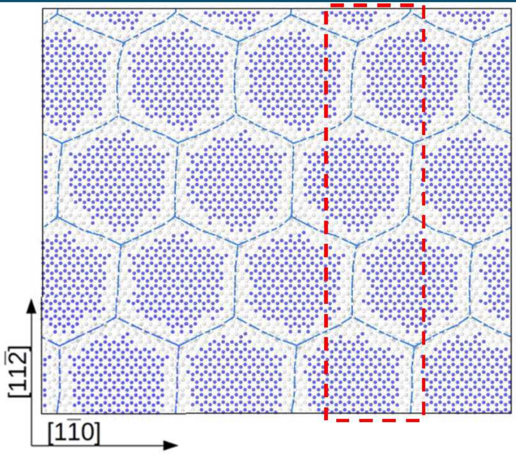
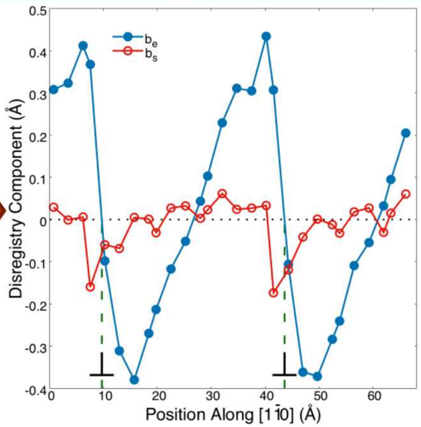
SAND2018-3482C

Georgia Tech Mechanical Engineering
The George W. Woodruff School of Mechanical Engineering

Interfacial Defect Structure of U-Zr Stacking Misfit Phase Boundaries

EN17.08.0





PRESENTED BY

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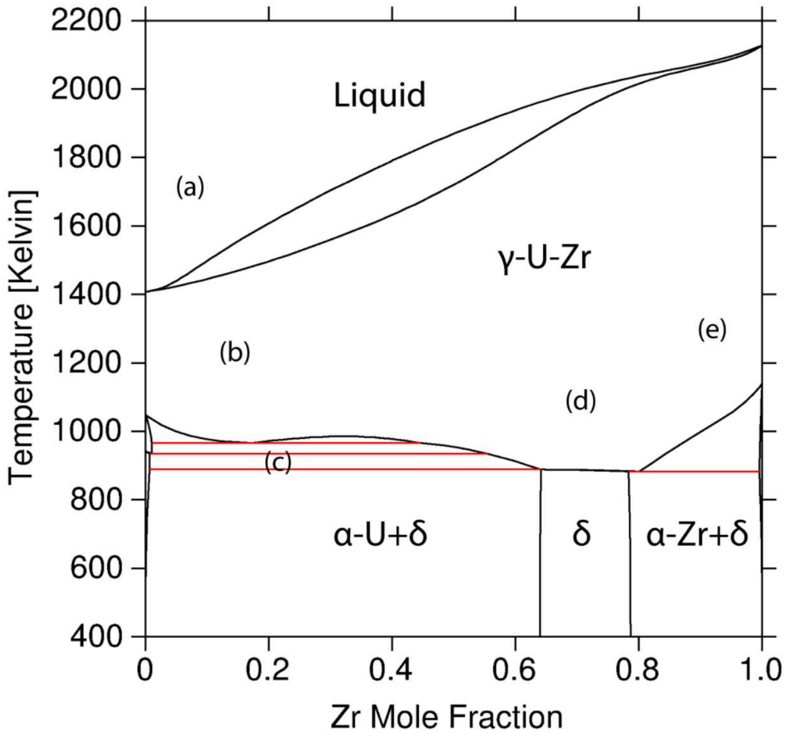
Talking Points

1. Miscible phase boundaries
2. Atomistic modeling of interfaces
3. Calculation and verification of the defect structures
4. Examining the effect of defect presences

Heterophase boundaries between miscible metals: U-Zr



(a
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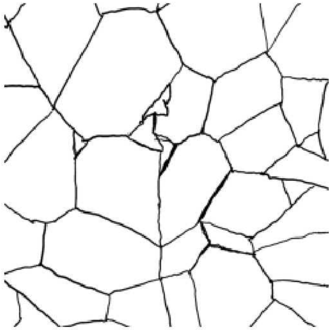
(b
)

(c)



(d
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(e
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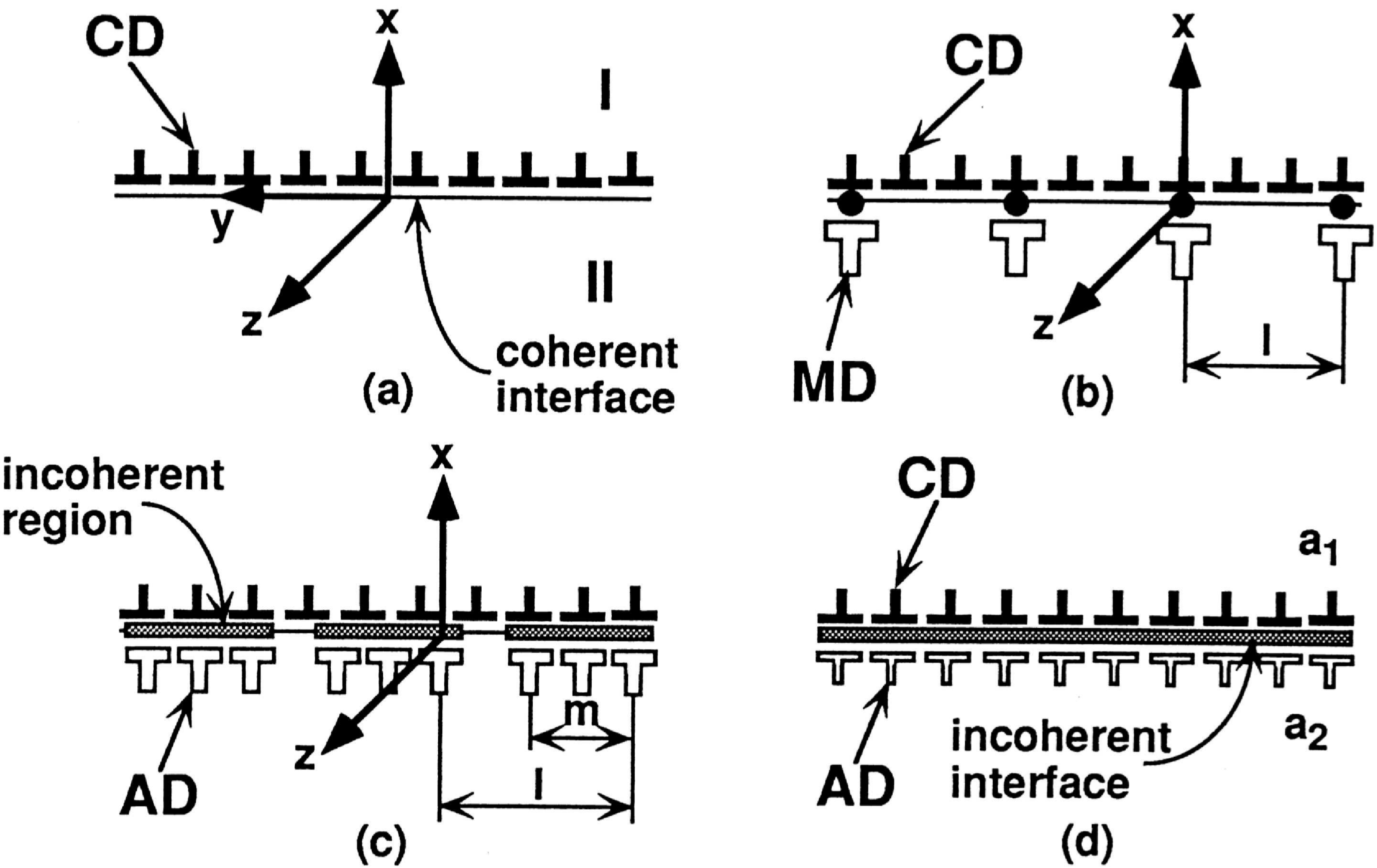
[Moore (2016)]

States of interfacial structure coherency



[Romanov (1998)]

Atomistic phase boundary modeling strategy

Build γ-U-Zr Interface Isotropic Commensurate Stretch

+

Introduce Misfit Strain Variations

$$\epsilon^{S,m} = 2\frac{m\lambda_1 - n\lambda_2}{m\lambda_1 + n\lambda_2}$$

LAMMPS Simulation Interface Optimization

+

γ-U-Zr MEAM Potential

Identify Interface Defect Structure (DXA)

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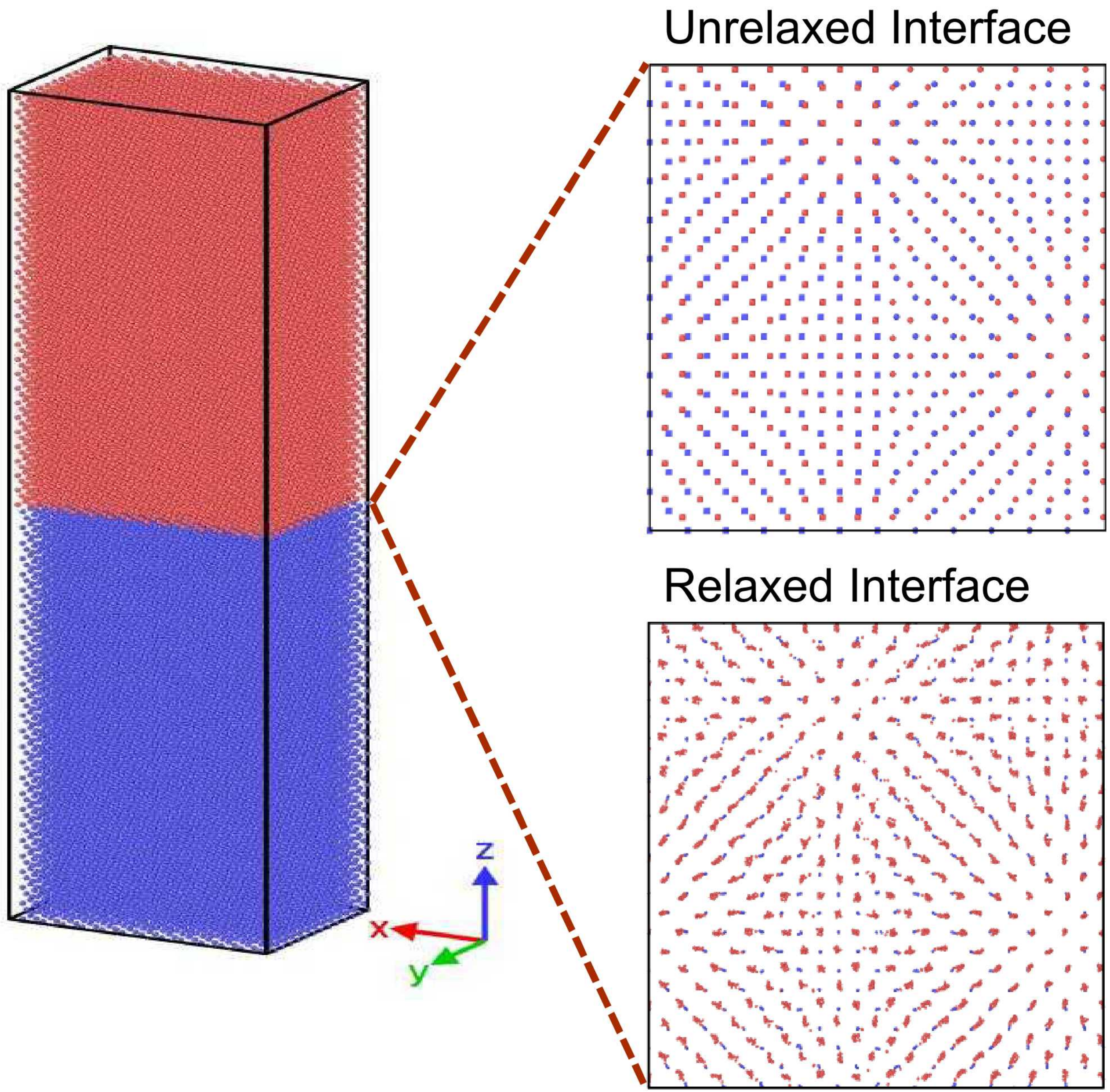
Verify Against
- Disregistry
- Quantized FB

+

Characterize Properties
- Energy
- Elastic Field

Construction → Simulation → Analysis

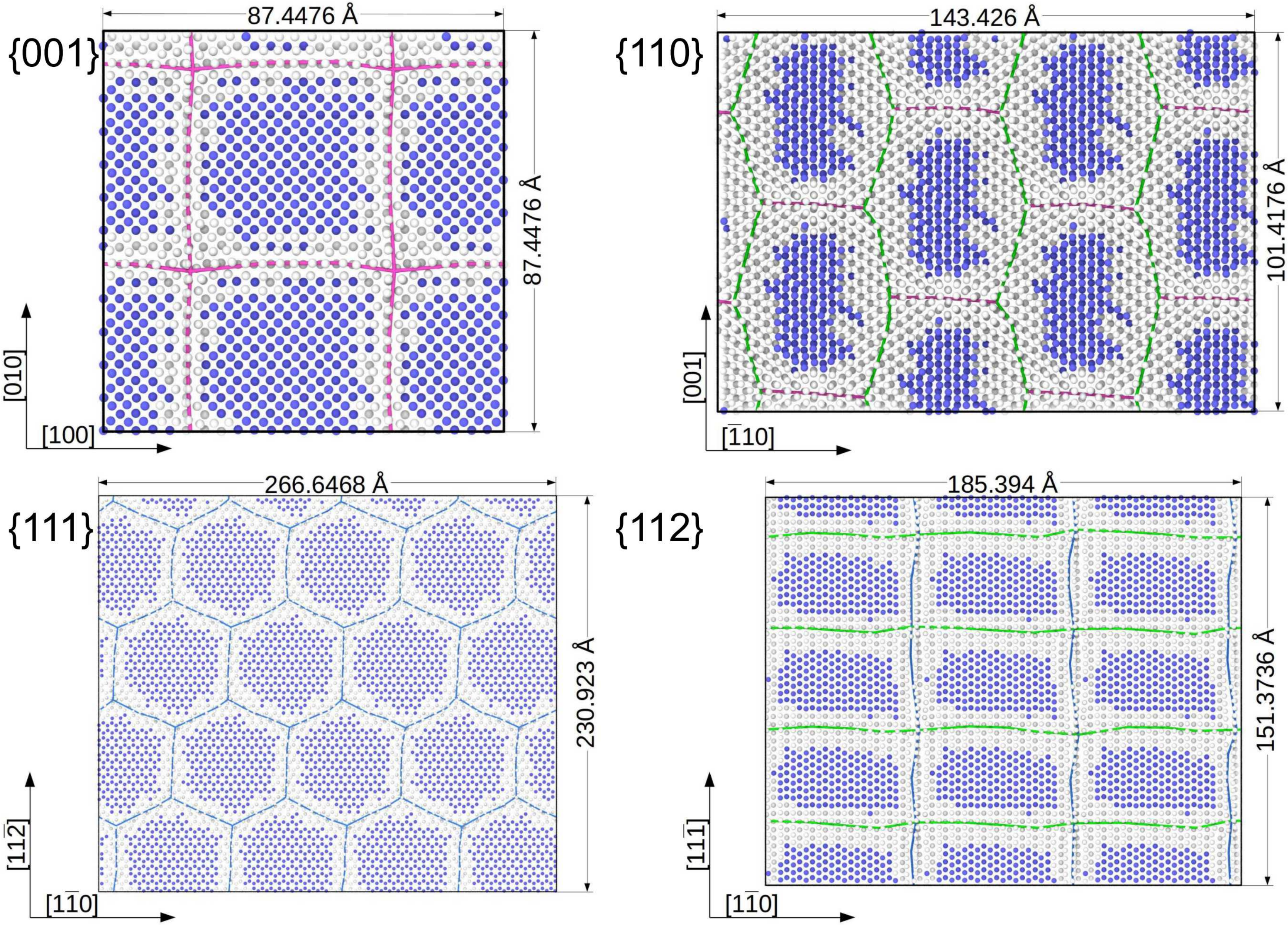
Example of atomistic phase boundary simulation



Interfacial Defect Structure

Identification & Verification

DXA dislocation network structure identification



Verification against disregistry analysis

Disregistry

$$\Delta\vec{r} = \vec{r}_{ij}^{\alpha} - \vec{r}_{ij}^{\beta}$$

Displacement Field

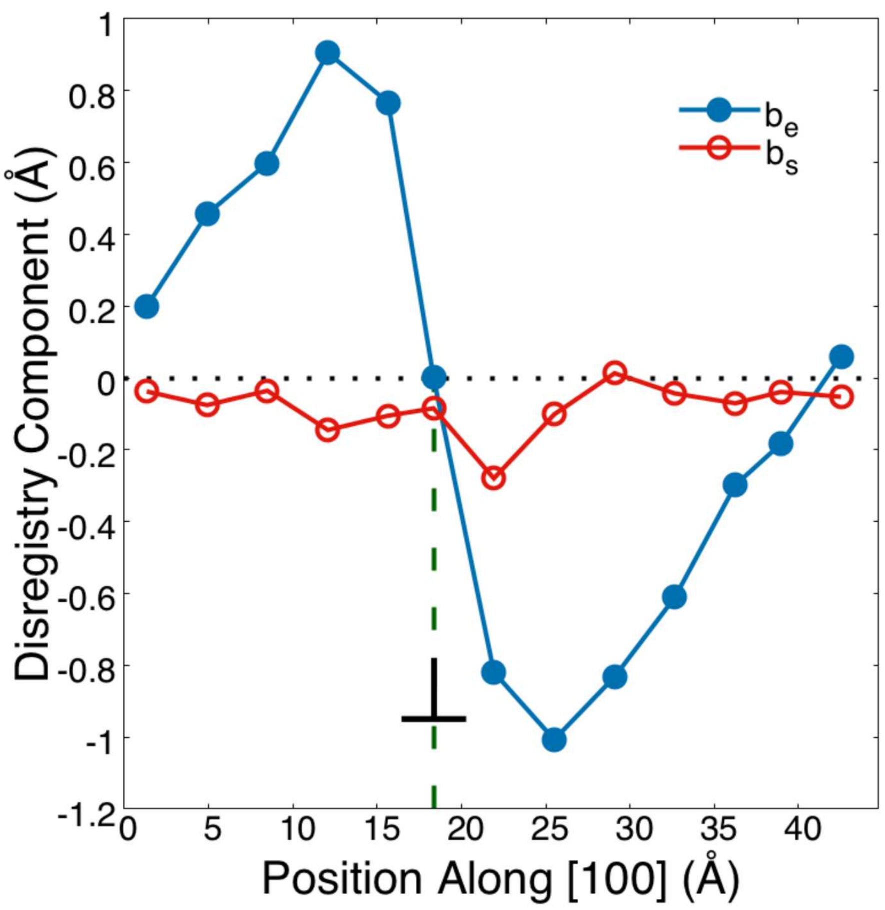
$$\Delta\vec{r} = \vec{r}_{ij}^{Rlx} - \vec{r}_{ij}^{unRlx}$$

Edge component

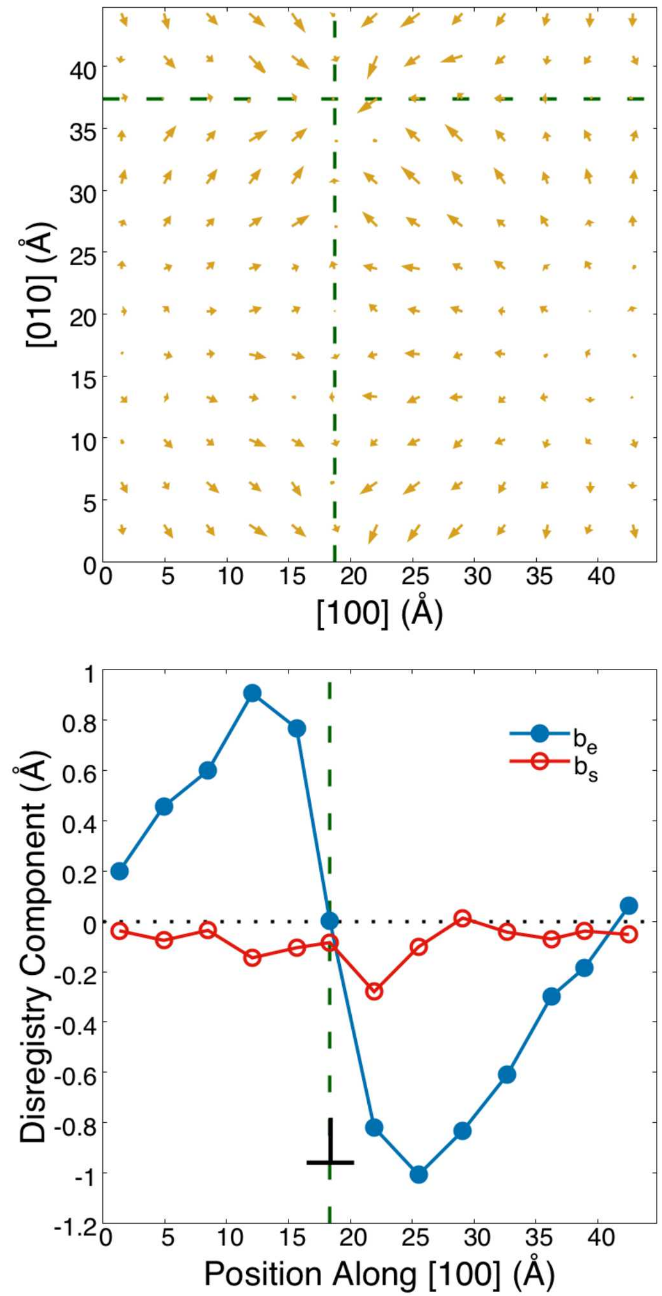
$$\vec{b}_e = \Delta\vec{r} \cdot \vec{n}$$

Screw component

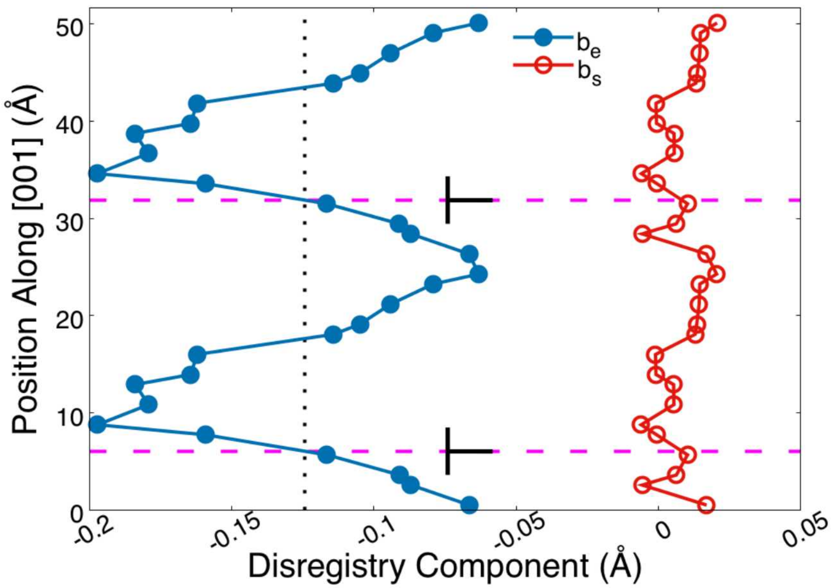
$$\vec{b}_s = \Delta\vec{r} \cdot \vec{\xi}$$

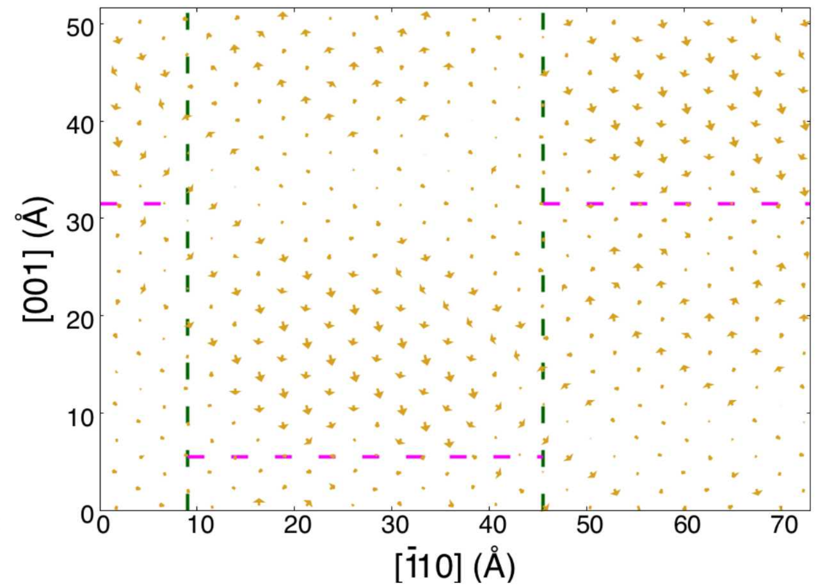


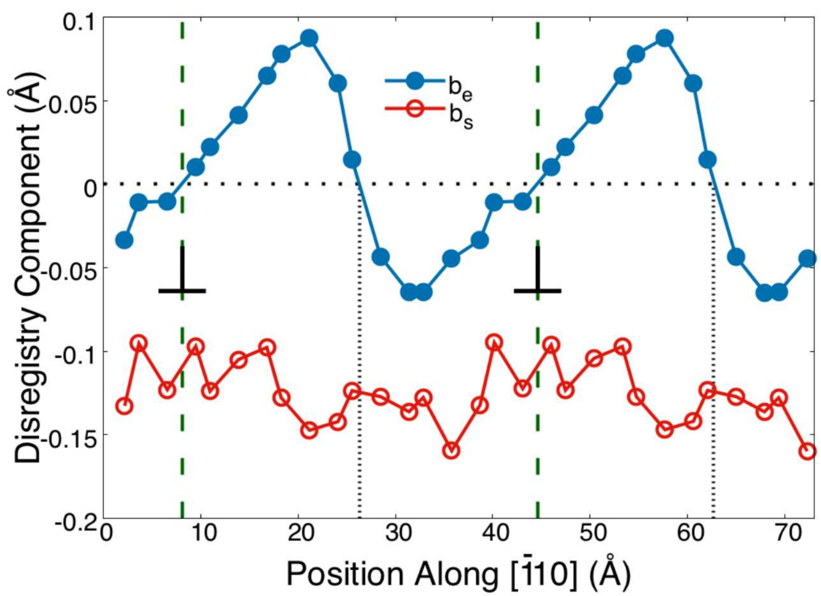
{001} disregistry analysis



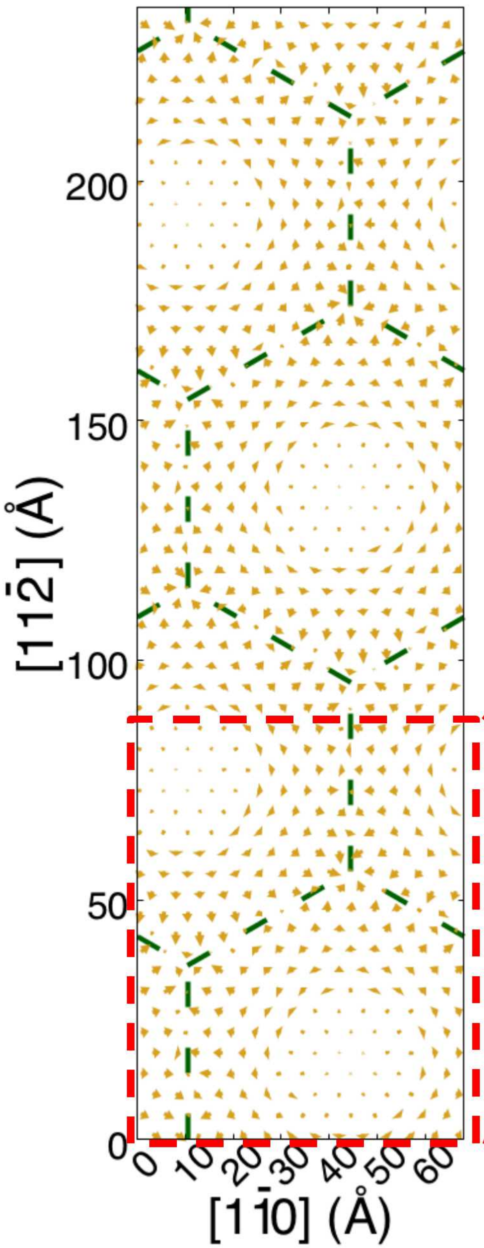
{110} disregistry analysis

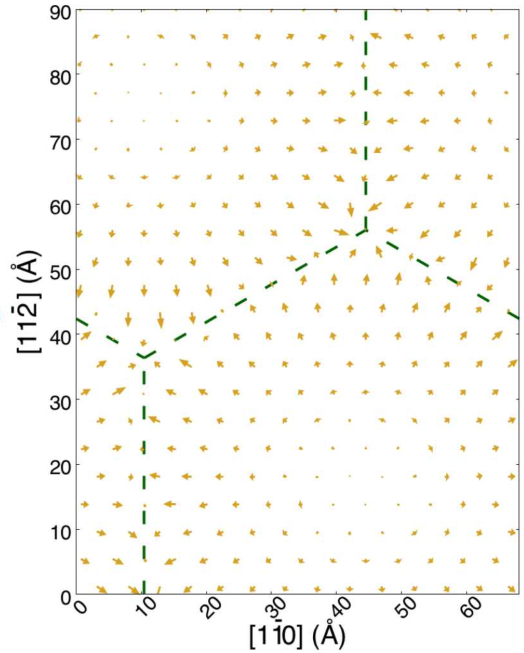


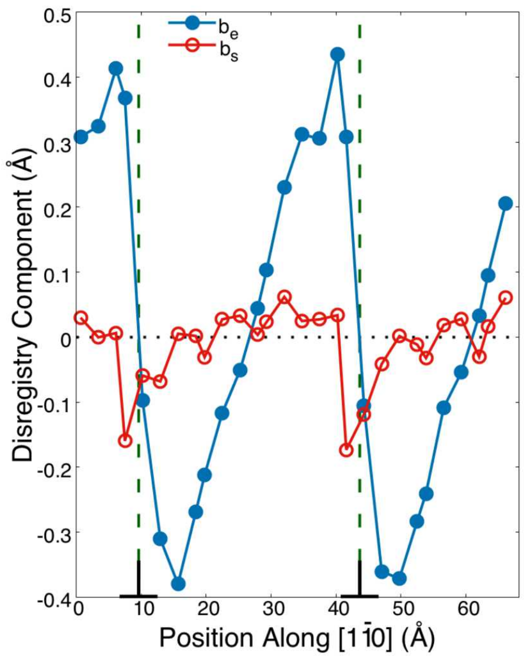




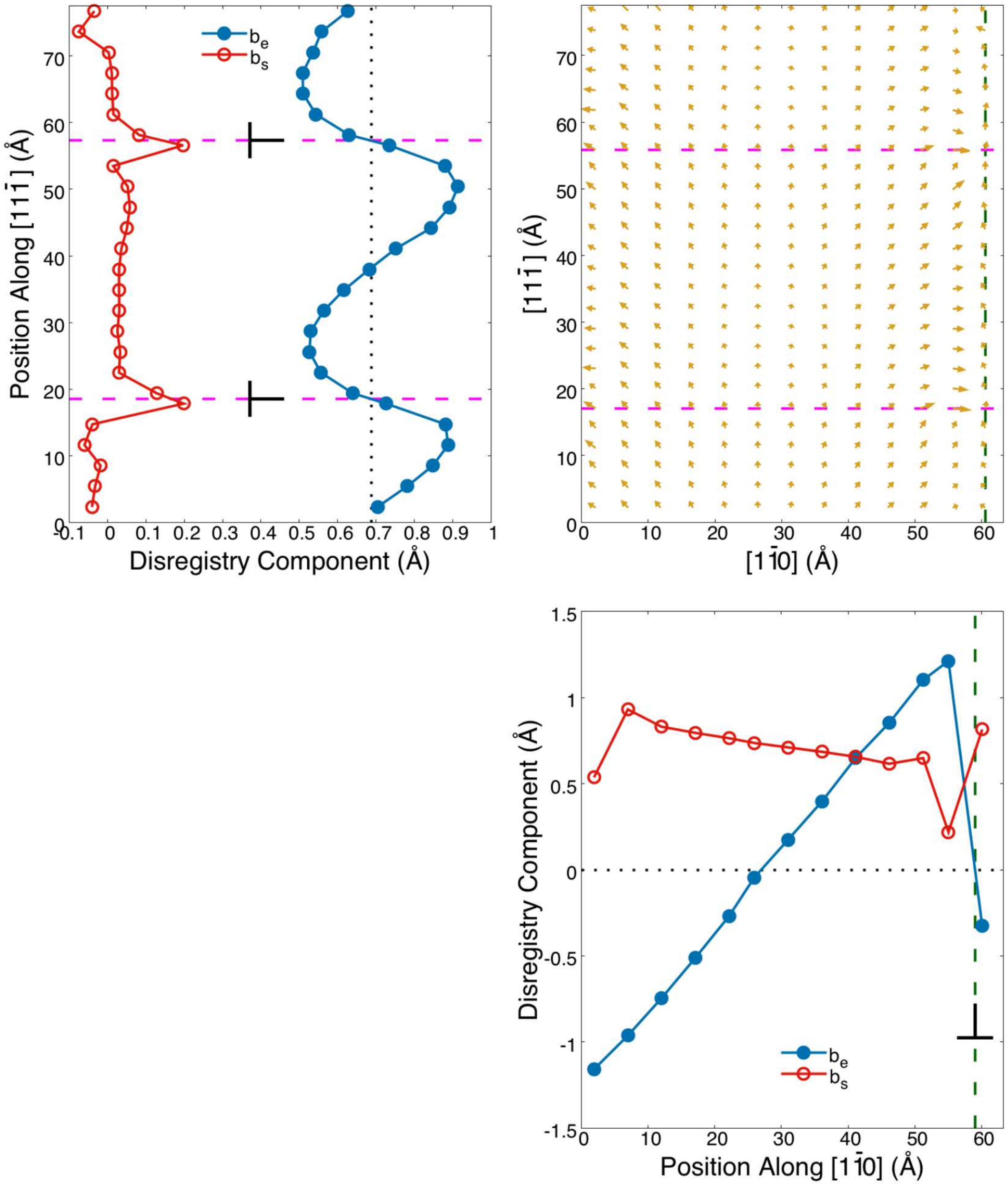
{111} disregistry analysis





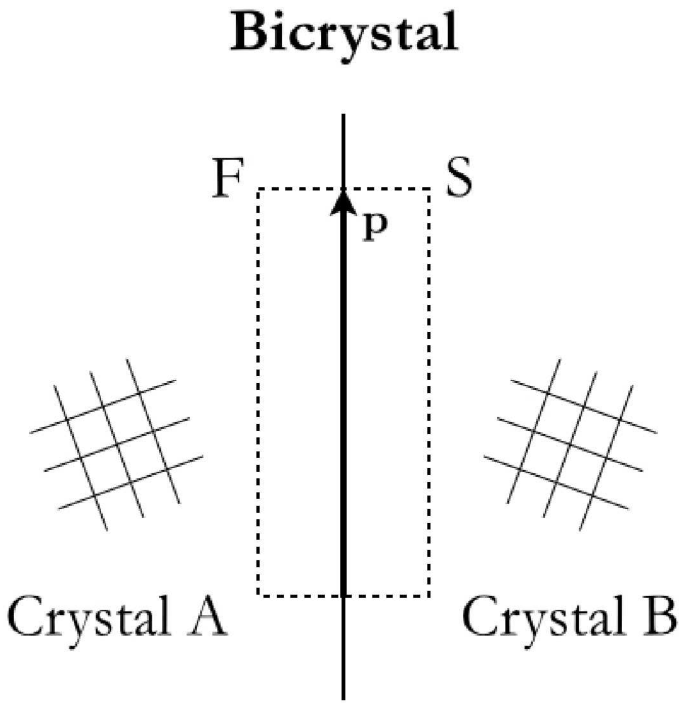


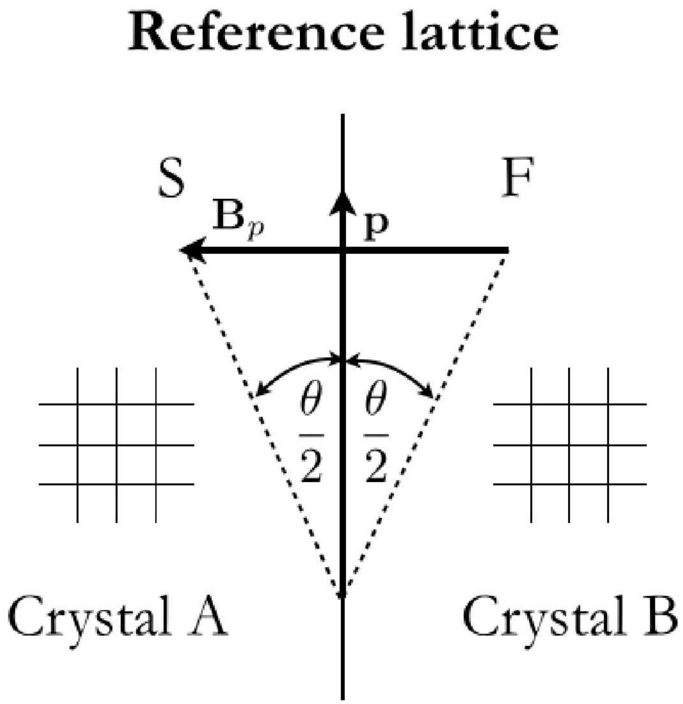
{112} disregistry analysis



Verification against quantized Frank-Bilby

$$(\mathbf{S}_a^{-1} - \mathbf{S}_b^{-1})\mathbf{p} = \sum_{i=1}^{N}\left(\frac{\mathbf{n} \times \xi_i}{d_i} \cdot \mathbf{p}\right)\mathbf{b}_i$$



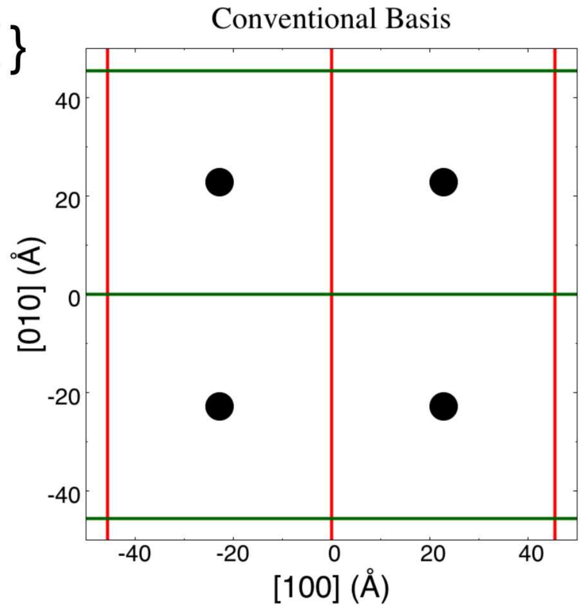


Quantized Frank-Bilby results

	$\boldsymbol{\xi}_1$	$d_1(\mathring{A})$	$\boldsymbol{\xi}_2$	$d_2(\mathring{A})$	$\boldsymbol{\xi}_3$	$d_3(\mathring{A})$
{001} DXA	$[010]$	43.7	$[100]$	43.7	-	-
{001} qFB Conventional	$[010]$	45.5	$[\bar{1}00]$	45.5	-	-
{001} qFB Primitive	$[00\bar{1}]$	45.5	$[01\bar{1}]$	32.17	$[010]$	45.5
{110} DXA	$[001]$	35.7	$[\bar{1}10]$	50.6	-	-
{110} qFB Conventional	$[001]$	74.2	$[00\bar{1}]$	74.2	$[\bar{1}10]$	52.5
{110} qFB Primitive	$[\bar{1}1\bar{1}]$	42.9	$[\bar{1}11]$	42.9	-	-
{111} DXA	$[11\bar{2}]$	66.7	$[\bar{1}2\bar{1}]$	66.7	$[\bar{2}11]$	66.7
{111} qFB Conventional	$[0\bar{1}1]$	60.0	$[10\bar{1}]$	60.0	$[\bar{1}10]$	60.0
{111} qFB Primitive	$[1\bar{1}0]$	60.0	$[01\bar{1}]$	60.0	$[\bar{1}01]$	60.0
{112} DXA	$[1\bar{1}0]$	37.8	$[11\bar{1}]$	61.8	-	-
{112} qFB Conventional	$[0\bar{2}1]$	49.8	$[20\bar{1}]$	49.8	$[\bar{1}10]$	78.8
{112} qFB Primitive	$[1\bar{1}0]$	39.4	$[11\bar{1}]$	64.3	$[\bar{1}\bar{1}1]$	64.3

Visualizing quantized Frank-Bilby results

{001}



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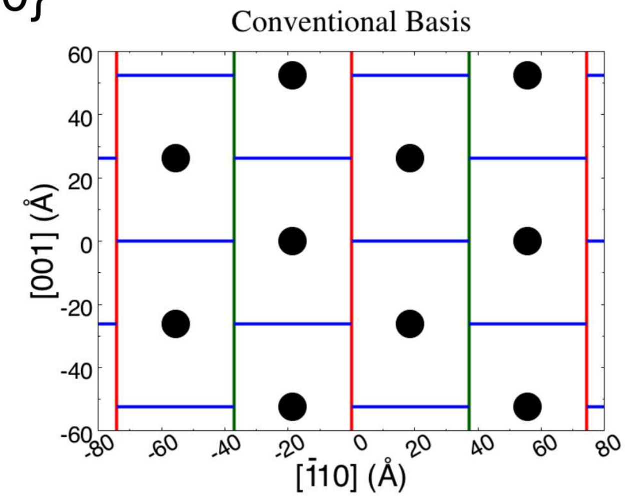

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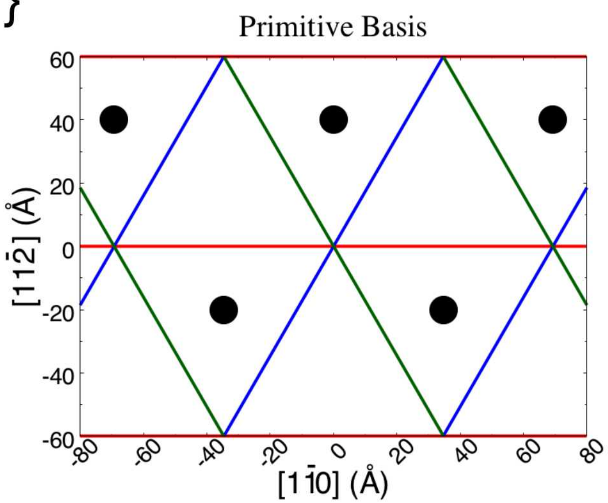

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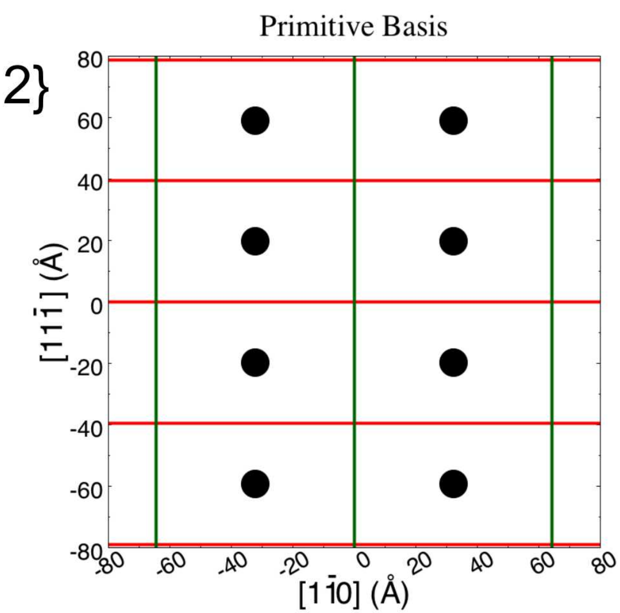
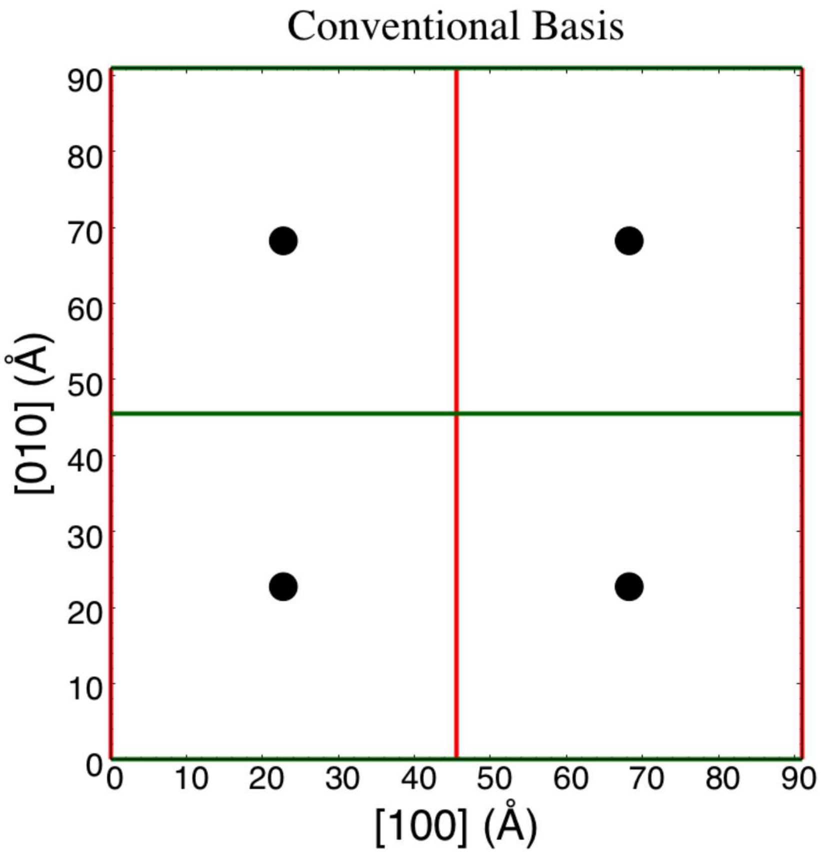
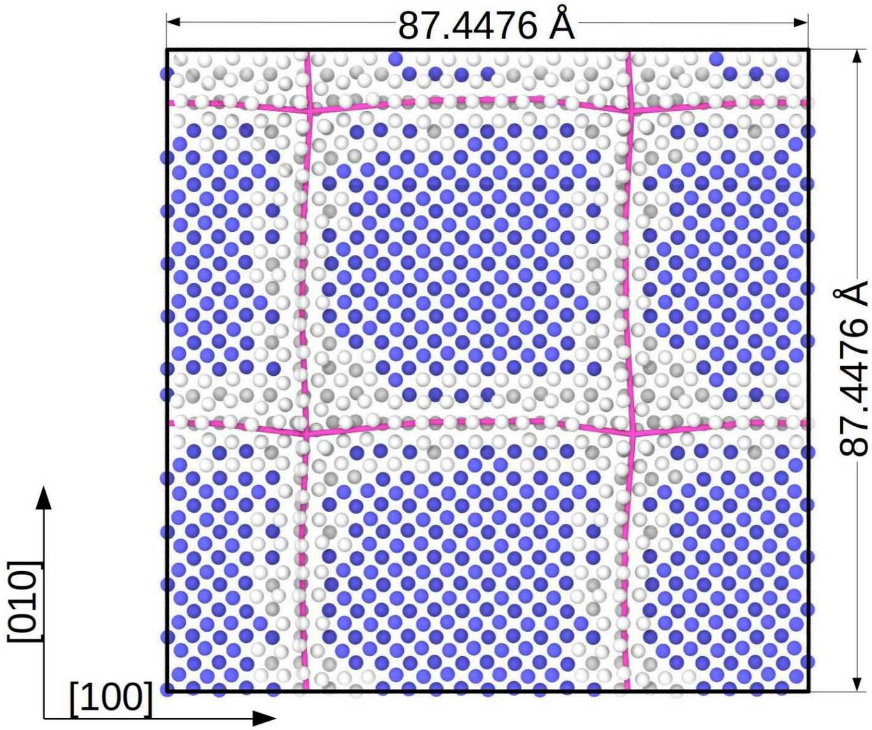
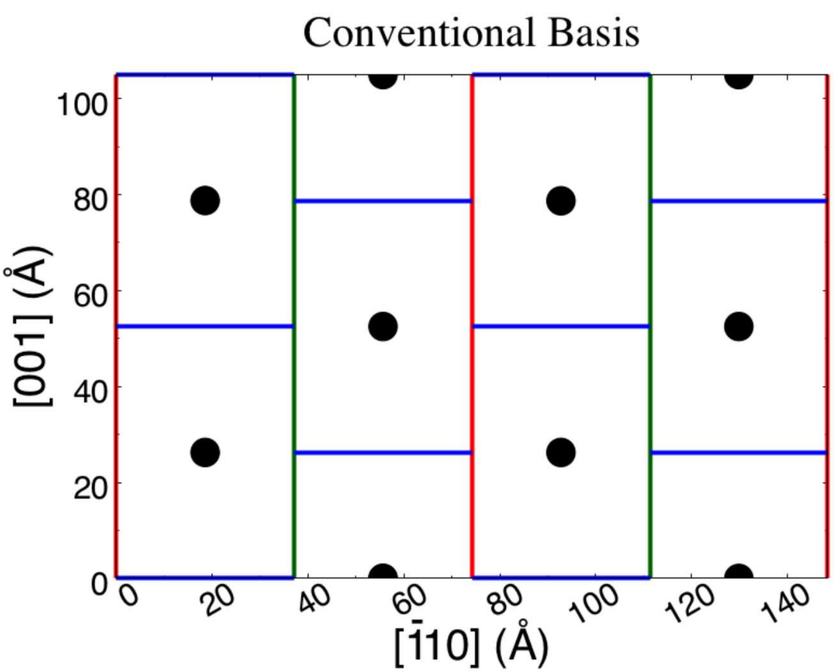


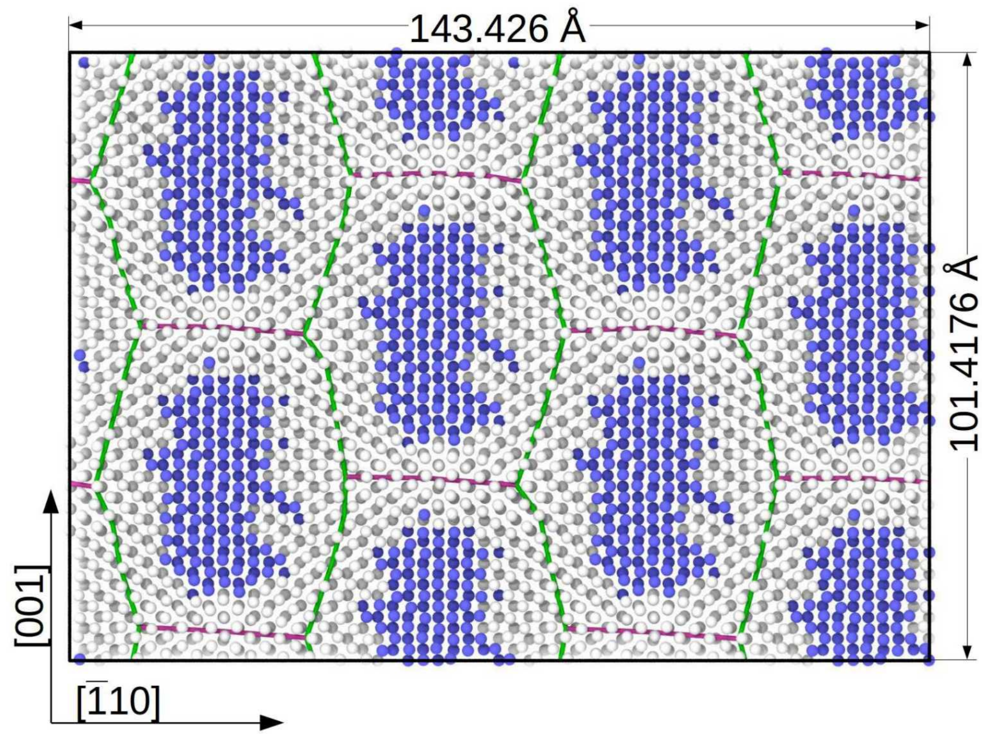
Comparing {001} dislocation network structures



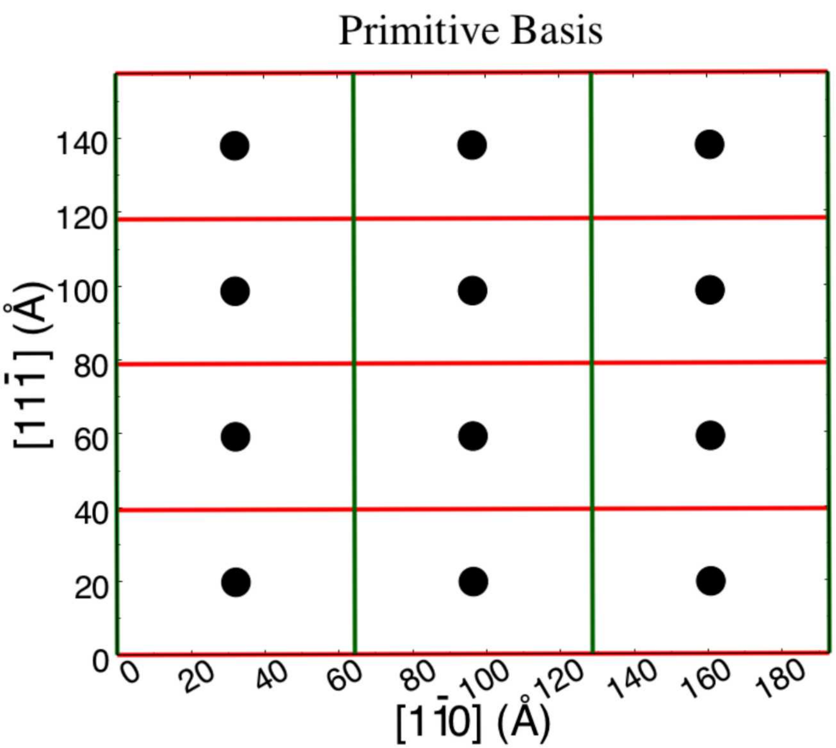


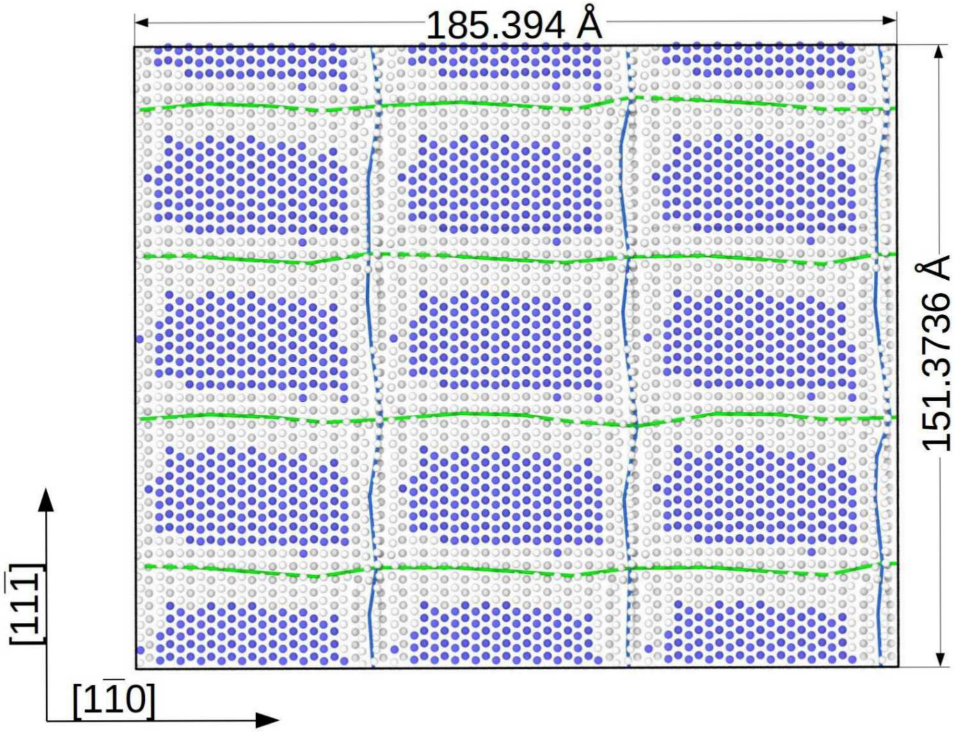
Comparing {110} dislocation network structures



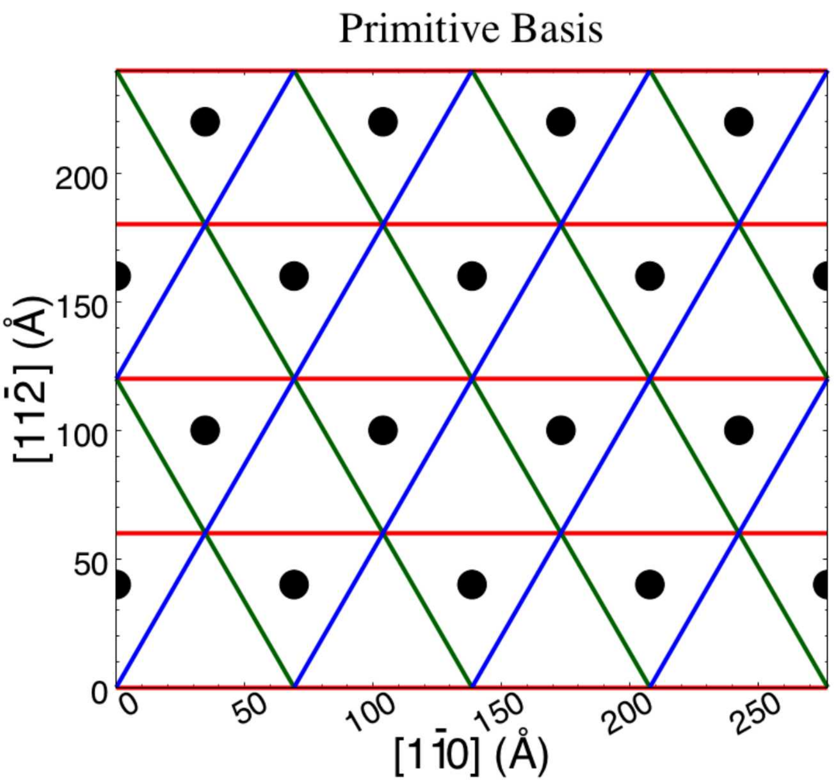


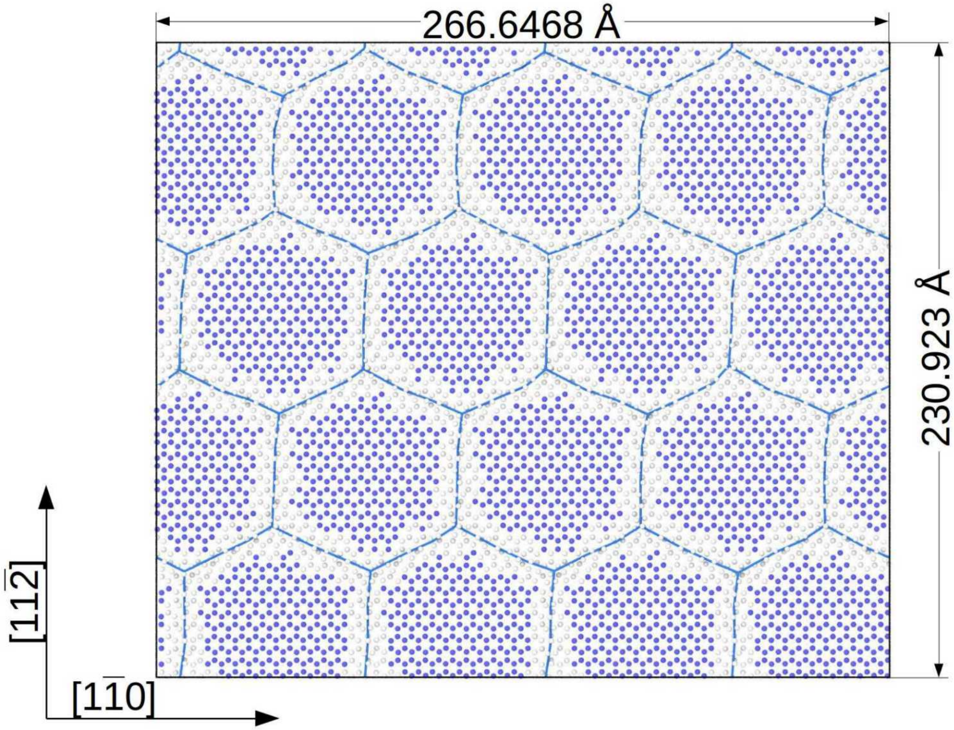
Comparing {112} dislocation network structures



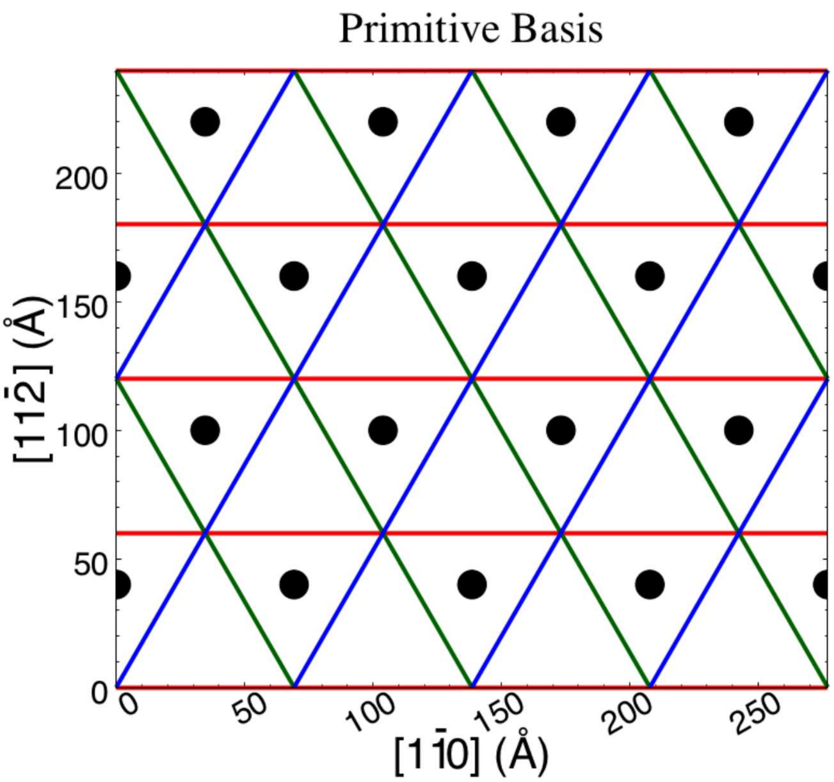


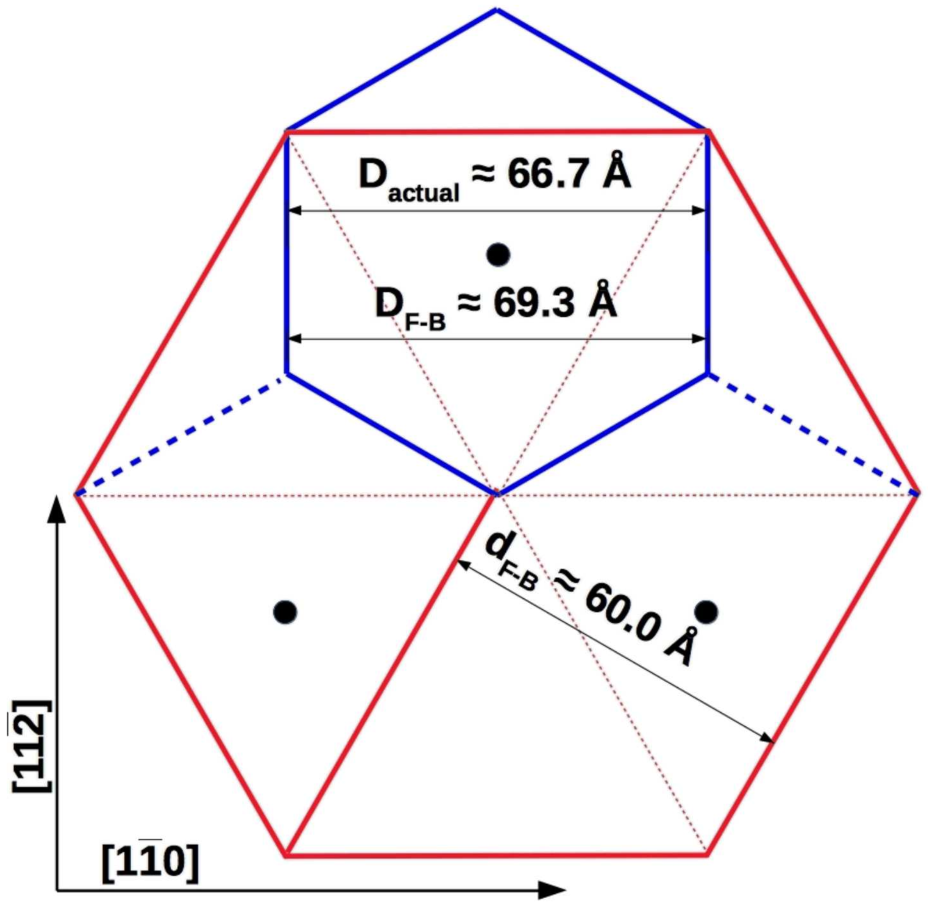
Comparing {111} dislocation network structures





{111} dislocation network deviations



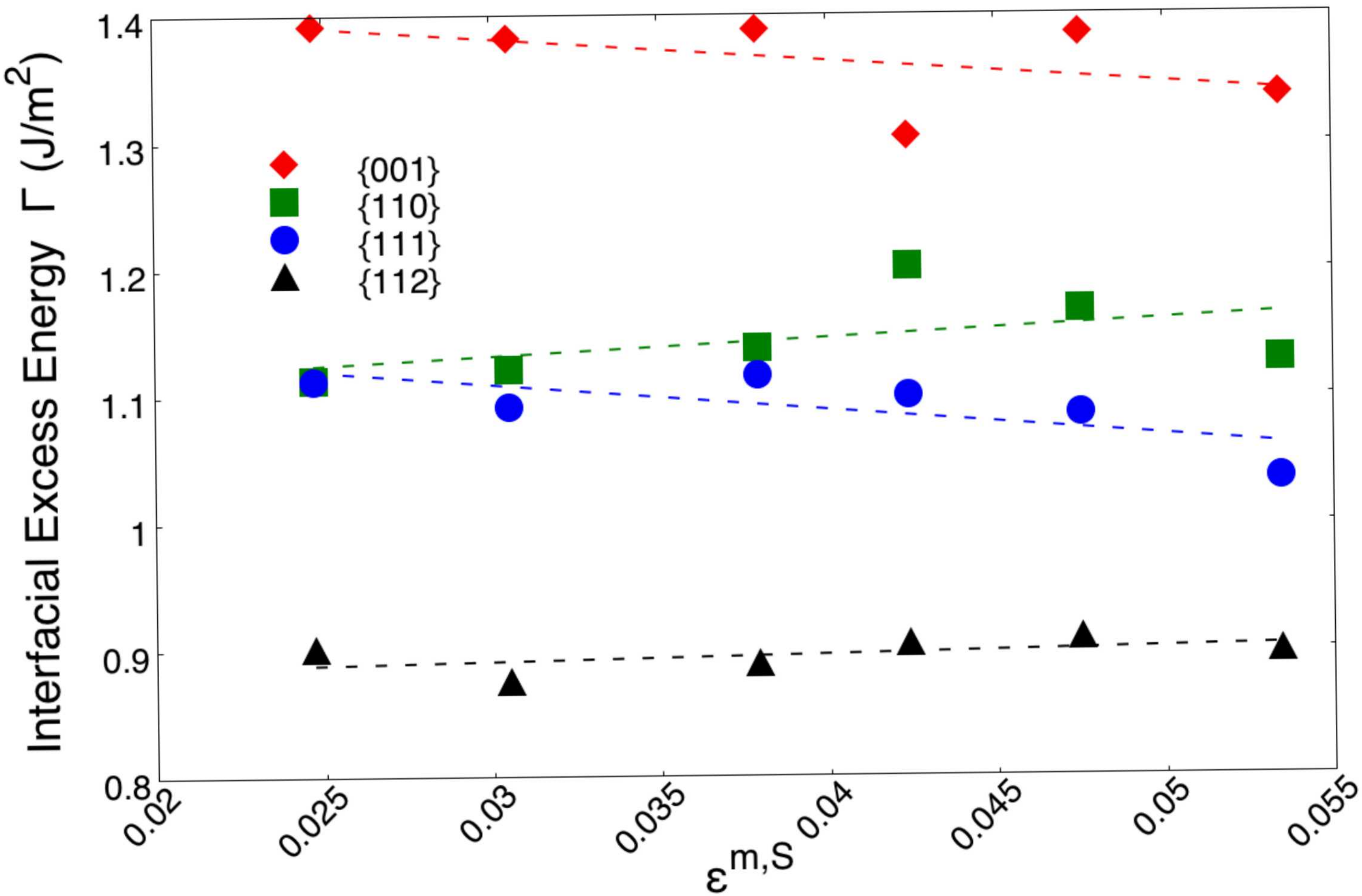


Mechanistic Effects of Defect Presence

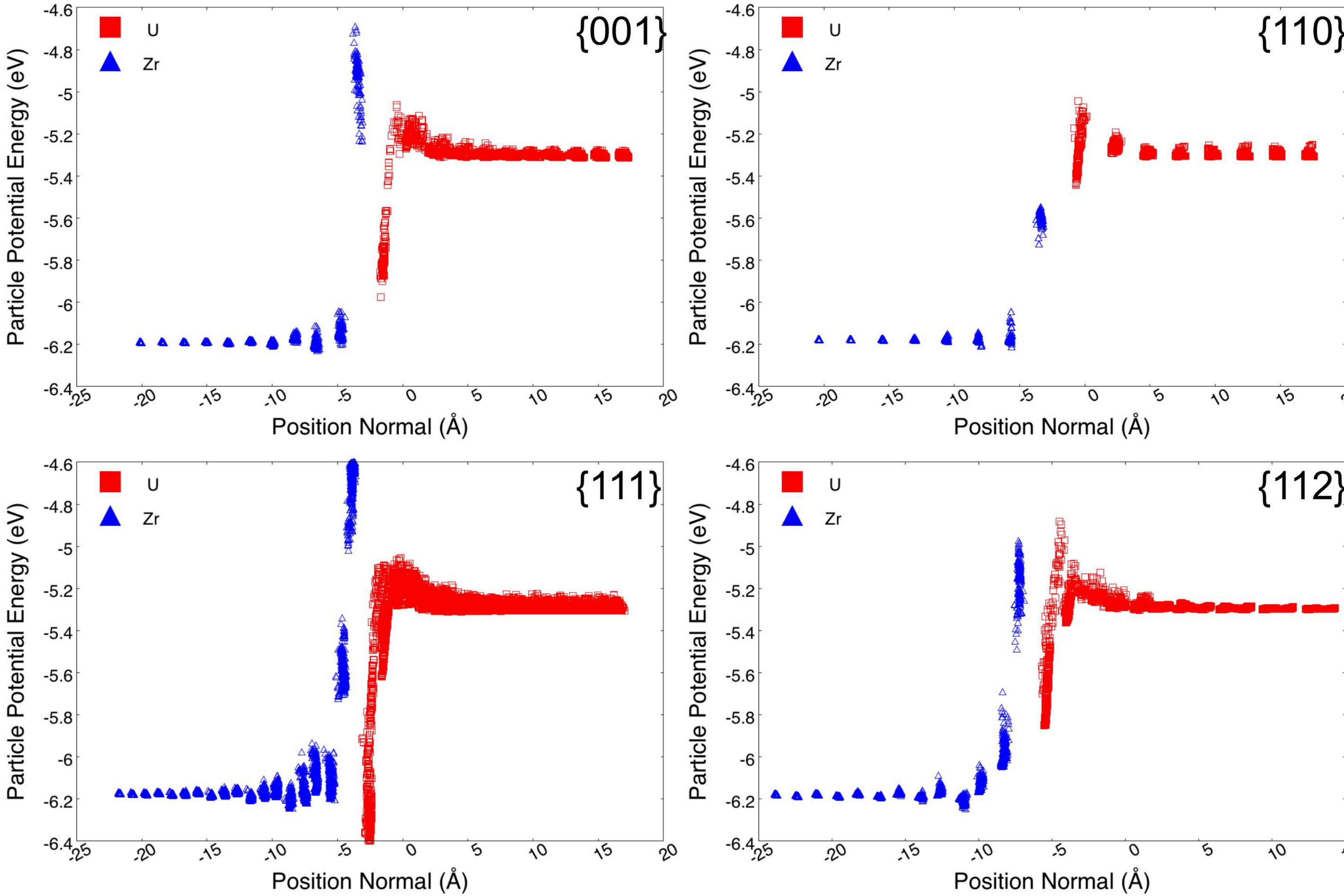
Interfacial Energetics & Elastic Fields

Interfacial excess energies at different defect contents

$$\Gamma = \frac{1}{2A}\left[\sum_{i=1}^{N_U}(e_U^i - e_U^{bulk}) + \sum_{i=1}^{N_{Zr}}(e_{Zr}^i - e_{Zr}^{bulk})\right]$$



Interfacial surface layer particle binding



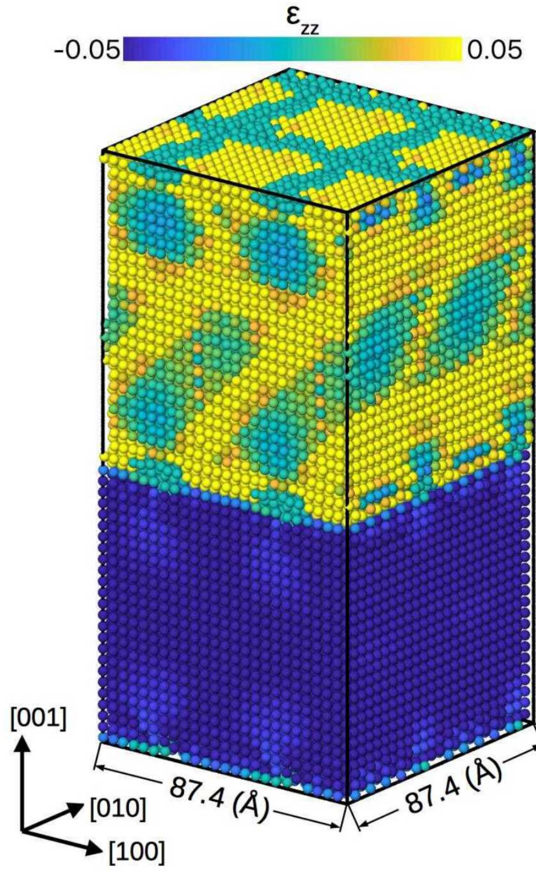
Dislocation presence generates elastic field

Per particle Eulerian-Almansi strain tensor

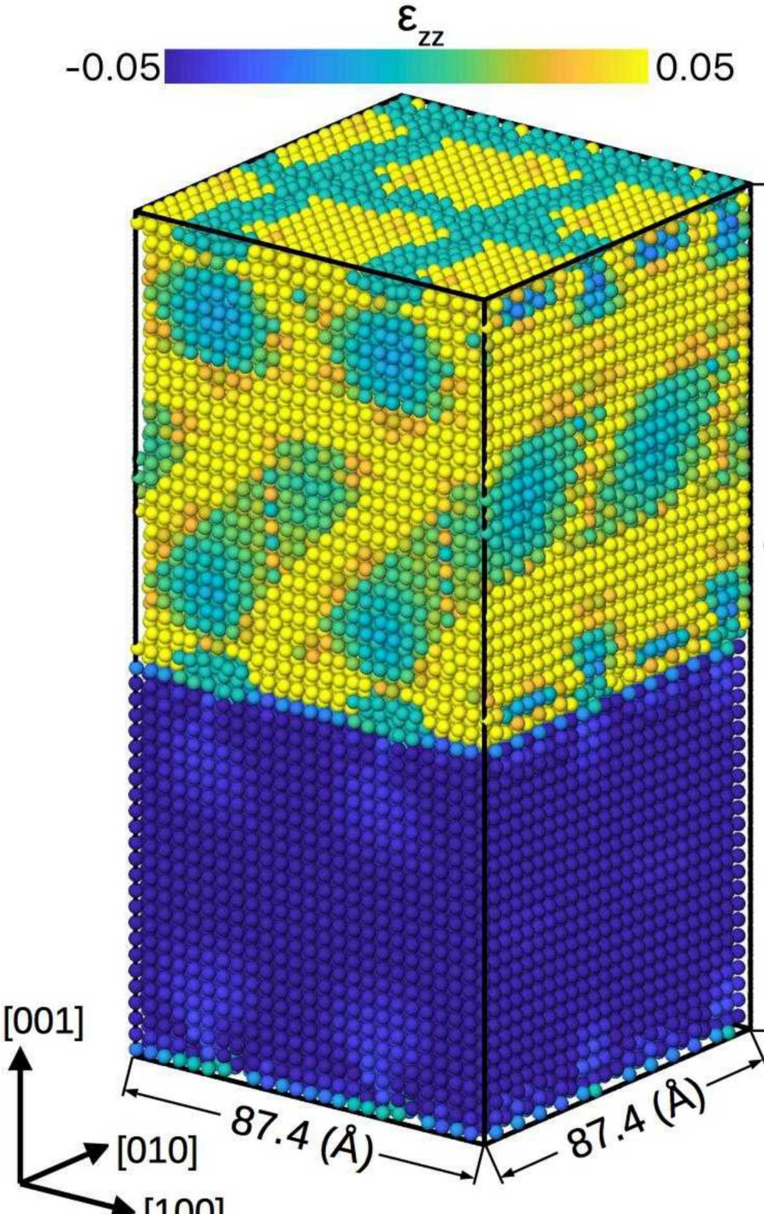
$$\mathbf{e} = \frac{1}{2}\left[\mathbf{I} - (\mathbf{F}^{\mathrm{e}})^{-\mathrm{T}}(\mathbf{F}^{\mathrm{e}})^{-1}\right]$$

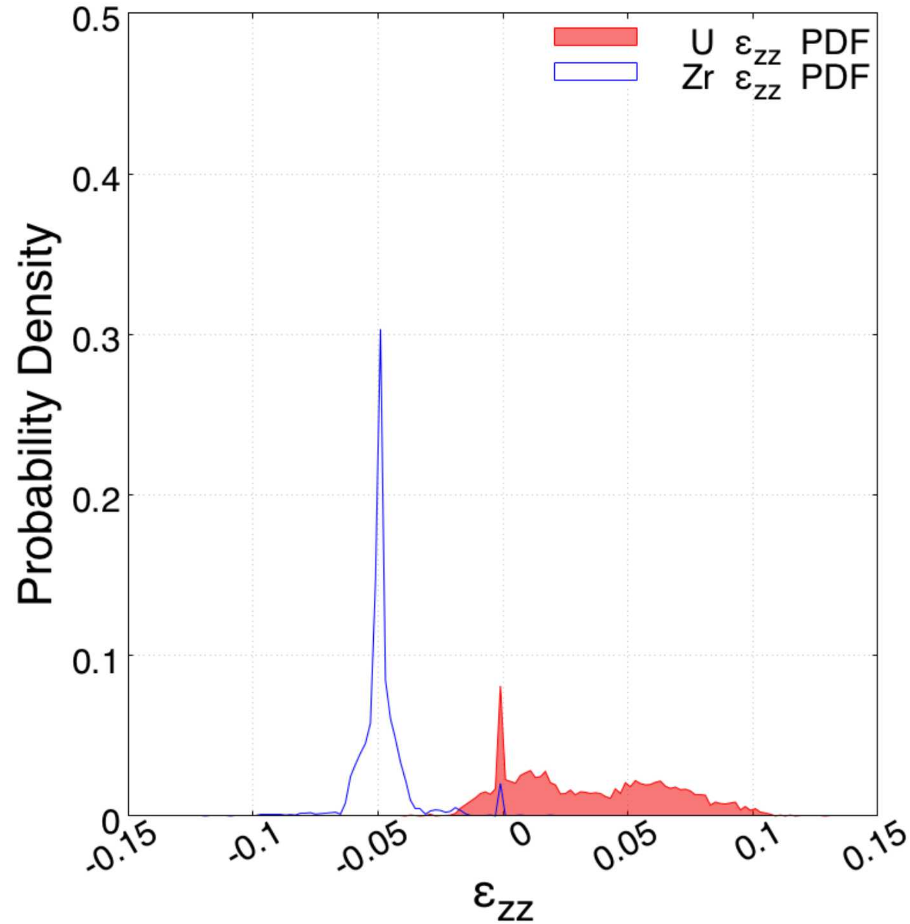
$$\mathbf{e} = \varepsilon, \quad \omega = 0$$

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \boxed{\varepsilon_{zz}} \end{bmatrix}$$

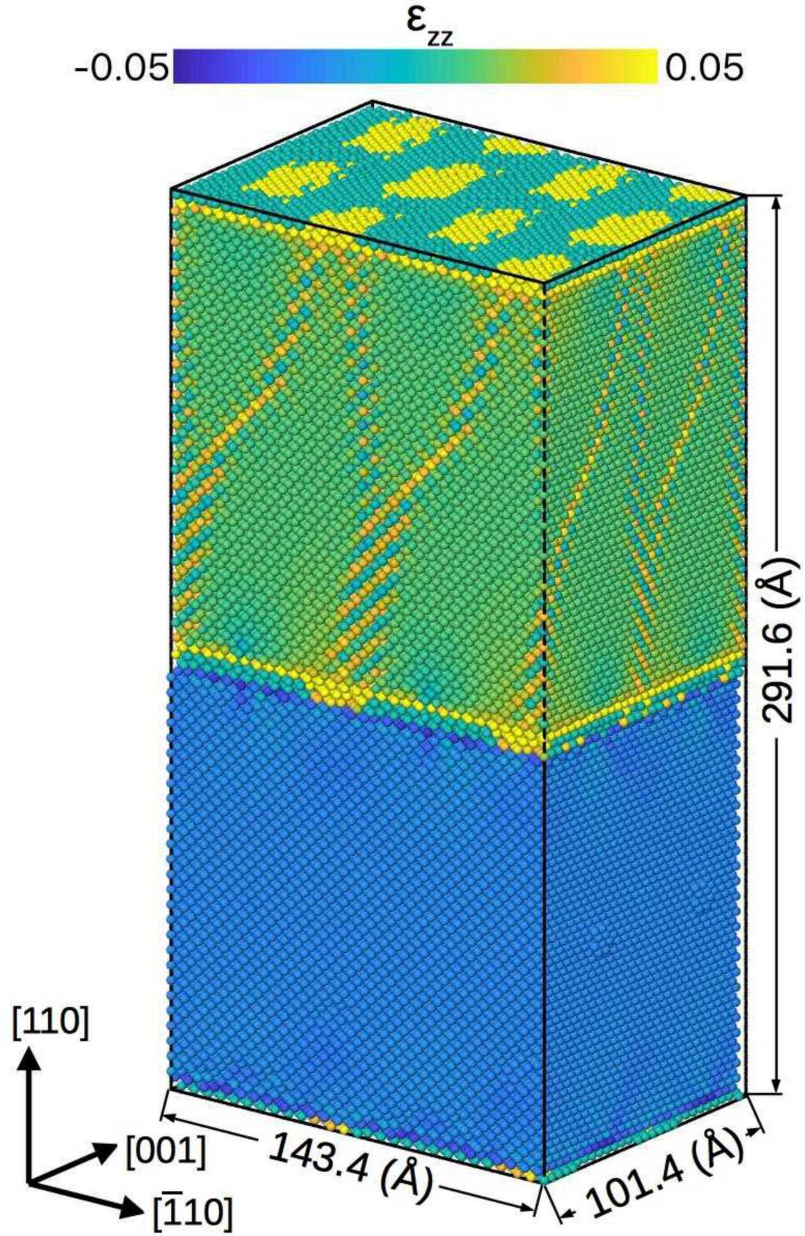


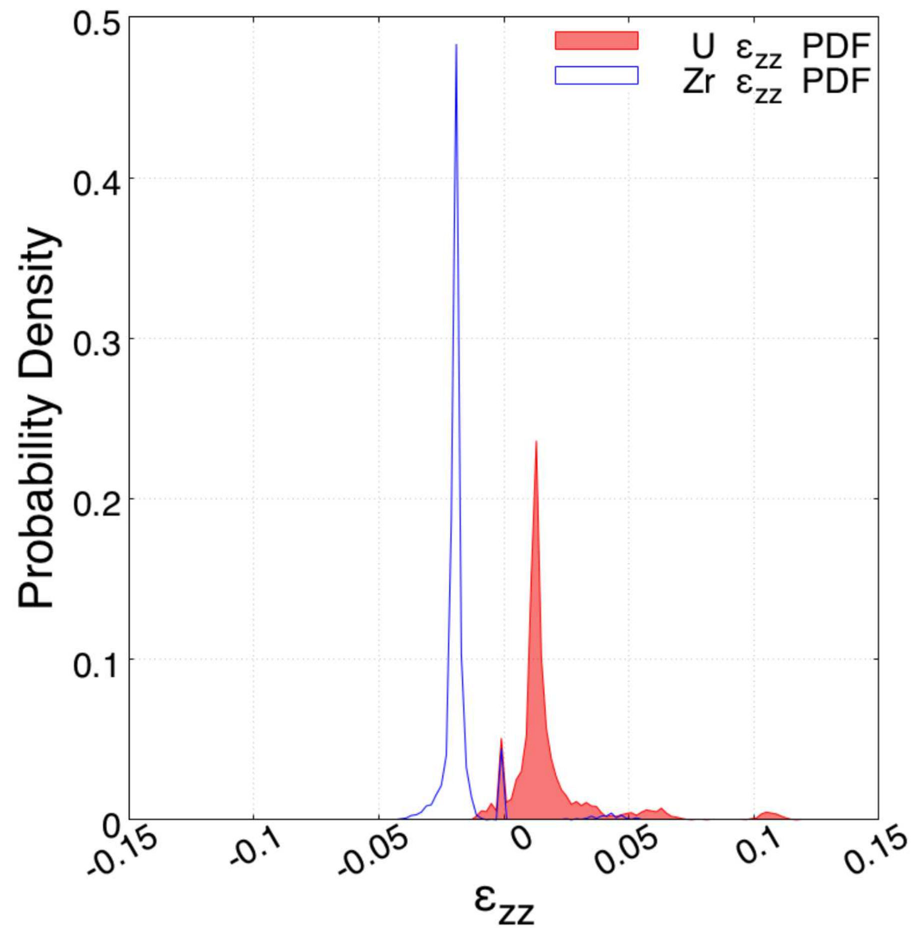
{001} residual strain field



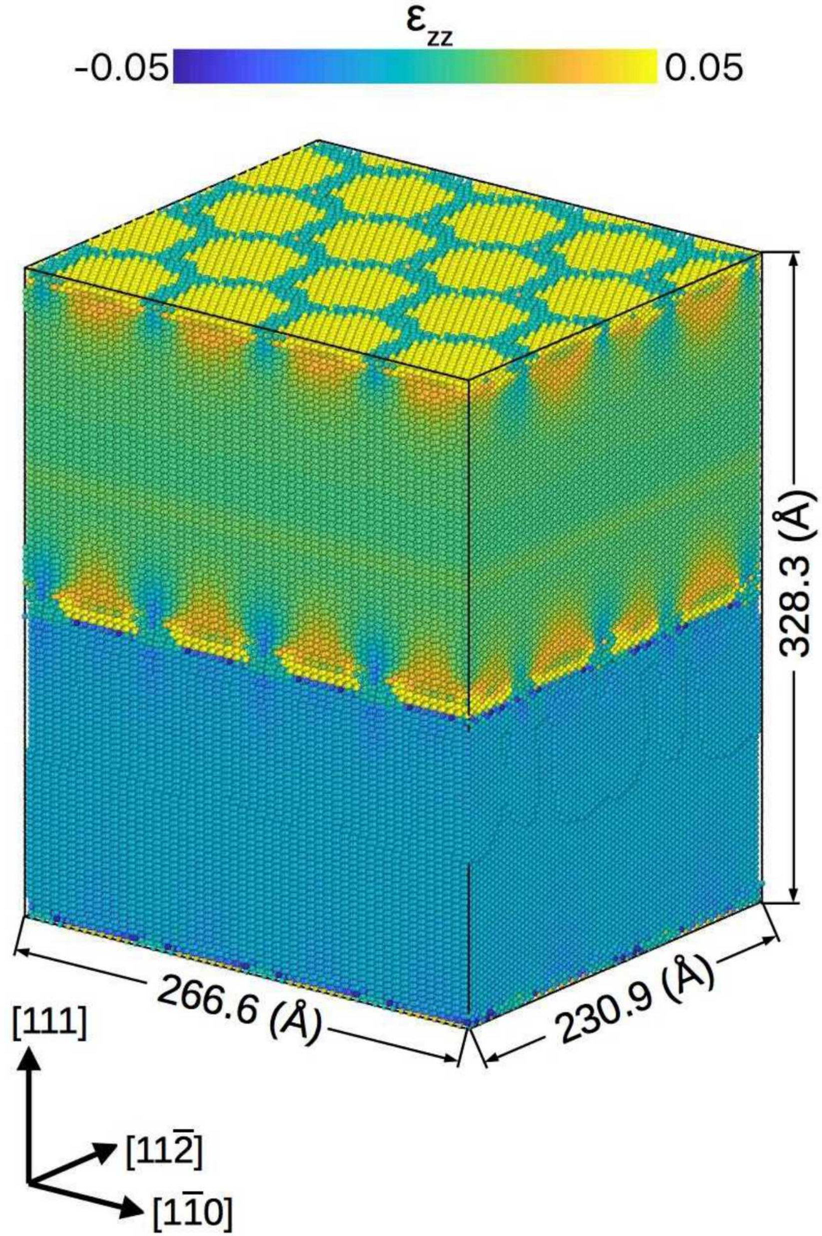


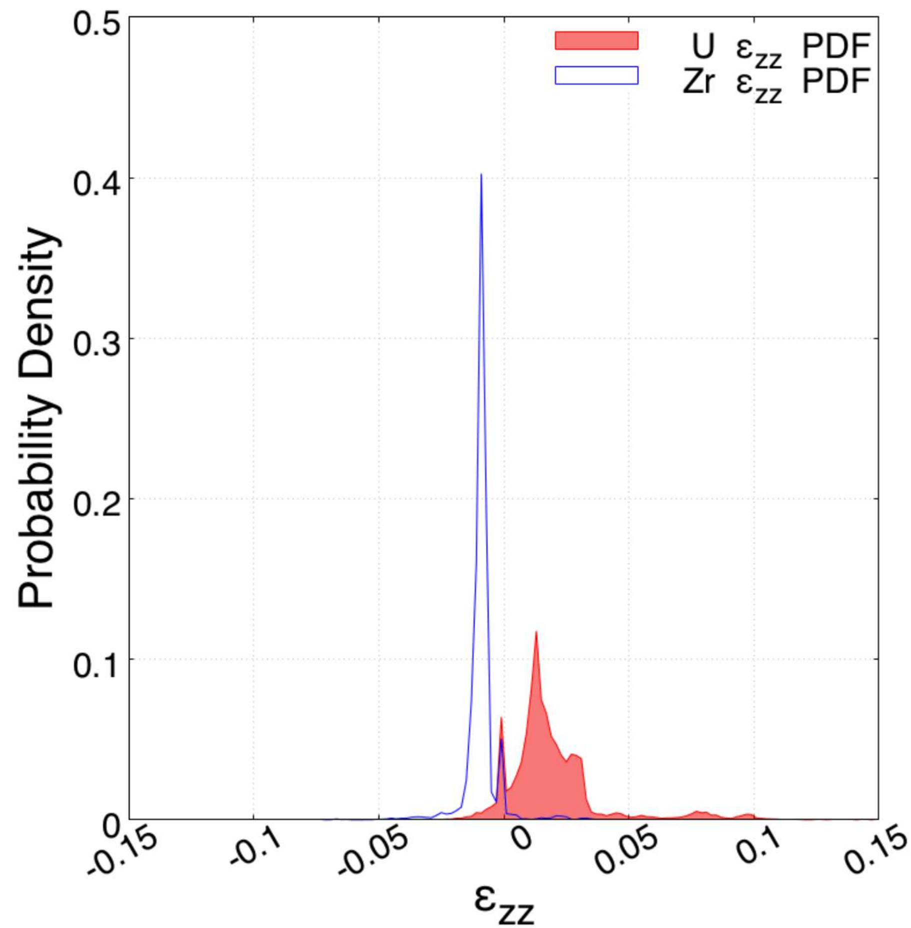
{110} residual strain field



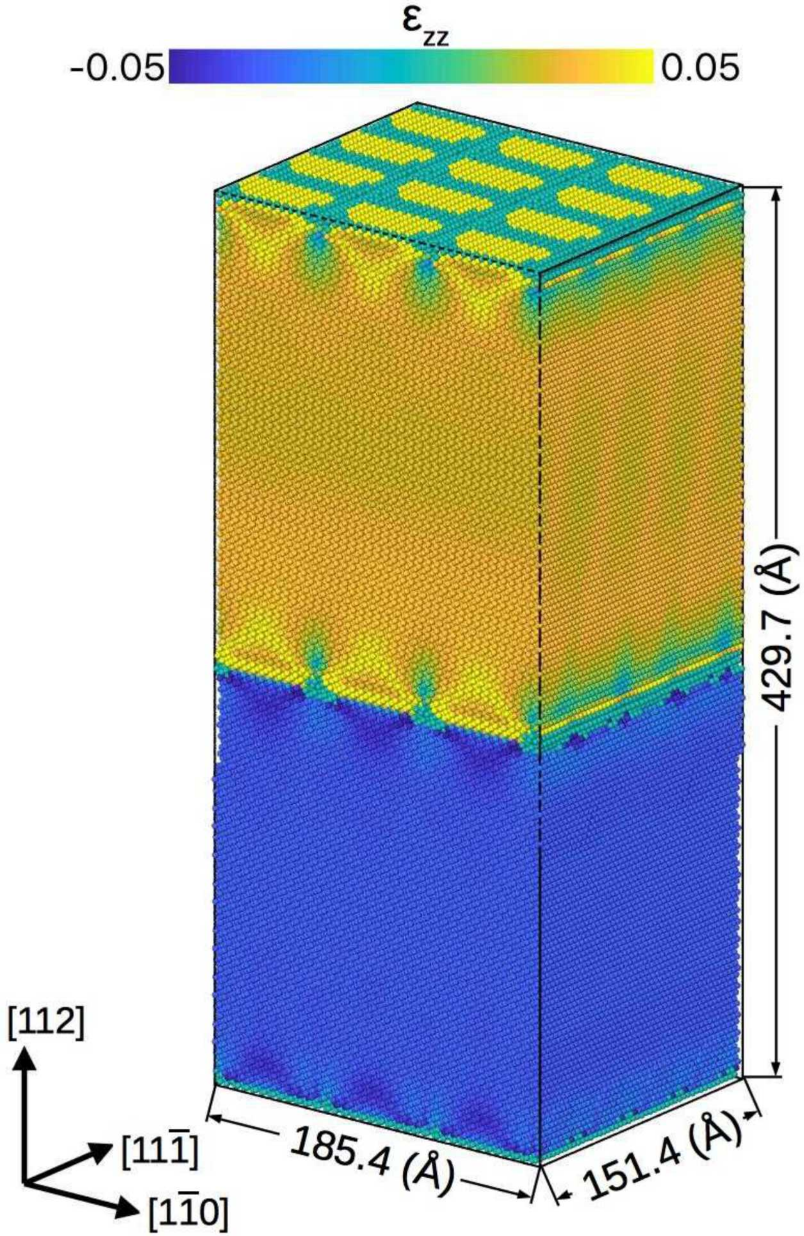


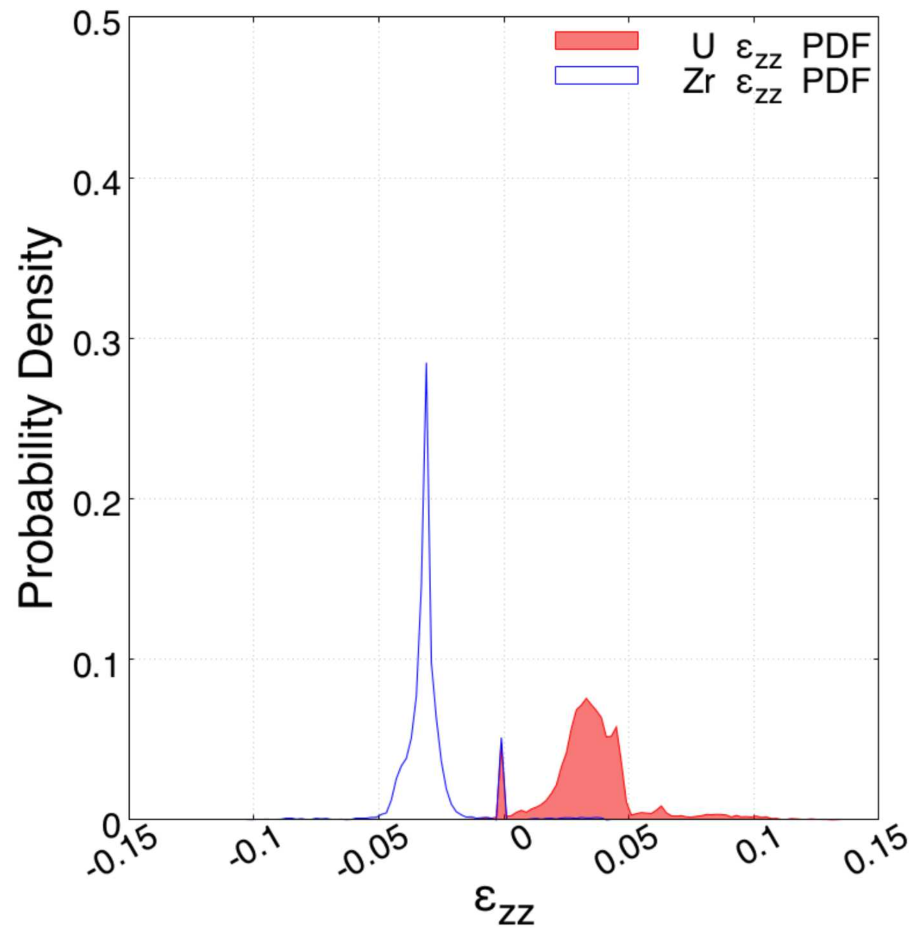
{111} residual strain field





{112} residual strain field





Conclusion

- Constructed various misfit stacking phase boundaries
- Identified & verified characteristic interfacial defect structures
- Examined mechanistic effects of dislocation networks
  - Interfacial excess energies
  - Residual strain fields

- Adapt phase boundary models to intergranular fracture
- Link boundary features to decohesion crack growth