

Continuum theory of crystalline defects and mechanical fields

Lecture: Field disclination mechanics and applications to interfacial defects in crystalline materials

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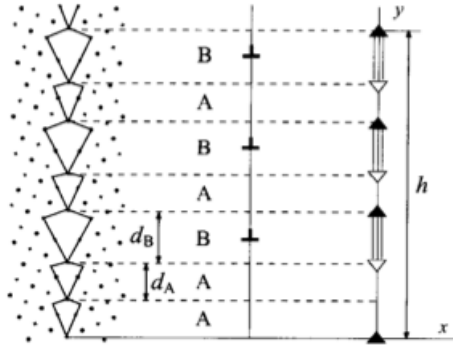
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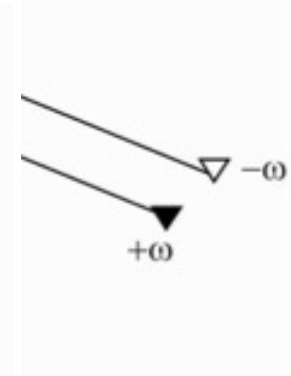
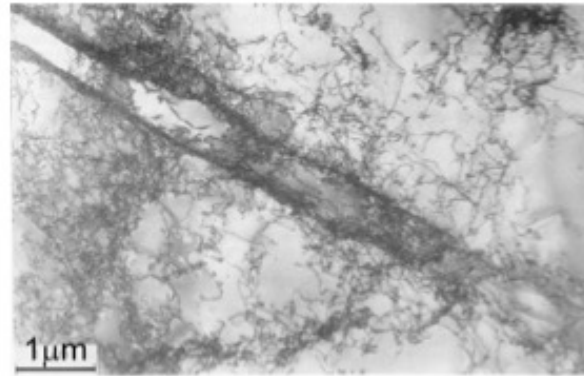
Elastic fields of disclinations seen as interfacial defects

Grain boundaries, GB defects,
Nanocrystalline metals,...



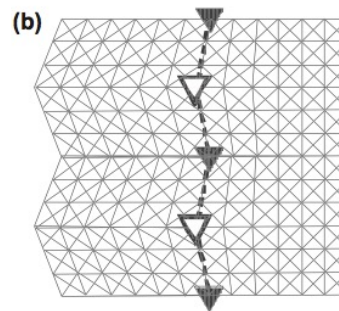
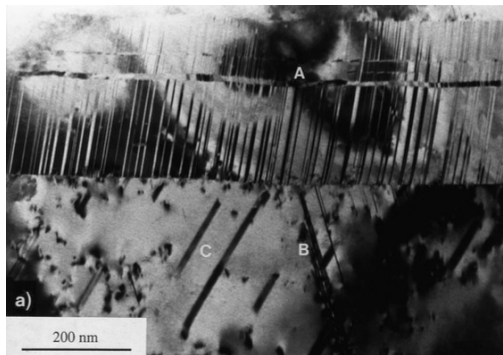
V. Yu. Gertsman et al. *Philos. Mag. A* 59 (1989)

Misorientation bands, micro bands,...



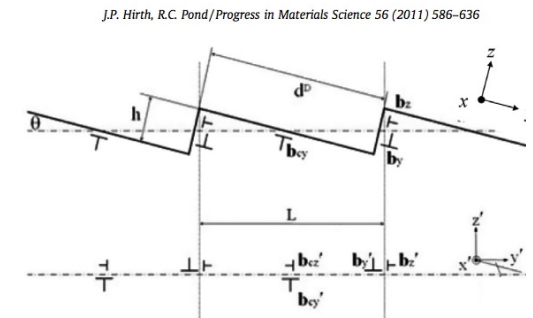
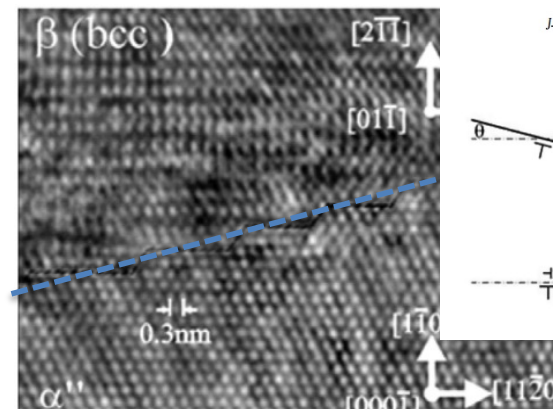
A.E. Romanov, A.L. Kolesnikova.
Prog. Mater. Sci (2009)

Twin boundaries and twin junctions



P. Müllner, A.H. King,
Acta Mater (2010)

GB terrace disconnection defects



J.P. Hirth, et al. *Acta Mater* (2006)

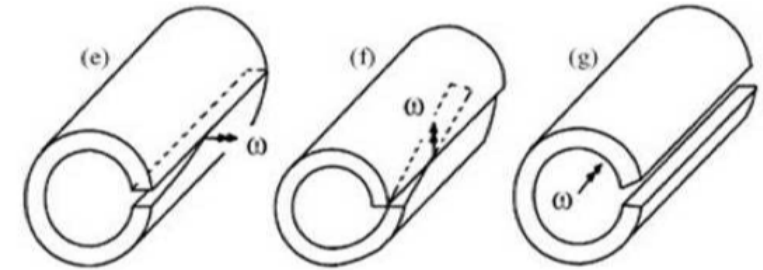
Outline

- Continuous theory of disclinations: field equations
- Spectral-based approach and applications
- Disclination mechanics within a couple stress theory
- References

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Kinematics of disclinations

- Discontinuity of rotation along a closed circuit C (and surface S inside it): Frank's vector Ω



V. Volterra, Ann. Sci. Ec. Norm. Sup. III 24, 401 (1907)

$$\left[\vec{\omega} \right] = \Omega = \int_C \kappa_e \cdot d\mathbf{x} = \int_S \text{curl} \kappa_e \cdot \mathbf{n} dS = \int_S \theta \cdot \mathbf{n} dS$$

$$\mathbf{b} = \int_C (\varepsilon_e - \kappa_e \times \mathbf{x}) \cdot d\mathbf{x} = \int_S (\alpha - \theta \times \mathbf{x}) \cdot \mathbf{n} dS$$

Anthony (1970), DeWit (1970, 1973)
Kossecka and DeWit (1977)
Fressengeas et al. (2011)

- Incompatibility of elastic curvature κ_e : $\theta = \text{curl} \kappa_e$
with $\text{div} \alpha + 2\vec{\theta} = 0$
- Incompatibility of elastic strain ε_e : $\text{curl} \varepsilon_e + \text{tr}(\kappa_e) \mathbf{I} - \kappa_e^t = \alpha$
- Elastic rotation tensor is multi-valued (undefined)

Elasto-static fields equations for defects in heterogeneous materials

- Stokes-Helmholtz decomposition Field Disclination Mechanics

$$\boldsymbol{\kappa}_e = \boldsymbol{\kappa}_e^\perp + \boldsymbol{\kappa}_e^{//} \quad \text{and}$$

Berbenni and Taupin (2018)

$$\boldsymbol{\varepsilon}_e = \boldsymbol{\varepsilon}_e^\perp + \boldsymbol{\varepsilon}_e^{//}$$

- Poisson-type equation for incompatible elastic fields

$$\Delta \boldsymbol{\kappa}_e^\perp = -\mathbf{curl} \, \boldsymbol{\theta}$$

$$\Delta \boldsymbol{\varepsilon}_e^\perp = -\mathbf{curl} \left(\alpha - \text{tr}(\boldsymbol{\kappa}_e^\perp) \mathbf{I} + \boldsymbol{\kappa}_e^{\perp t} \right)$$

- Lippmann-Schwinger integral equation for compatible elastic strain

$$\varepsilon_{ij}^{e,||}(\mathbf{x}) = \langle \varepsilon^{e,||} \rangle_{ij} - \int_V \Gamma_{ijkl}^0(\mathbf{x} - \mathbf{x}') \tau_{kl}(\mathbf{x}') dV' \quad \text{with} \quad \begin{cases} \tau_{ij} = T_{ij}^\perp + \delta C_{ijkl} \varepsilon_{kl}^{e,||} \\ T_{ij}^\perp = C_{ijkl} \varepsilon_{kl}^{e,\perp} \end{cases}$$

- Continuous theory of disclinations: field equations
- **Spectral-based approach and applications**
- Disclination mechanics within a couple stress theory
- References

Spectral approach of elasto-static field equations

- Incompatible fields: Field Dislocation and Disclination Mechanics

$$\begin{cases} \tilde{\mathbf{K}}_{ij}^{e,\perp}(\xi) = \frac{i}{\xi^2} \xi_k \left(\mathbf{e}_{jkl} \tilde{\theta}_{il}(\xi) \right) & \forall \xi \neq \mathbf{0} \\ \tilde{\mathbf{K}}_{ij}^{e,\perp}(\mathbf{0}) = \mathbf{0} \end{cases} \quad \text{Berbenni and Taupin (2018)}$$

$$\begin{cases} \tilde{\boldsymbol{\varepsilon}}_{ij}^{e,\perp}(\xi) = \frac{i}{\xi^2} \xi_k \mathbf{e}_{jkl} \left(\tilde{\alpha}_{il}(\xi) + \tilde{\mathbf{K}}_{li}^{e,\perp}(\xi) - \delta_{il} \tilde{\mathbf{K}}_{pp}^{e,\perp}(\xi) \right) & \forall \xi \neq \mathbf{0} \\ \tilde{\boldsymbol{\varepsilon}}_{ij}^{e,\perp}(\mathbf{0}) = \mathbf{0} \end{cases}$$

- Lippmann-Schwinger-type equation with incompatibilities:

$$\boldsymbol{\varepsilon}_{ij}^{e,\parallel}(\mathbf{x}) = \langle \boldsymbol{\varepsilon}^{e,\parallel} \rangle_{ij} - \int_V \Gamma_{ijkl}^0(\mathbf{x} - \mathbf{x}') \tau_{kl}(\mathbf{x}') dV' \quad \Rightarrow$$

$$\begin{cases} \tilde{\boldsymbol{\varepsilon}}^{e,\parallel}(\xi) = -\tilde{\Gamma}^0(\xi) : \boldsymbol{\tau}(\xi) & \forall \xi \neq \mathbf{0} \\ \tilde{\boldsymbol{\varepsilon}}^{e,\parallel}(\mathbf{0}) = \langle \boldsymbol{\varepsilon}^{e,\parallel} \rangle \end{cases}$$

$$\tilde{\Gamma}_{ijkl}^0(\xi) = \frac{1}{4} \left(\tilde{G}_{ik}^0(\xi) \xi_l \xi_j + \tilde{G}_{jk}^0(\xi) \xi_l \xi_i + \tilde{G}_{il}^0(\xi) \xi_k \xi_j + \tilde{G}_{jl}^0(\xi) \xi_k \xi_i \right)$$

$$\begin{cases} \tilde{G}_{ik}^0(\xi) = \left(\xi_j C_{ijkl}^0 \xi_l \right)^{-1} & \forall \xi \neq \mathbf{0} \\ \tilde{G}_{ik}^0(\mathbf{0}) = \mathbf{0} \end{cases}$$

- Iterative scheme to solve Lippmann-Schwinger equation using FFT

FFT-based algorithm

Initialization (θ, α being known)

- 1: $\tilde{\theta} \leftarrow \text{FFT}(\theta) \quad \tilde{\alpha} \leftarrow \text{FFT}(\alpha)$
- 2: Solve 1st Poisson's equation to obtain $\tilde{\mathbf{K}}^{e,\perp}$

$$\begin{cases} \tilde{\mathbf{K}}_{ij}^{e,\perp}(\xi) = \frac{i}{\xi^2} \xi_k \left(\mathbf{e}_{jkl} \tilde{\theta}_{il}(\xi) \right) & \forall \xi \neq 0 \\ \tilde{\mathbf{K}}_{ij}^{e,\perp}(0) = 0 \end{cases}$$
- 3: Solve 2nd Poisson's equation to obtain $\tilde{\boldsymbol{\varepsilon}}^{e,\perp}$

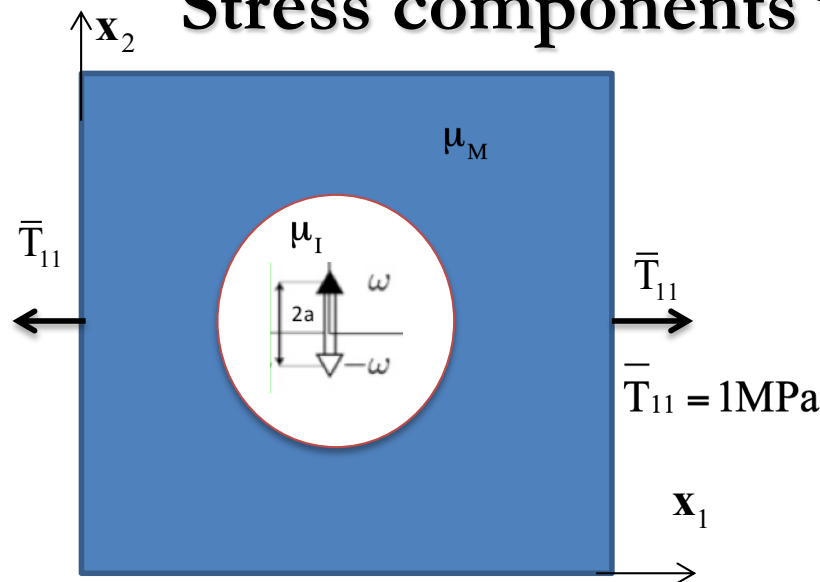
$$\begin{cases} \tilde{\varepsilon}_{ij}^{e,\perp}(\xi) = \frac{i}{\xi^2} \xi_k \mathbf{e}_{jkl} \left(\tilde{\alpha}_{il}(\xi) + \tilde{\mathbf{K}}_{li}^{e,\perp}(\xi) - \delta_{il} \tilde{\mathbf{K}}_{pp}^{e,\perp}(\xi) \right) \\ \forall \xi \neq 0 & \tilde{\varepsilon}_{ij}^{e,\perp}(0) = 0 \end{cases}$$
- 4: $\boldsymbol{\varepsilon}^{e,\perp} \leftarrow \text{FFT}^{-1}(\tilde{\boldsymbol{\varepsilon}}^{e,\perp})$
- 5: $\mathbf{T}^\perp \leftarrow \mathbf{C} : \boldsymbol{\varepsilon}^{e,\perp}$
- 6: $\boldsymbol{\varepsilon}_0^{e,\parallel} \leftarrow \langle \boldsymbol{\varepsilon}^{e,\parallel} \rangle = \mathbf{C}^{0^{-1}} : \bar{\mathbf{T}}$
- 7: $\mathbf{T}_0 \leftarrow \mathbf{C} : \boldsymbol{\varepsilon}_0^{e,\parallel} + \mathbf{T}^\perp$

Iteration n+1: ($\mathbf{T}_n$ and $\boldsymbol{\varepsilon}_n^{e,\parallel}$ being known)

- 8: $\tilde{\mathbf{T}}_n = \text{FFT}(\mathbf{T}_n)$
- 9: Convergence test (stress equilibrium):

$$e_n = \frac{\|\mathbf{div}(\mathbf{T}_n)\|_2}{|\langle \mathbf{T}_n \rangle|} = \frac{\|\xi \cdot \tilde{\mathbf{T}}_n(\xi)\|_2}{|\tilde{\mathbf{T}}_n(0)|} \leq \epsilon$$
- 10: $\tilde{\boldsymbol{\tau}}_n(\xi) \leftarrow \tilde{\mathbf{T}}_n(\xi) - \overline{(\mathbf{C}^0 : \boldsymbol{\varepsilon}_n^{e,\parallel}(\xi))}$
- 11: $\tilde{\boldsymbol{\varepsilon}}_{n+1}^{e,\parallel}(\xi) \leftarrow -\tilde{\Gamma}^0(\xi) : \tilde{\boldsymbol{\tau}}_n(\xi) \quad \forall \xi \neq 0$
 $\tilde{\boldsymbol{\varepsilon}}_{n+1}^{e,\parallel}(0) \leftarrow \langle \boldsymbol{\varepsilon}^{e,\parallel} \rangle$
- 12: $\boldsymbol{\varepsilon}_{n+1}^{e,\parallel} \leftarrow \text{FFT}^{-1}(\tilde{\boldsymbol{\varepsilon}}_{n+1}^{e,\parallel}(\xi))$
- 13: $\mathbf{T}_{n+1} \leftarrow \mathbf{C} : \boldsymbol{\varepsilon}_{n+1}^{e,\parallel} + \mathbf{T}^\perp$

Application to wedge disclination dipoles: Stress components with a circular inhomogeneity



Rotation discontinuity (wedge disclination dipole, Frank pseudo-vector: $\pm\omega = \pm 5/6 \text{ rad}$)

Disclination densities (on 1 pixel)
(dipole at $x_2 = \pm a$): $\theta_{33}(\mathbf{x}) = \pm\omega / \delta^2$

Mesh: 1024×1024 pixels

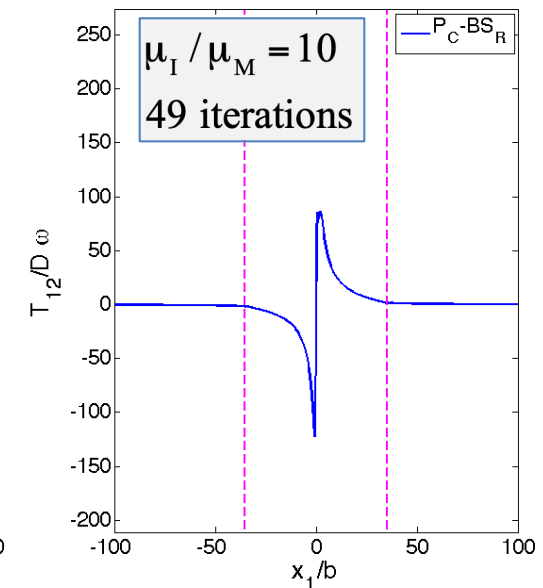
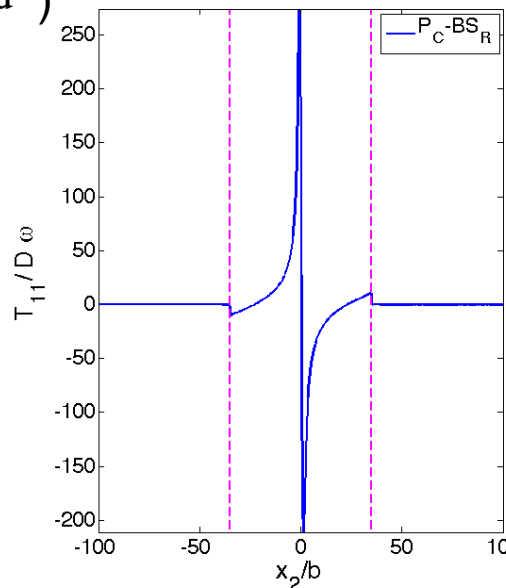
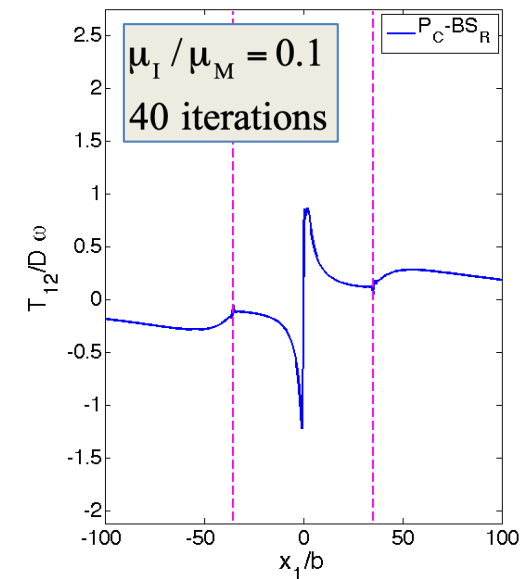
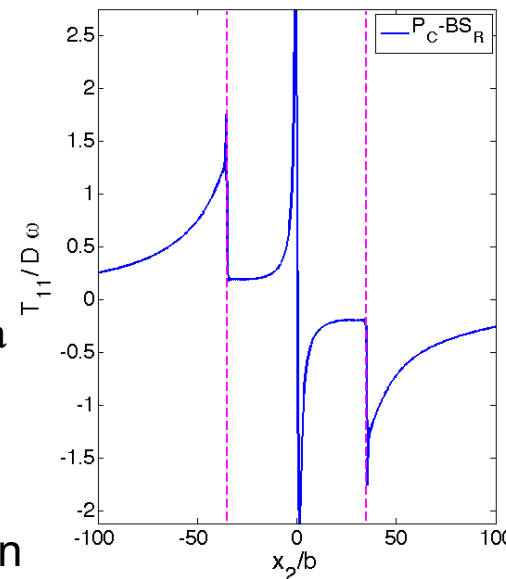
Pixel size: $\delta_1 = \delta_2 = \delta \simeq 0.44b$

Inclusion radius: $R = 80\delta$

$\mu_M = 2.3001 \times 10^3 \text{ MPa}$; $\nu_M = \nu_I = 0.3647$

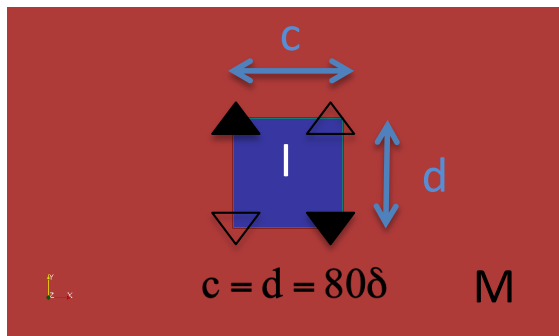
$\mu_0 = 0.505(\mu_M + \mu_I)$; $D = \frac{\mu_M}{2\pi(1-\nu_M)}$
 $\varepsilon = 10^{-6}$

Convergence criteria:



Application to nanotwin modeled as wedge disclination quadrupole

Squared inclusion



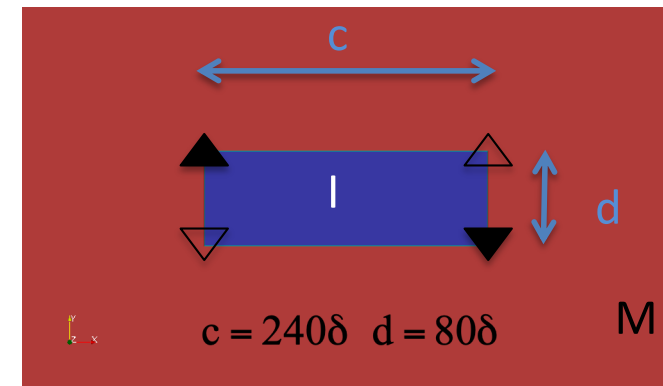
Mesh: 1024×1024 pixels

Pixel size: $\delta_1 = \delta_2 = \delta \approx 0.44b$

Convergence criteria: $\varepsilon = 10^{-5}$

Imposed loading: $\bar{T}_{11} = 1\text{MPa}$

Rectangular inclusion size:



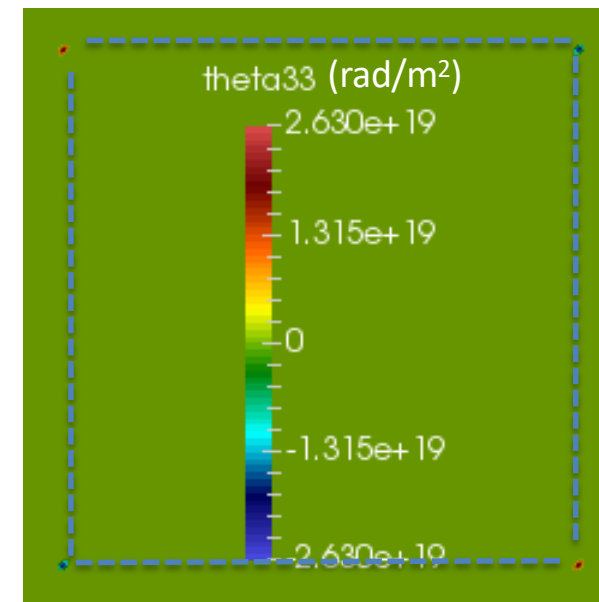
Linear elastic properties:

$$\mu_M = 2.3001 \times 10^3 \text{MPa}; \nu_M = \nu_I = 0.3647$$

$$\mu_0 = 0.505(\mu_M + \mu_I); D = \frac{\mu_M}{2\pi(1 - \nu_M)}$$

Disclination quadrupole densities (on 4 pixels)
(dipole at $x_2 = \pm d/2$ and at $x_1 = \pm c/2$): $\theta_{33}(\mathbf{x}) = \pm\omega / \delta^2$

Rotation discontinuity (wedge disclination quadrupole, Frank vector: $\pm\omega = \pm 5/6 \text{rad}$)

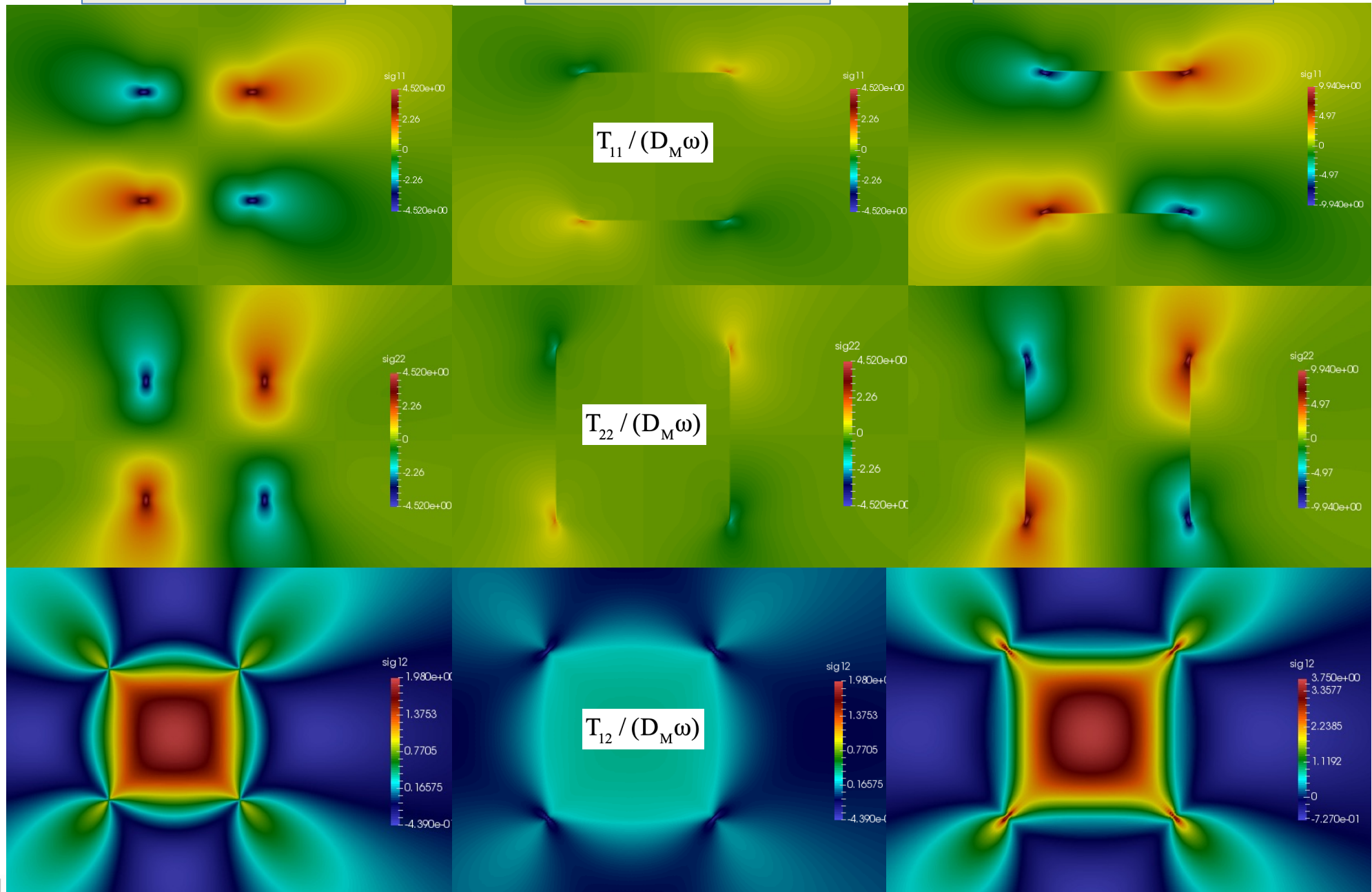


Stresses: squared wedge disclination quadrupole

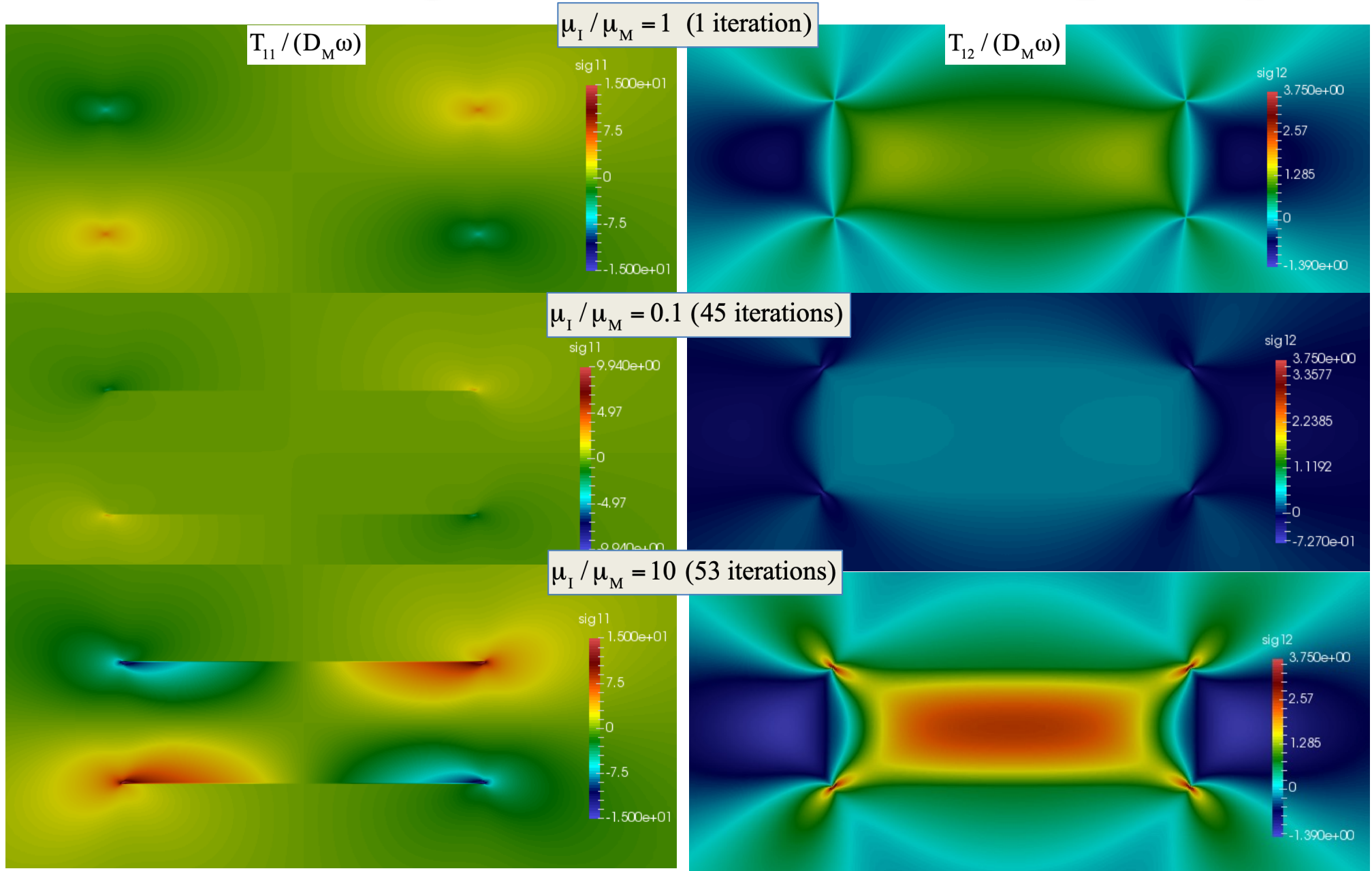
$\mu_I / \mu_M = 1$ (1 iteration)

$\mu_I / \mu_M = 0.1$ (41 iterations)

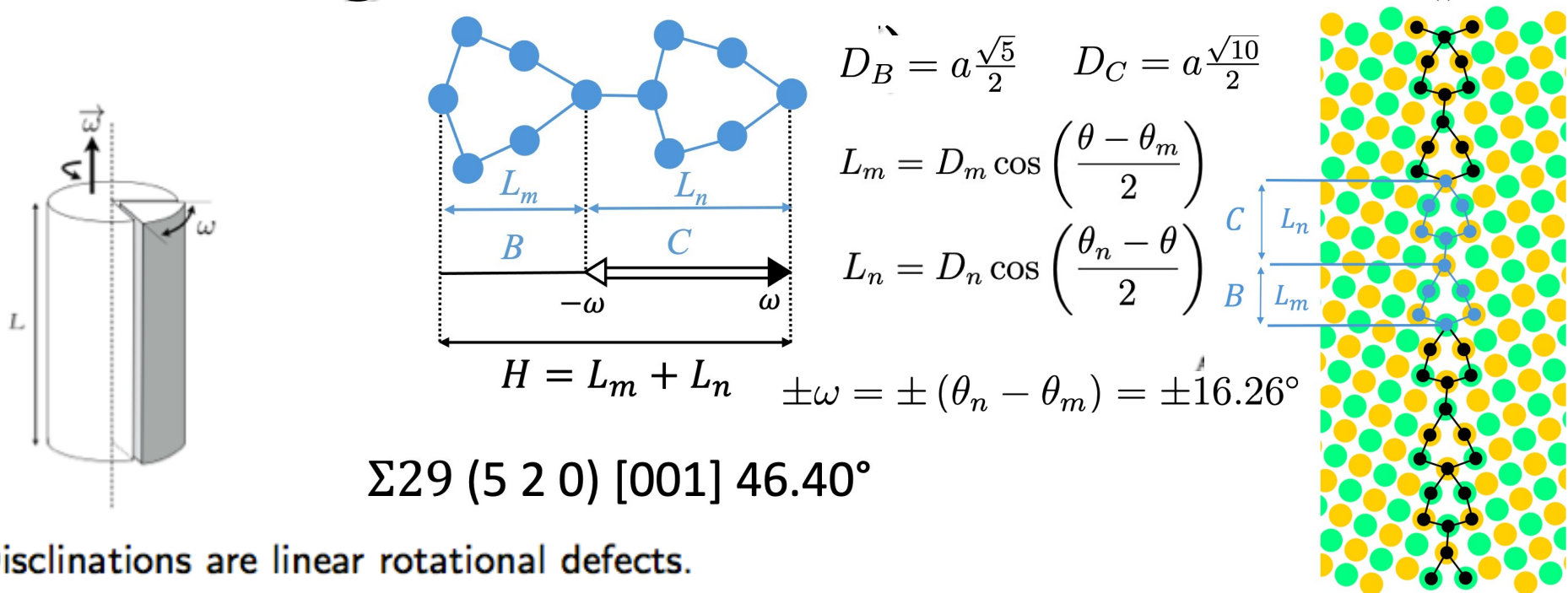
$\mu_I / \mu_M = 10$ (59 iterations)



Stresses: rectangular wedge disclination quadrupole



Application to Grain boundaries (GB): Modeling of HAGB using the disclination structural unit model



Disclinations are linear rotational defects.

- Exist only in a screened state by configuring straight disclinations in dipoles or other multipole configurations.

Decomposing GB into a contiguous and alternating sequence of special (favored) m majority and n minority structural units.

Boundary is represented in the form of a complex wall of disclinations combined into dipoles associated with the **minority structural units**.

Structural units:

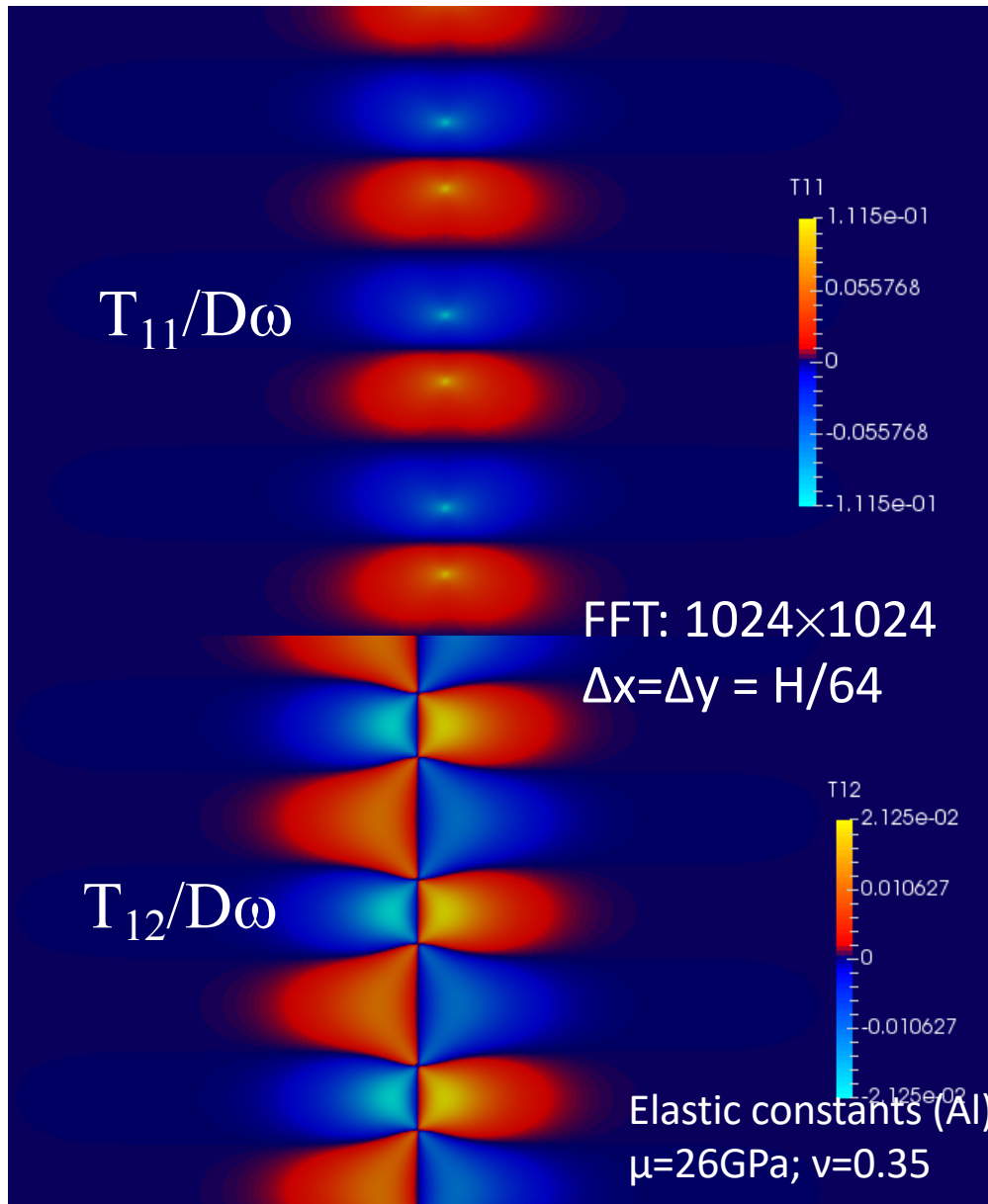
$$\Theta_A = 0^\circ$$

$$\Theta_B = 36.87^\circ$$

$$\Theta_C = 53.13^\circ$$

$$\Theta_D = 90^\circ$$

Stresses and strains for a symmetric tilt [001] GB



Application (stresses):

[AAAB.AAAB]

Example: Al [001]

$\Sigma 41(5\ 4\ 0)$

$\Theta = 12.68^\circ$ (5 4 0)

Period: $a[-4\ 5\ 0]$

$a = 4.0495 \text{ \AA}$

DSU model (Nazarov-Romanov 1989):

$\omega = 36.87^\circ$

$D_A = a\sqrt{2}/2$

$D_B = a\sqrt{5}/2$

$L_A = 0.5D_A \cos((\Theta - \Theta_A)/2)$

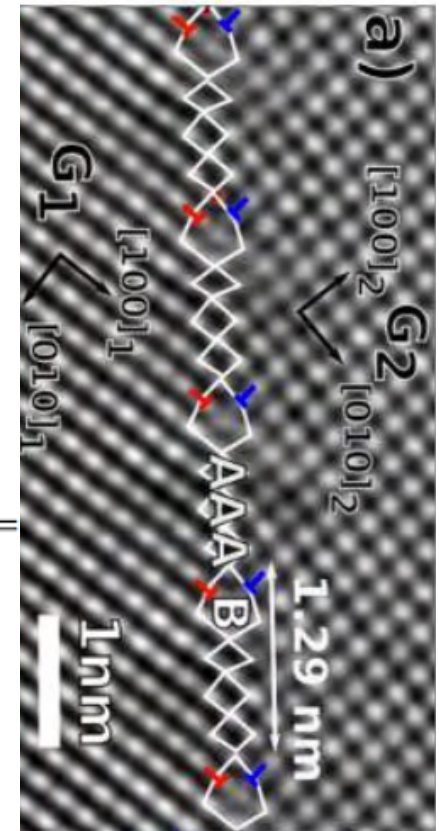
$L_B = 0.5D_B \cos((\Theta_B - \Theta)/2)$

$M = 3$

$N = 1$

$H = M(2L_A) + N(2L_B)$

$\theta_{33}(\mathbf{x}) = \pm \omega / \delta^2$

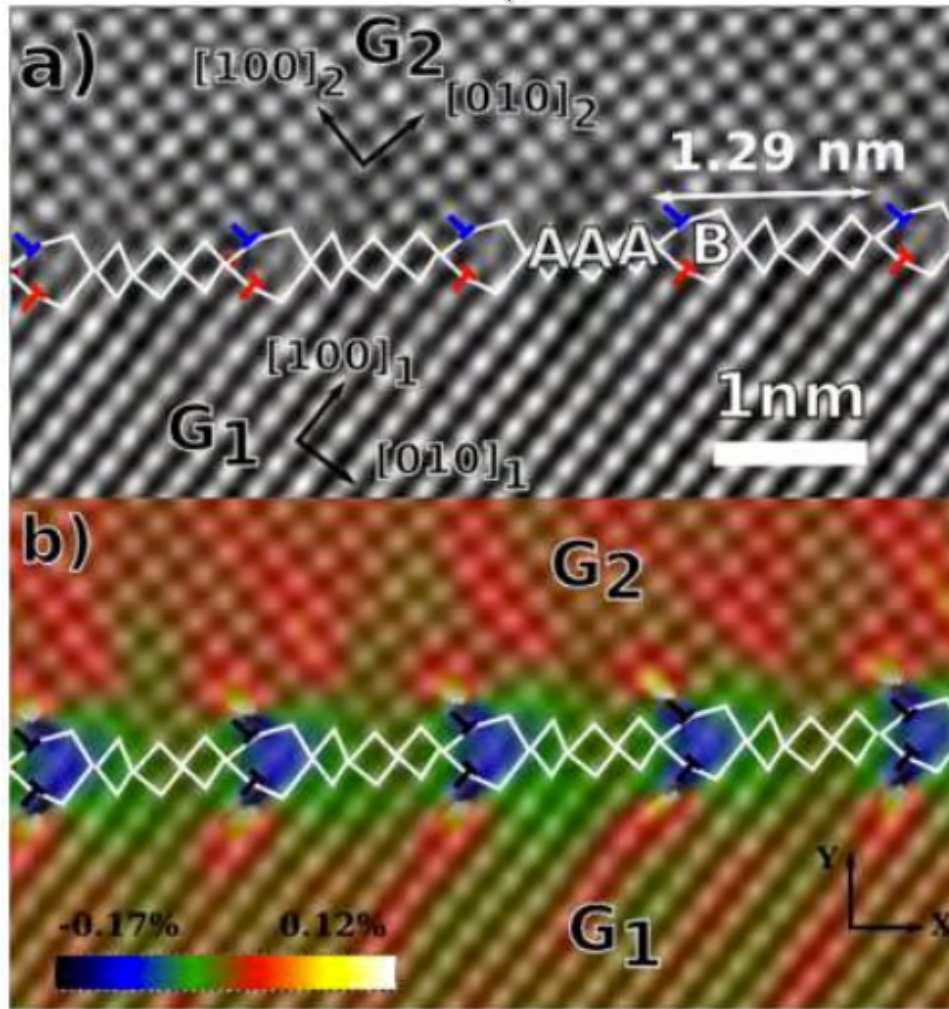


HRTEM

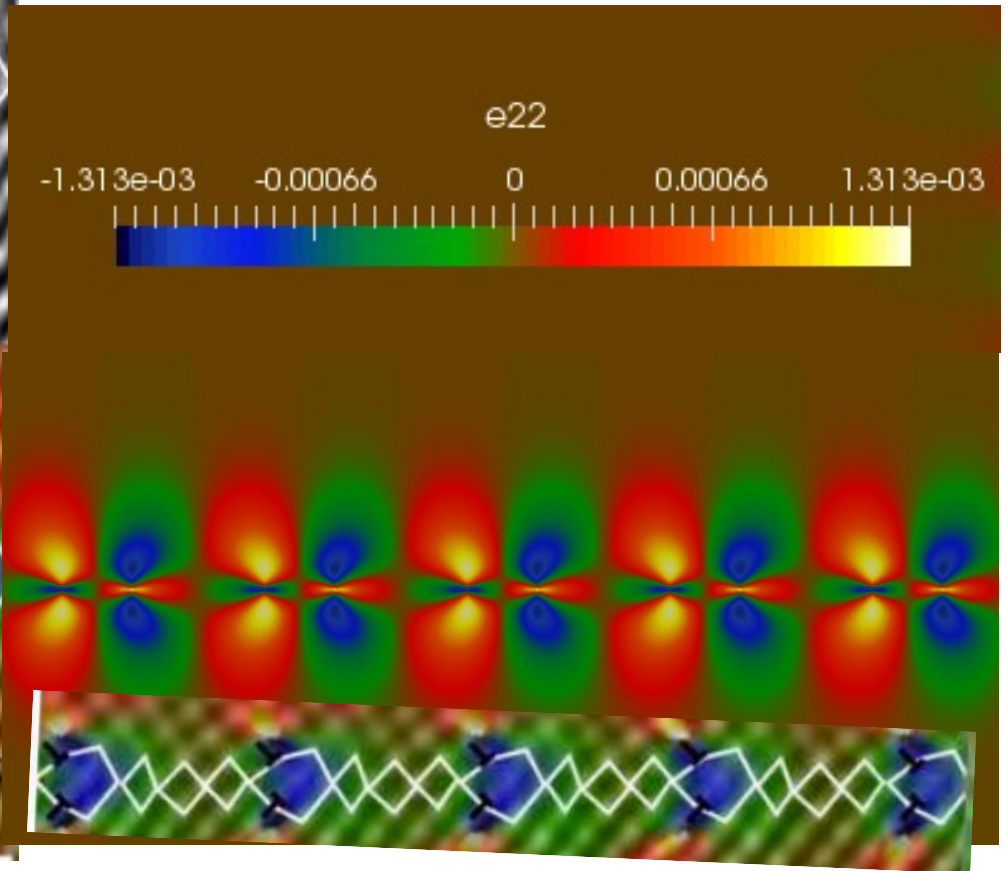
Rajabzadeh et al.

Acta Mater (2014)

Comparisons with HR-TEM measurements (GPA method): axial strain



FFT simulation: 1024×1024
 $\Delta x = \Delta y = H/64$ $\theta_{33}(\mathbf{x}) = \pm \omega / \delta^2$



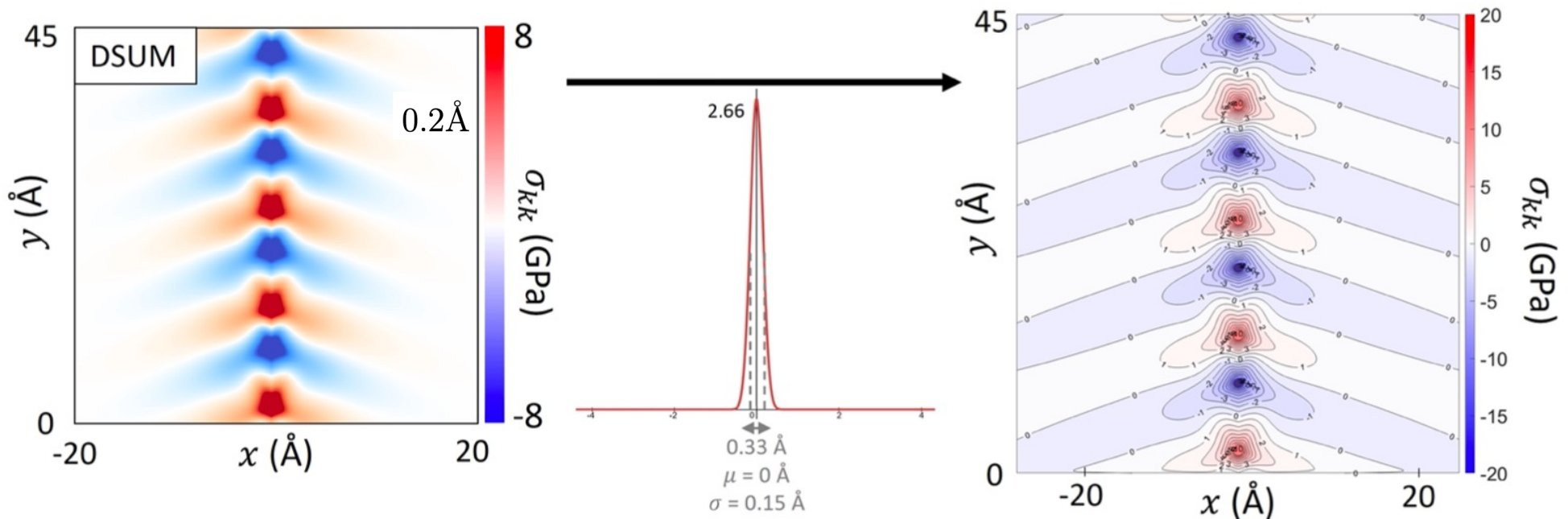
HRTEM + GPA from: A. Rajabzadeh *PhD University Toulouse* (2013)

Disclination density for FFDM-FFT

$$\omega = \omega_3 = \int_S \theta_{33} dS$$

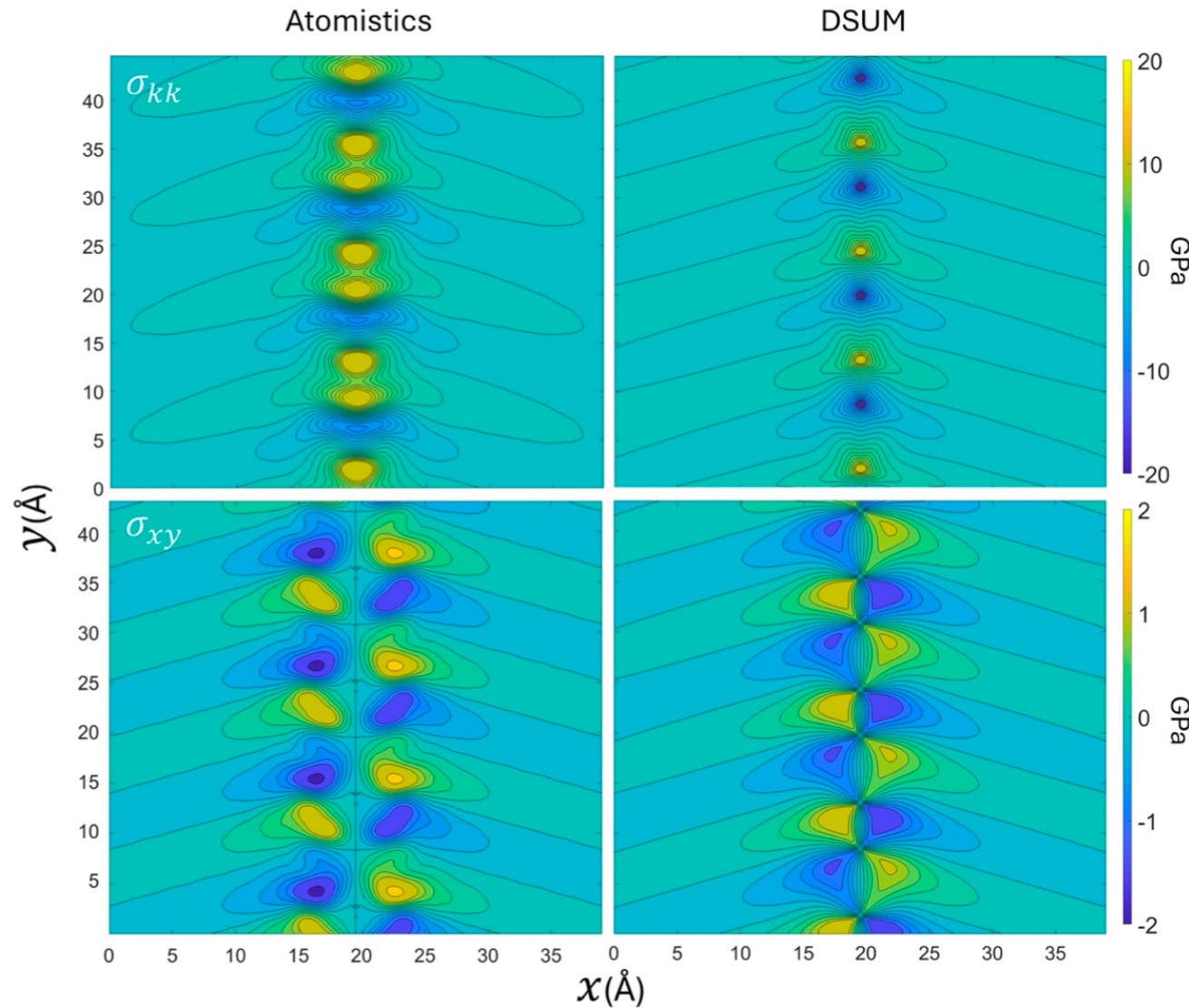
$$\theta_{33} = \pm \frac{\omega}{2\pi\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right)$$

$$\theta_{33} = 0 \text{ if } r \geq d$$



Wazne et al. *Mechanics Research Communications* (2025)

Comparisons between atomistic and anisotropic FFT simulations (Ag)



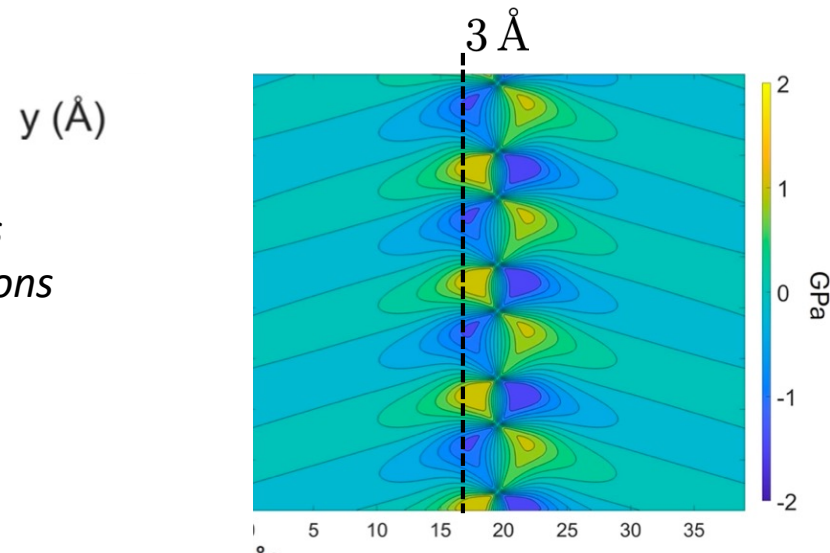
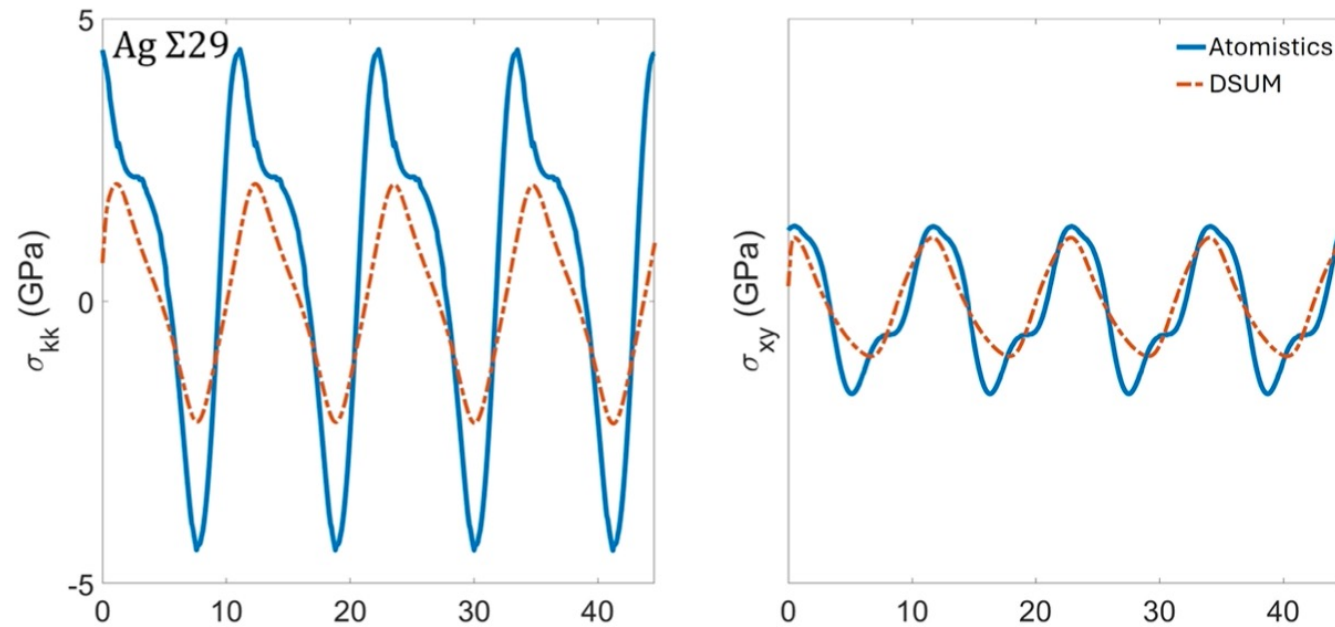
$\Sigma 29 (5\ 2\ 0) [001] 46.40^\circ$

1024×1024 pixels

Wazne et al. *Mechanics Research Communications* (2025)

$A = 3.21$ (Zener ratio)
Ag : FCC

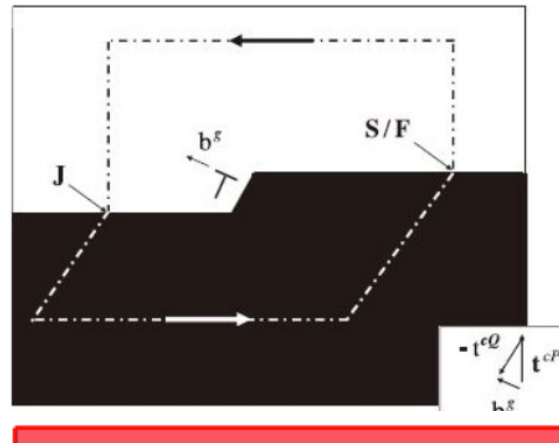
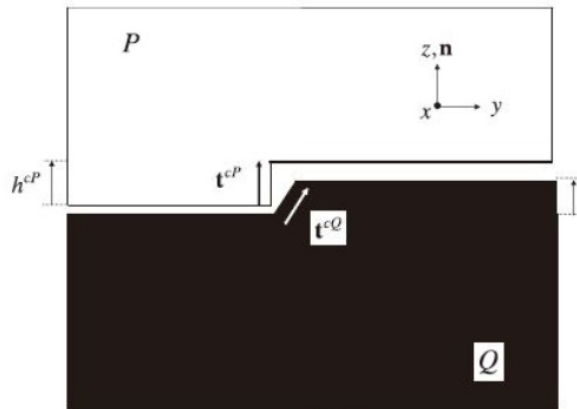
Comparisons between atomistic and anisotropic FFT simulations (Ag)



Wazne et al. *Mechanics Research Communications* (2025)

Applications to dislocation/disclination defects:

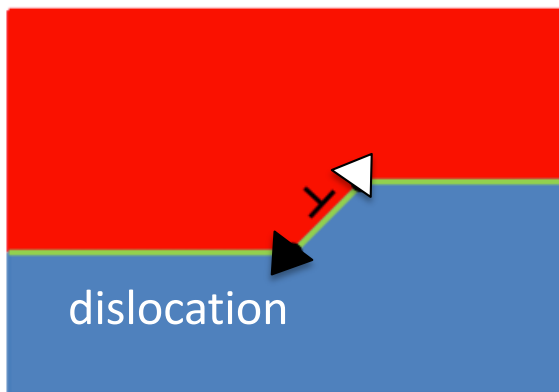
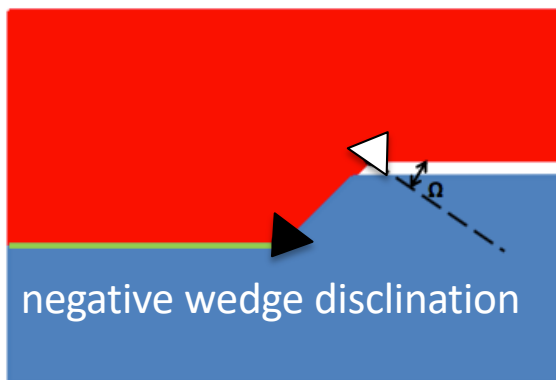
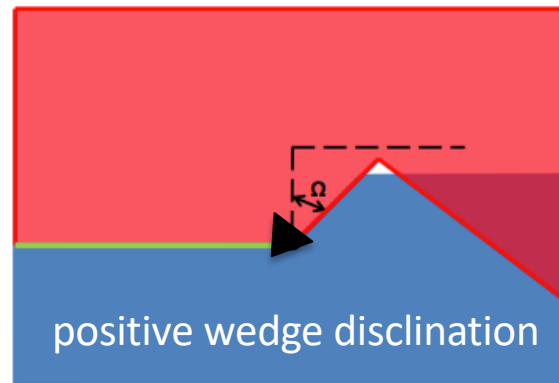
Pond and Hirth's disconnection



Burgers circuit to define the equivalent Burgers vector of the disconnection
Hirth et al. (2006)

Continuum defect mechanics
description of the
disconnection
defect
**1 disclination dipole
+ 1 dislocation**

Pixel size: $\delta_1 = \delta_2 = \delta \simeq 0.44b$



$$\theta_{33}(\mathbf{x}) = \pm \omega / \delta^2 \quad \text{with } \omega = \pi / 4$$

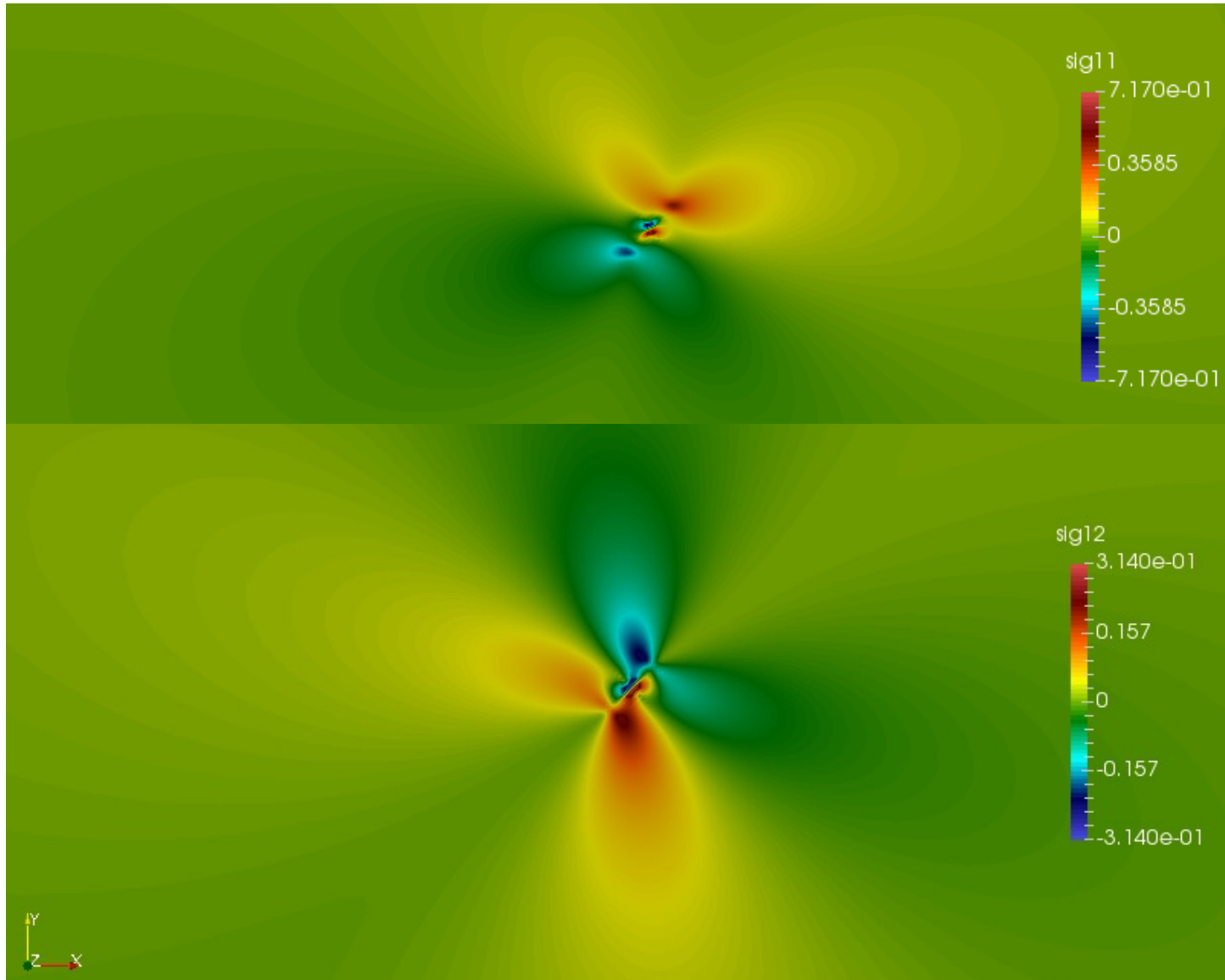
$$a = a_{\text{Cu}} = 0.3615 \text{ nm}$$

$$\alpha_{13}(\mathbf{x}) = a \cdot \cos\left(\frac{\pi}{4}\right) / \delta^2$$

$$\alpha_{23}(\mathbf{x}) = a \cdot \sin\left(\frac{\pi}{4}\right) / \delta^2$$

Predicted stress field by FFT

Mesh: 512×512 pixels



Isotropic elastic constants for Copper:

$$E_{\text{Cu}} = 130 \text{ GPa}$$

$$\nu_{\text{Cu}} = 0.34$$

Elastic energy / pixel :

$$E_1 = 12.3 \text{ (MJ/m}^3\text{)}$$

- Continuous theory of disclinations: field equations
- Spectral-based approach and applications
- **Disclination mechanics within a couple stress theory**
- References

Constitutive relationships related to couple stress theory (Mindlin-Tiersten)

- Couple stress theory (Mindlin-Tiersten, 1962) with centrosymmetry

$$\Psi = \frac{1}{2} \boldsymbol{\epsilon}_e : \mathbf{C} : \boldsymbol{\epsilon}_e + \frac{1}{2} \boldsymbol{\kappa}_e^D : \mathbf{A} : \boldsymbol{\kappa}_e^D$$

- Isotropic centro-symmetric materials (4 material's elastic constants):

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{jk} \delta_{il})$$
$$A_{ijkl} = A_1 \delta_{ik} \delta_{jl} - A_2 \delta_{jk} \delta_{il}$$



$$T_{ij}^{sym} = C_{ijkl} \epsilon_{kl}^e = \lambda \epsilon_{kk}^e \delta_{ij} + 2\mu \epsilon_{ij}^e$$
$$m_{ij}^D = A_{ijkl} \kappa_{kl}^{eD} = A_1 \kappa_{ij}^{eD} - A_2 \kappa_{ji}^{eD}$$

with m_{ij} : couple stress tensor

Equilibrium equations

- Linear and angular balance momentum equations (without body forces and couples) (see: Mindlin-Tiersten)

$$\begin{aligned}\operatorname{div} \mathbf{T} &= 0 \text{ in } V, \\ \operatorname{div} \mathbf{m}^D - \mathbf{X} : \mathbf{T} &= 0 \text{ in } V\end{aligned}$$

- Reduction to a single equilibrium equation (Mindlin-Tiersten)

$$\operatorname{div} \mathbf{T}^{sym} + \frac{1}{2} \operatorname{curl} (\operatorname{div} \mathbf{m}^D) = 0 \text{ in } V$$

$$\operatorname{div} \mathbf{C} : \boldsymbol{\epsilon}_e^{\parallel} + \frac{1}{2} \operatorname{curl} (\operatorname{div} (\mathbf{A} : \boldsymbol{\kappa}_e^{D\parallel})) + \mathbf{f}^{\perp} = 0$$

$$\text{with } \mathbf{f}^{\perp} = \operatorname{div} \mathbf{C} : \boldsymbol{\epsilon}_e^{\perp} + \frac{1}{2} \operatorname{curl} (\operatorname{div} (\mathbf{A} : \boldsymbol{\kappa}_e^{D,\perp}))$$

- Indicial equilibrium equation form (homogeneous isotropic elasticity)

$$C_{ijkl}^0 w_{k,lj} + \frac{1}{4} e_{ikl} e_{prs} A_{lmpq}^0 w_{s,rqm} + C_{ijkl}^0 \epsilon_{kl,j}^{e,\perp} + \frac{1}{2} e_{ikl} A_{lmpq}^0 \kappa_{pq,m}^{eD,\perp} = 0$$

Fourier transform formulation

- Fourier transform (F.T.) of incompatible fields (Poisson's PDE)

$$\begin{cases} \tilde{\mathbf{K}}_{ij}^{e,\perp}(\boldsymbol{\xi}) = \frac{i}{\xi^2} \xi_k \left(\mathbf{e}_{jkl} \tilde{\theta}_{il}(\boldsymbol{\xi}) \right) & \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \tilde{\mathbf{K}}_{ij}^{e,\perp}(\mathbf{0}) = \mathbf{0} \end{cases}$$

$$\begin{cases} \tilde{\boldsymbol{\varepsilon}}_{(ij)}^{e,\perp}(\boldsymbol{\xi}) = \frac{i}{\xi^2} \xi_k \mathbf{e}_{(j)kl} \left(\tilde{\alpha}_{(i)l}(\boldsymbol{\xi}) + \tilde{\mathbf{K}}_{l(i)}^{e,\perp}(\boldsymbol{\xi}) - \delta_{(i)l} \tilde{\mathbf{K}}_{pp}^{e,\perp}(\boldsymbol{\xi}) \right) & \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \tilde{\boldsymbol{\varepsilon}}_{ij}^{e,\perp}(\mathbf{0}) = \mathbf{0} \end{cases}$$

- Resolution of a generalized Navier type- PDE in Fourier space (up to 4th order derivatives)

$$C_{ijkl}^0 \xi_l \xi_j \tilde{w}_k(\boldsymbol{\xi}) - \frac{1}{4} e_{ikl} e_{prs} A_{lmpq}^0 \xi_r \xi_q \xi_m \xi_k \tilde{w}_s(\boldsymbol{\xi}) = i C_{ijkl}^0 \xi_j \tilde{\varepsilon}_{kl}^{e,\perp}(\boldsymbol{\xi}) + \frac{1}{2} e_{ikl} A_{lmpq}^0 \xi_m \xi_k \tilde{\kappa}_{pq}^{eD,\perp}(\boldsymbol{\xi})$$

Fourier transform formulation (cont'd)

- Solution displacement field in Fourier space $\tilde{\mathbf{w}}(\boldsymbol{\xi})$ (compatible part):

$$\tilde{w}_i(\boldsymbol{\xi}) = \tilde{G}_{ik}(\boldsymbol{\xi}) \tilde{f}_k^\perp(\boldsymbol{\xi})$$

with $\tilde{f}_i^\perp(\boldsymbol{\xi}) = iC_{ijkl}^0 \xi_j \tilde{\epsilon}_{kl}^{e,\perp}(\boldsymbol{\xi}) + \frac{1}{2} e_{ikl} A_{lmpq}^0 \xi_m \xi_k \tilde{\kappa}_{pq}^{eD,\perp}(\boldsymbol{\xi})$

- Non local Green function in Fourier space (size dependent solution):

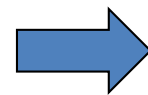
$$\tilde{G}_{ik}(\boldsymbol{\xi}) = \frac{1}{\mu \xi^2} \left[\frac{1}{1 + l^2 \xi^2} (\delta_{ik} - \xi_i \xi_k) + \frac{\mu}{\lambda + 2\mu} \xi_i \xi_k \right] \forall \boldsymbol{\xi} \neq \mathbf{0}$$

$$\tilde{G}_{ik}(\mathbf{0}) = 0$$

- (Internal) stress and couple stress fields:

$$\tilde{\epsilon}_{ij}^{e,\parallel}(\boldsymbol{\xi}) = \frac{1}{2} i (\xi_j \tilde{w}_i(\boldsymbol{\xi}) + \xi_i \tilde{w}_j(\boldsymbol{\xi}))$$

$$\tilde{\kappa}_{ij}^{eD,\parallel}(\boldsymbol{\xi}) = -\frac{1}{2} e_{ikl} \xi_j \xi_k \tilde{w}_l(\boldsymbol{\xi})$$



$$\left\{ \begin{array}{l} \tilde{T}_{ij}(\boldsymbol{\xi}) = C_{ijkl}^0 \tilde{\epsilon}_{kl}^e(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \tilde{T}_{ij}(\mathbf{0}) = 0 \\ \tilde{m}_{ij}^D(\boldsymbol{\xi}) = A_{ijkl}^0 \tilde{\kappa}_{kl}^{eD}(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \tilde{m}_{ij}^D(\mathbf{0}) = 0 \end{array} \right.$$

Straight disclinations: defect line along the x_3 -axis

- Elastic rotation discontinuity (classic wedge disclination and dipoles)

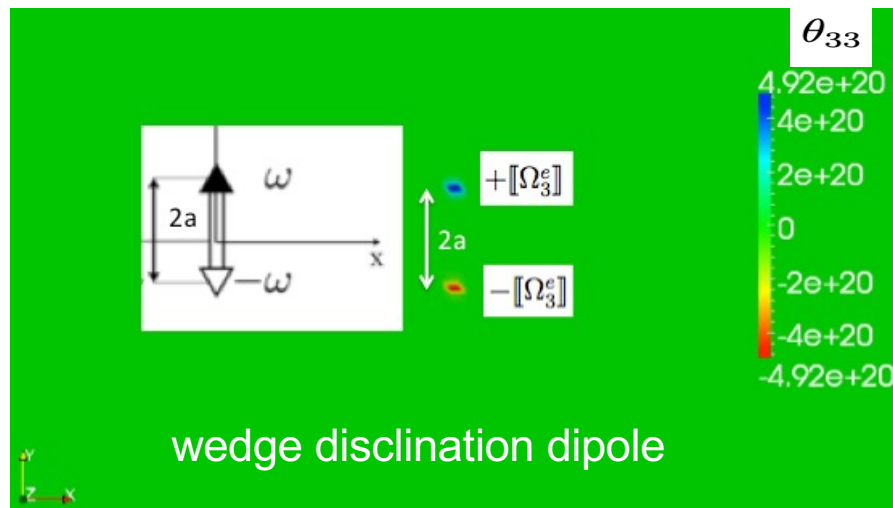
$$[\Omega_3^e] = \Omega_{3+}^e - \Omega_{3-}^e = \omega$$

- Material length scale parameter: $A_1 \approx \mu b^2$
- For wedge disclination, A_2 vanishes

$$\omega = \omega_3 = \int_S \theta_{33} dS$$

$$\theta_{33} = \pm \frac{\omega}{2\pi\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right)$$

$$\theta_{33} = 0 \quad \text{if } r \geq d$$



Copper

$$\sigma = 0.1r_0.$$

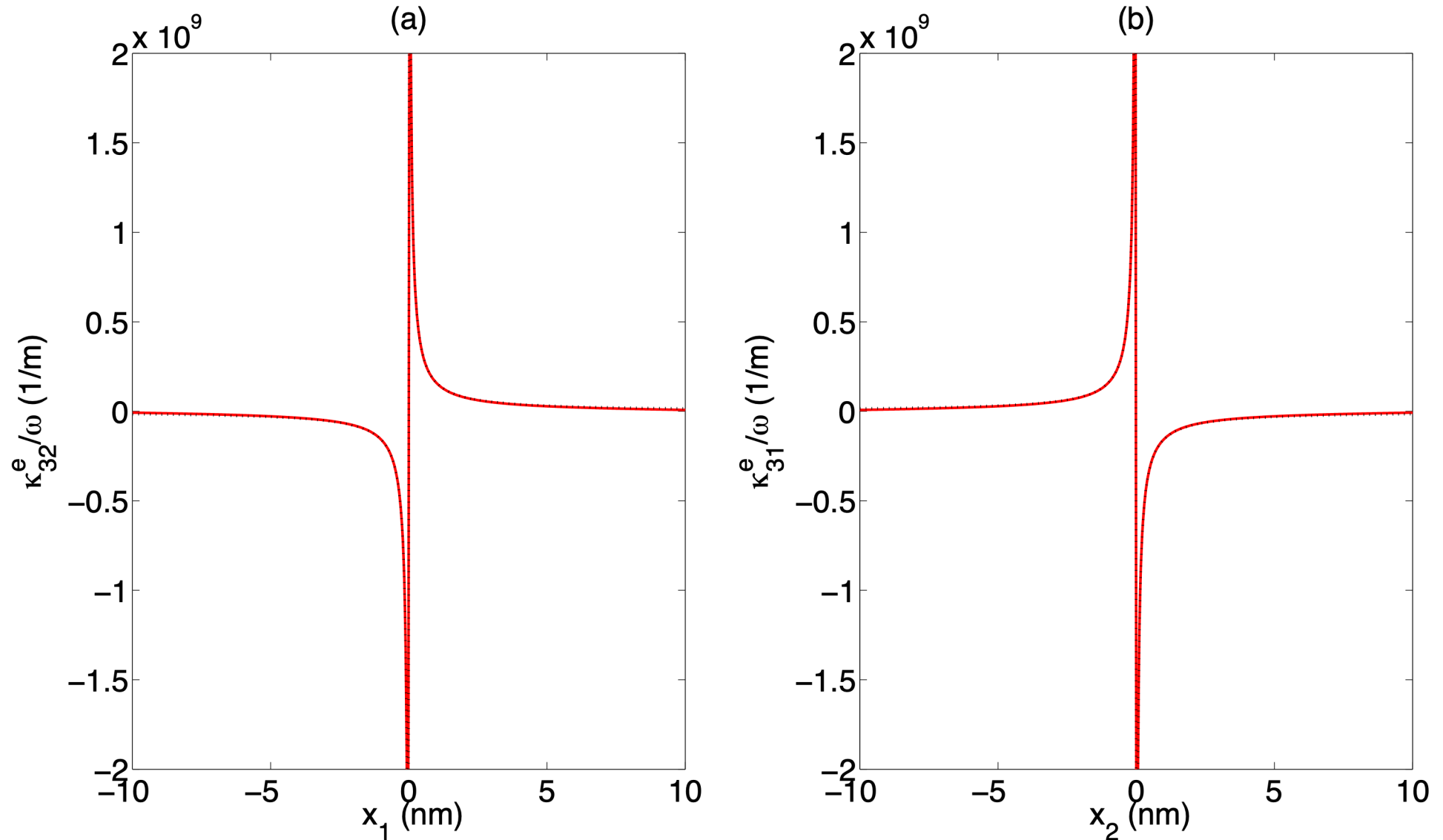
$$b = 0.25563\text{nm}$$

$$\mu = 47800\text{MPa}$$

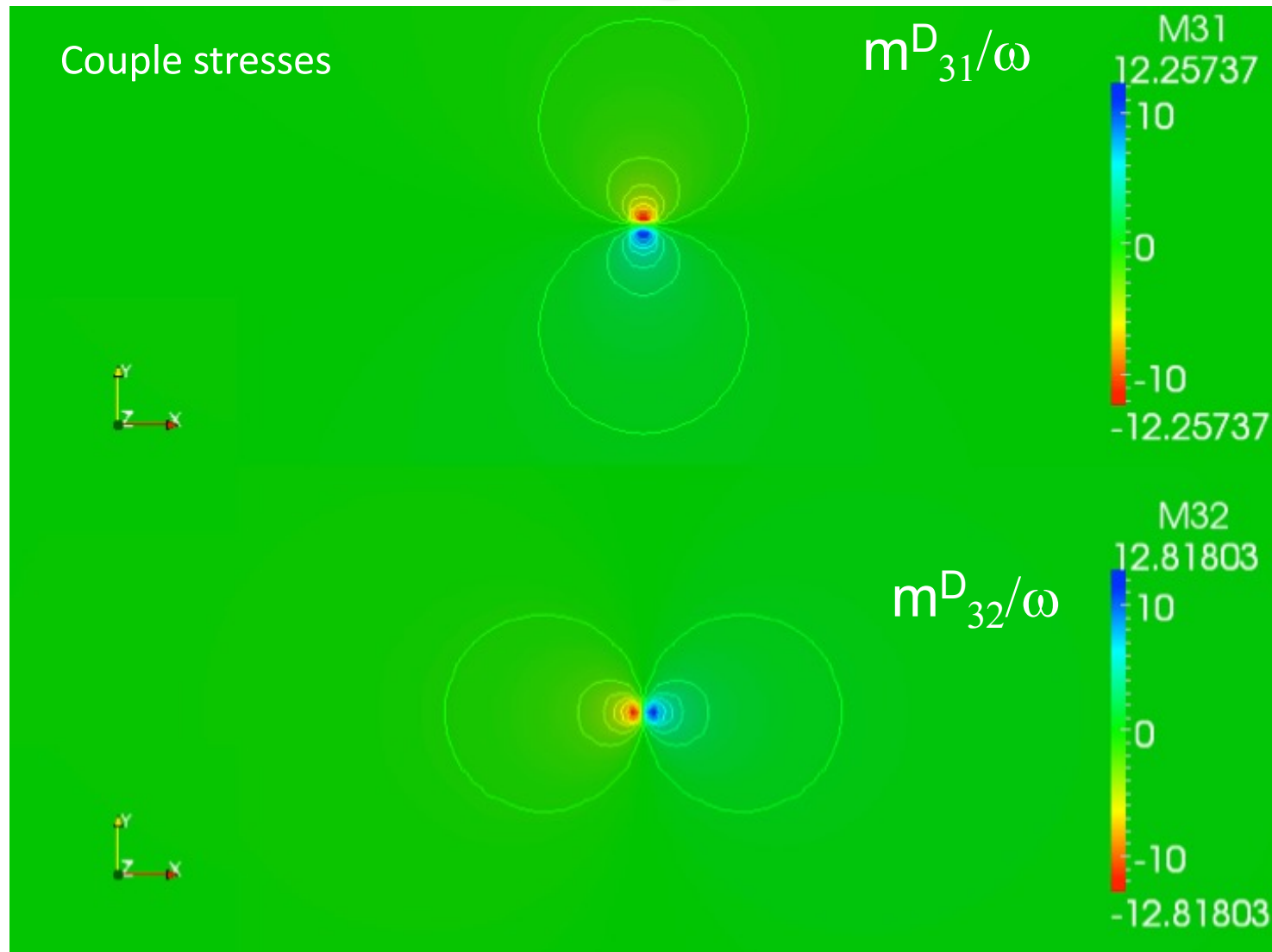
$$r_0 = 0.5b$$

$$\nu = 0.34$$

Elastic curvatures of a single centered wedge disclination (comparisons with analytical results)

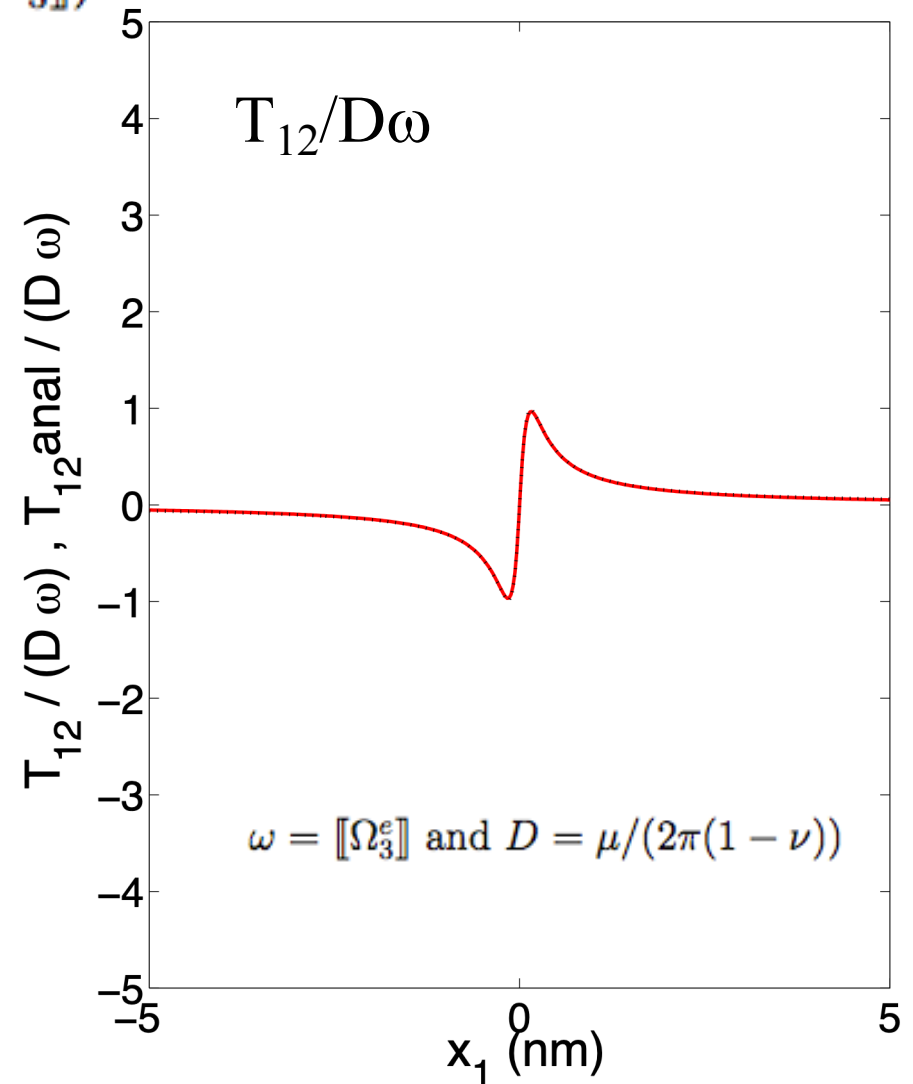
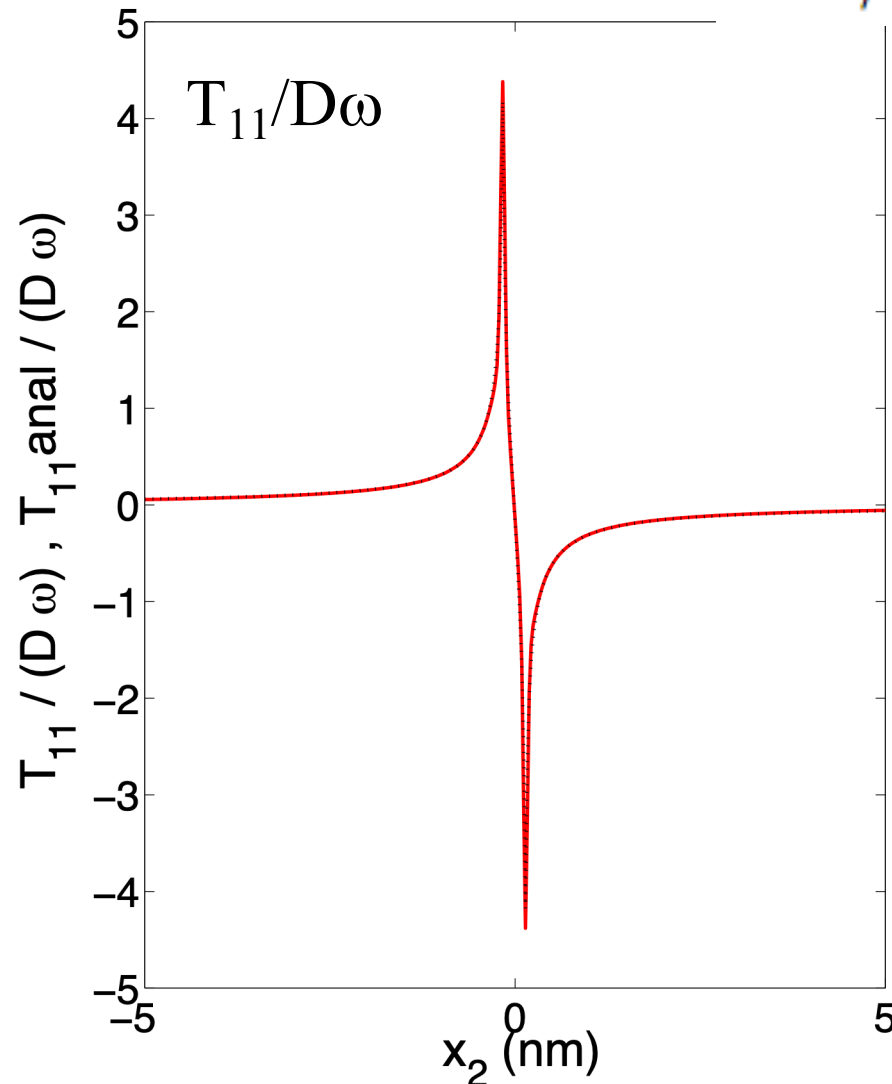


Non-zero couple stress contours for a single centered wedge disclination

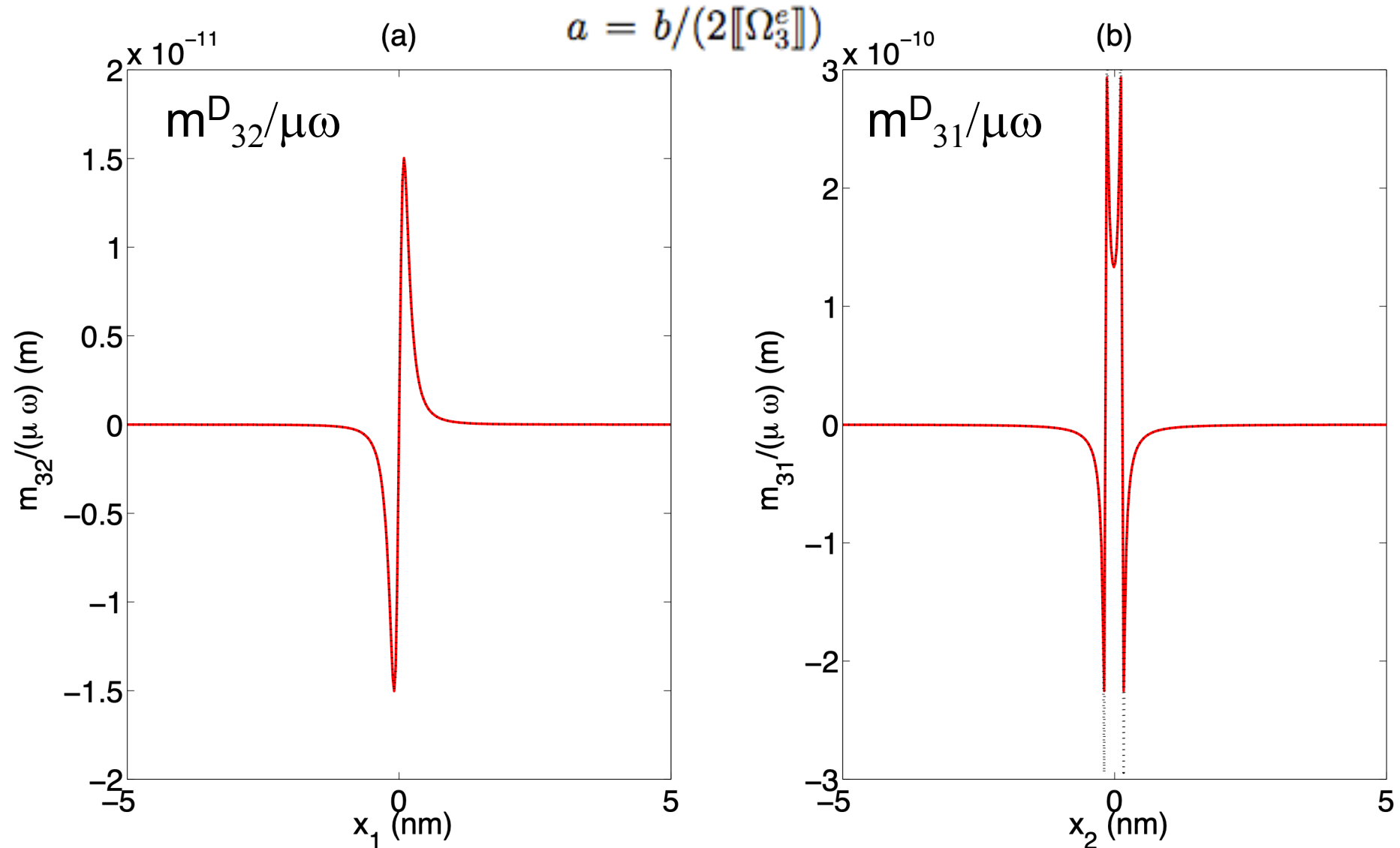


Stress comparisons with analytical solutions: Wedge disclination dipole (isotropic elasticity)

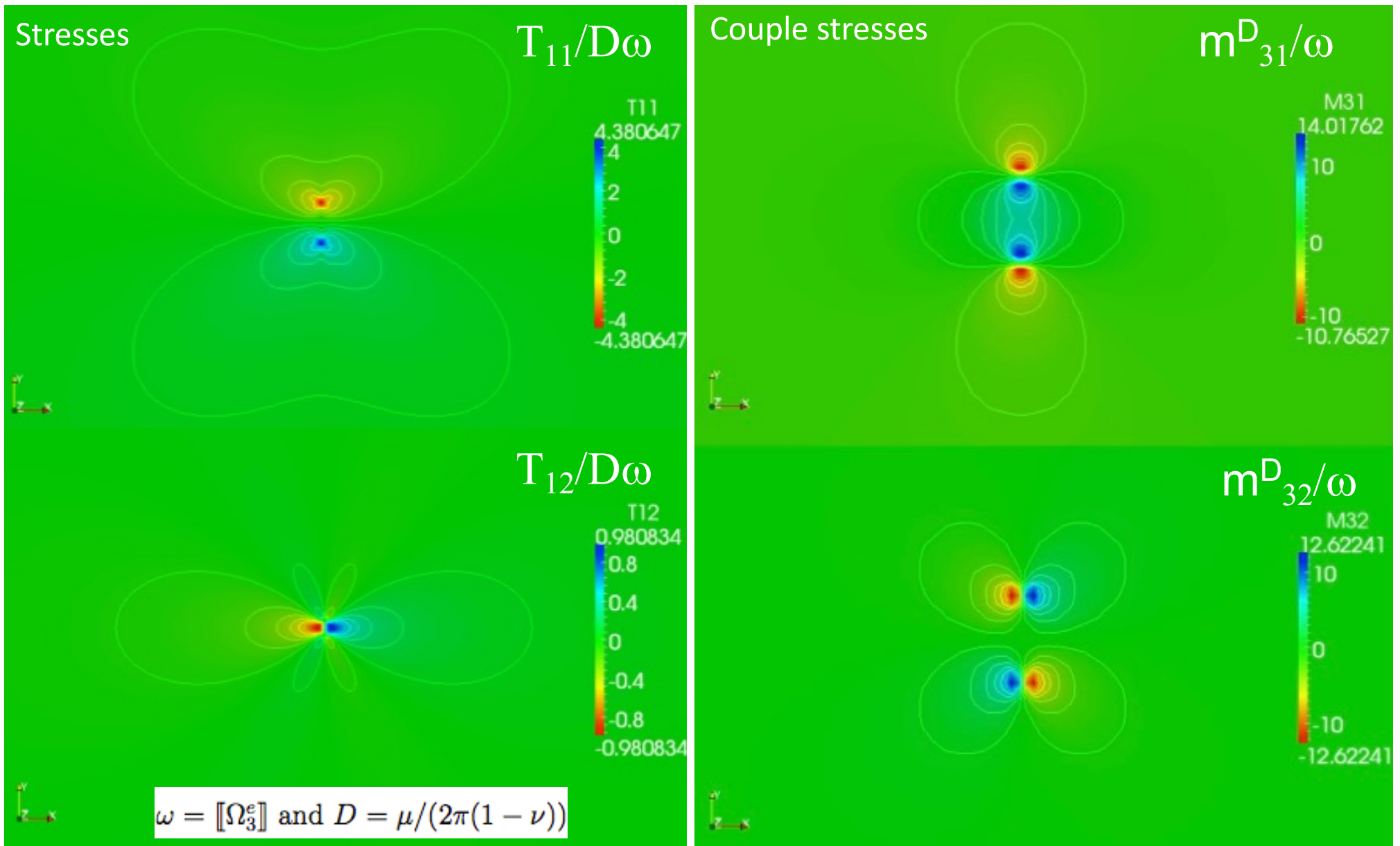
$$a = b/(2[\![\Omega_3^e]\!])$$



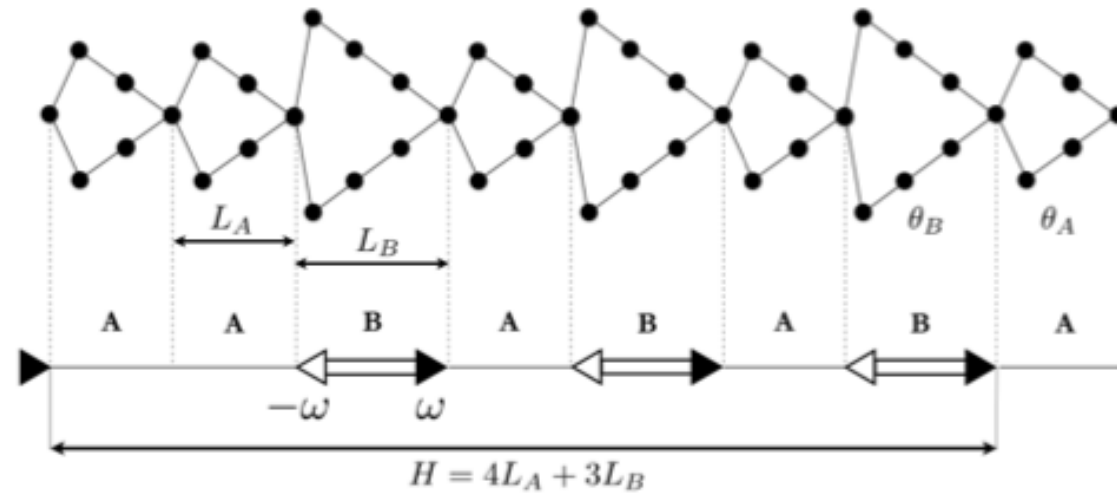
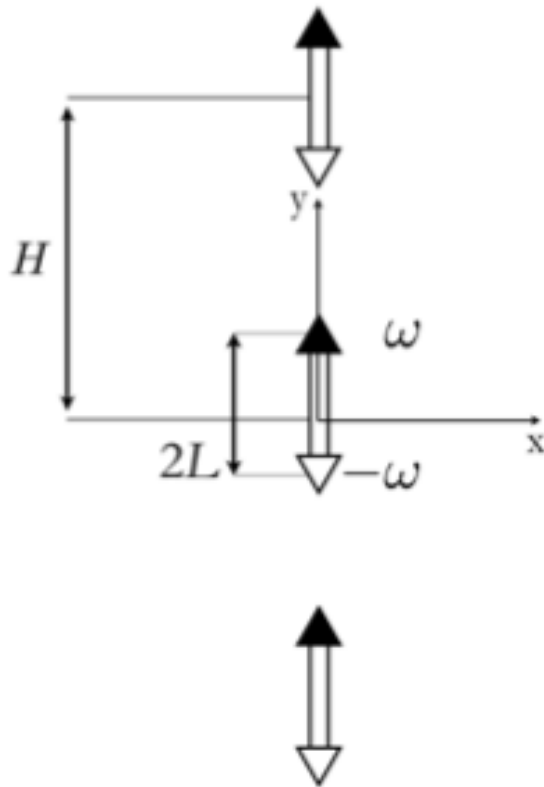
Couple stress comparisons with analytical solutions: Wedge disclination dipole



Couple stress contours : Wedge disclination dipole



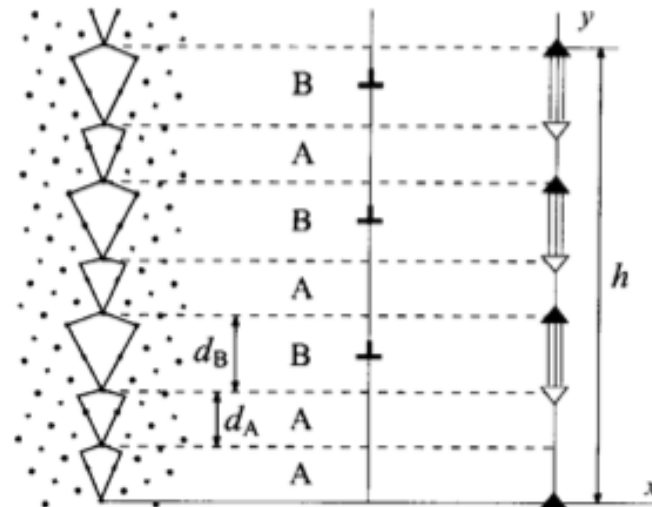
Application: Grain Boundaries (GBs)



AABABAB.AABABAB

Example: Cu [001] $\Sigma 149(10\ 7\ 0)$

$\theta = 20.02^\circ$

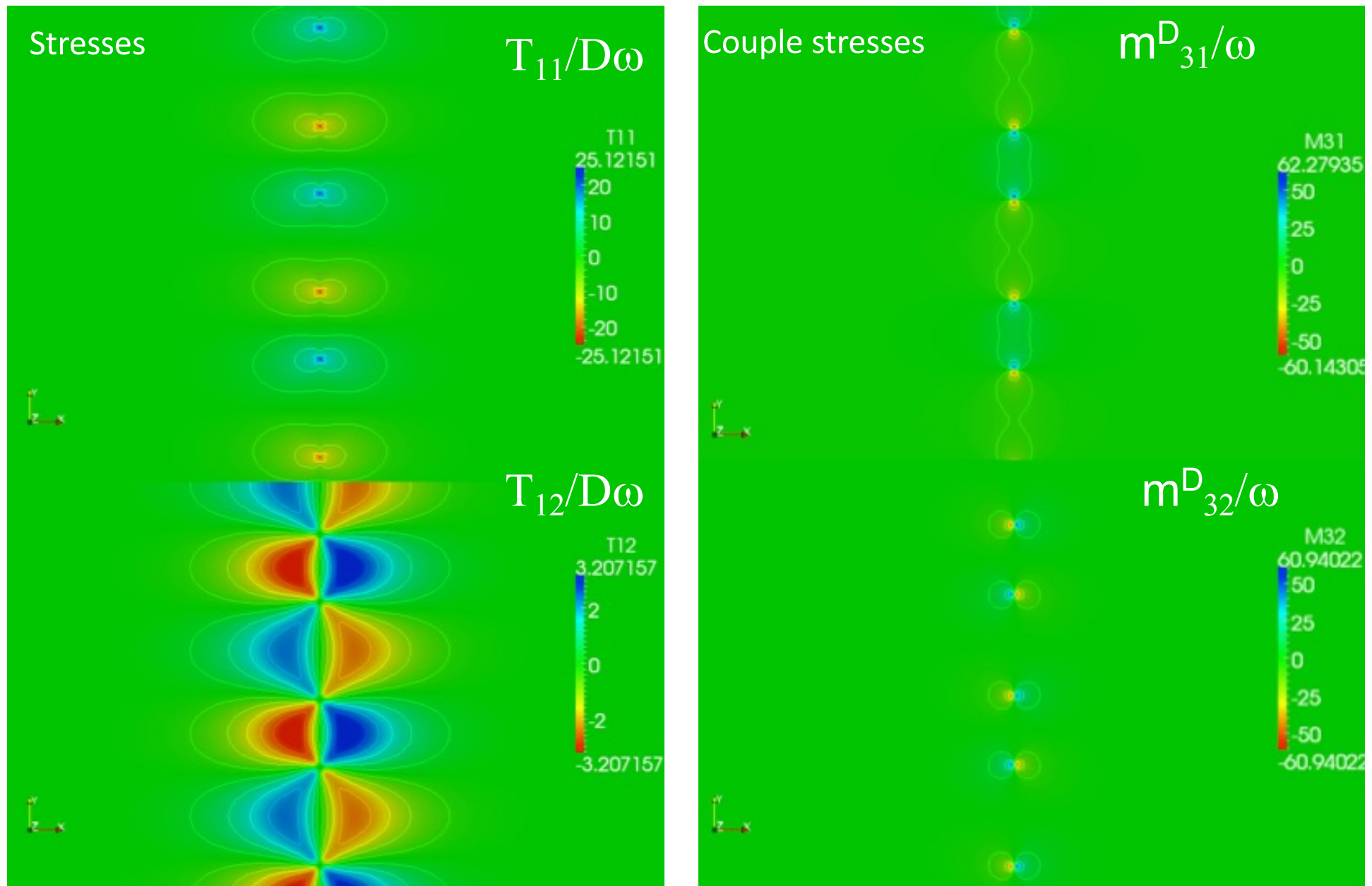


$d_A = 0.25287\text{nm}$

$d_B = 0.38344\text{nm}$

$\omega = 0.6435\text{ rad. } (=36.87^\circ)$

Stress and couple stress contours for a GB



- Continuous theory of disclinations: field equations
- Spectral-based approach and applications
- Disclination mechanics within a couple stress theory
- **References**

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