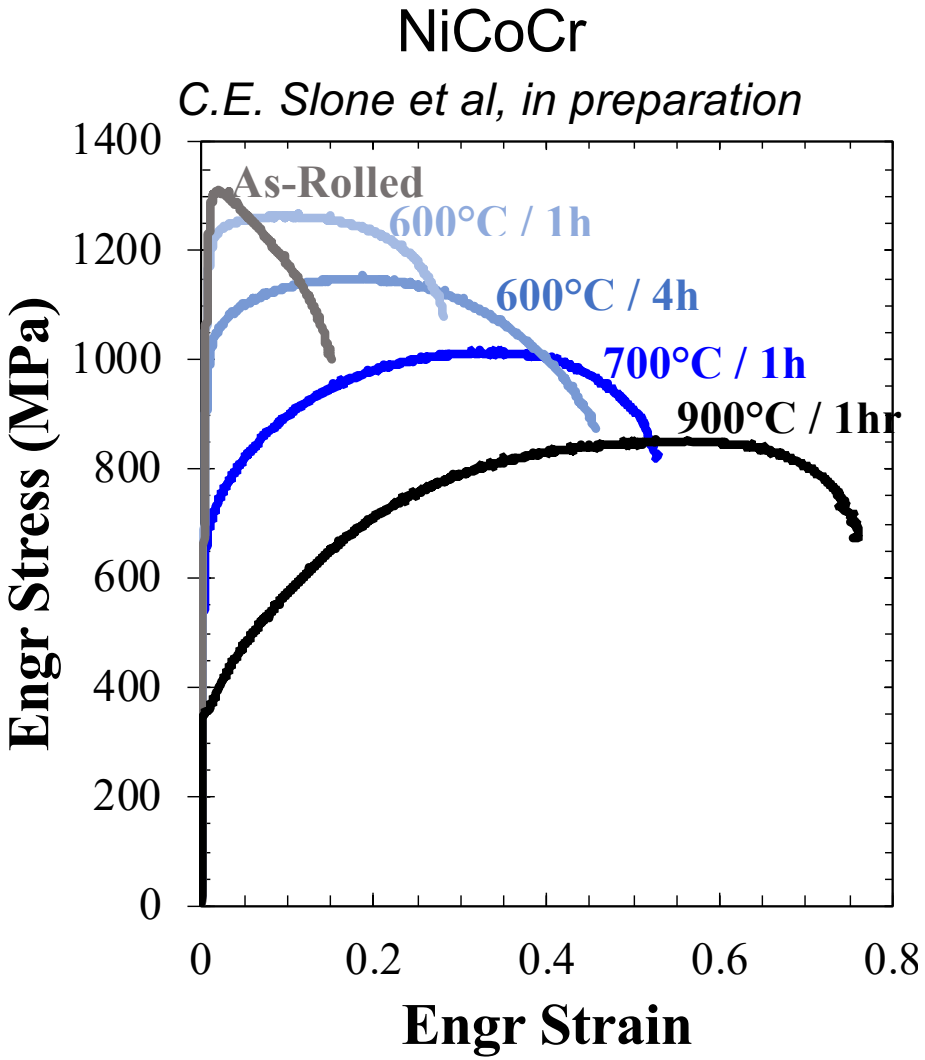
Twin structures, high dislocation density…

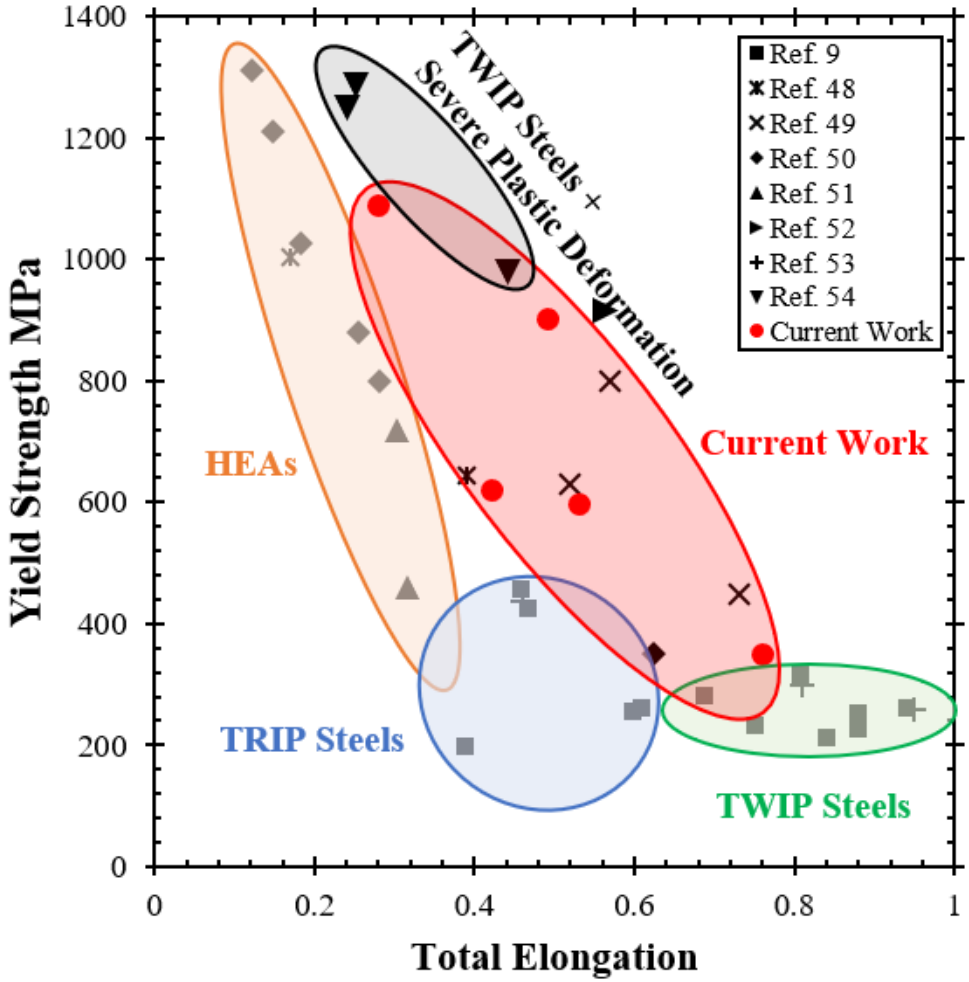
and HCP phase…

still present in Non-RX grains !

C.E. Slone et al, Acta Mater, 165 (2019)

Partially RX Microstructures: NiCoCr vs. Cantor Alloy





Partially RX microstructures offer route to achieve much higher strengths while retaining significant ductility

Conclusions

- High entropy FCC based alloys have conventional dislocation cores with highly variable dissociation distances:
  - SFE in concentrated solutions is a spatially varying quantity
  - Measurement of SFE from dissociation distance is problematic
- Twinning prominent at larger strains in both Cantor and NiCoCr – contributing to strong work hardening and large ductility
- In NiCoCr, HCP phase transformation at twins and stacking faults may impart further enhancement in work hardening
- Extreme strength and ductility can be achieved in partially-recrystallized states (both NiCoCr and IN740H)
- Alloy design crucially aided by advanced characterization and modeling