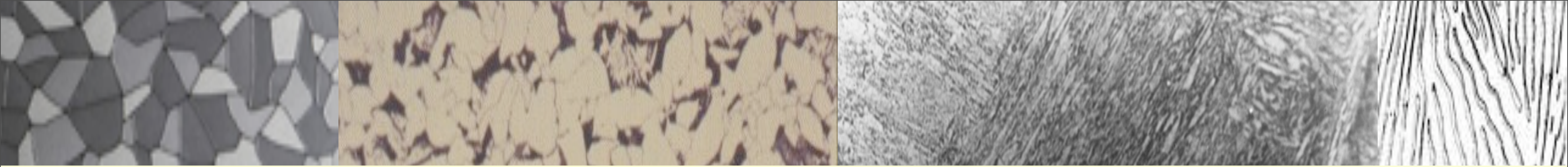


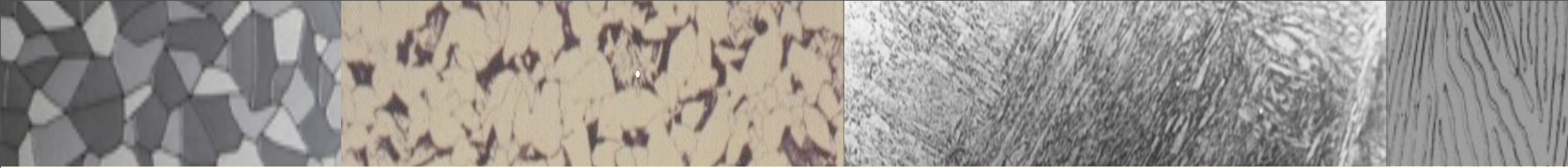
Dynamical heterogeneities, jamming and plasticity in solid-solid nucleation

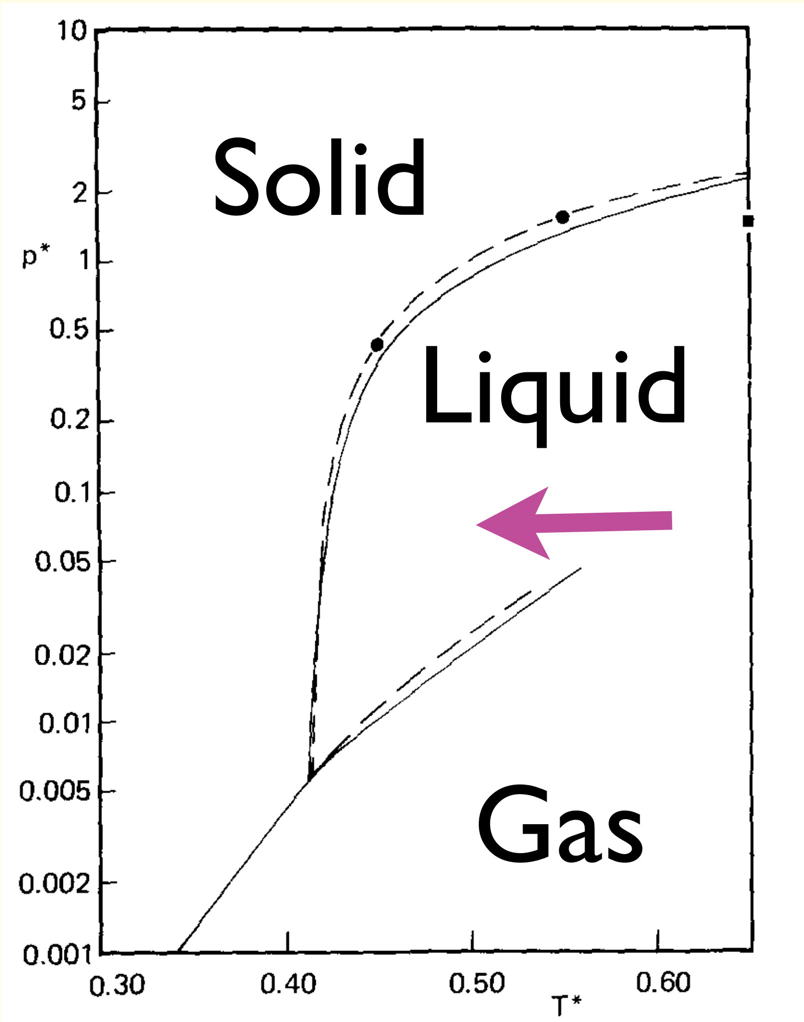
Surajit Sengupta (IACS & SNBNCBS, Kolkata)

Collaborators:

M. Rao (RRI & NCBS, Bangalore)
Jayee Bhattacharya, Arya Paul (SNBNCBS)

Glasses10 KITP (April 12 - July 9, 2010)

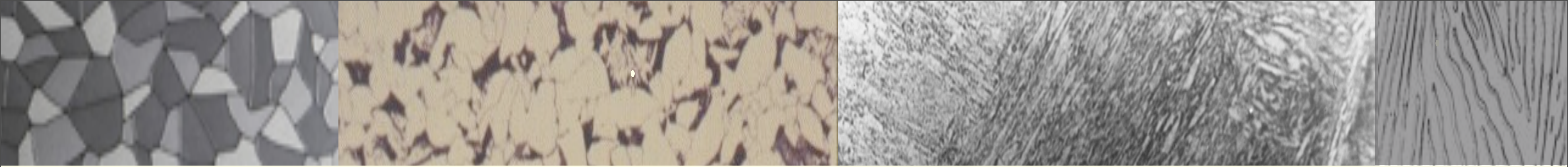


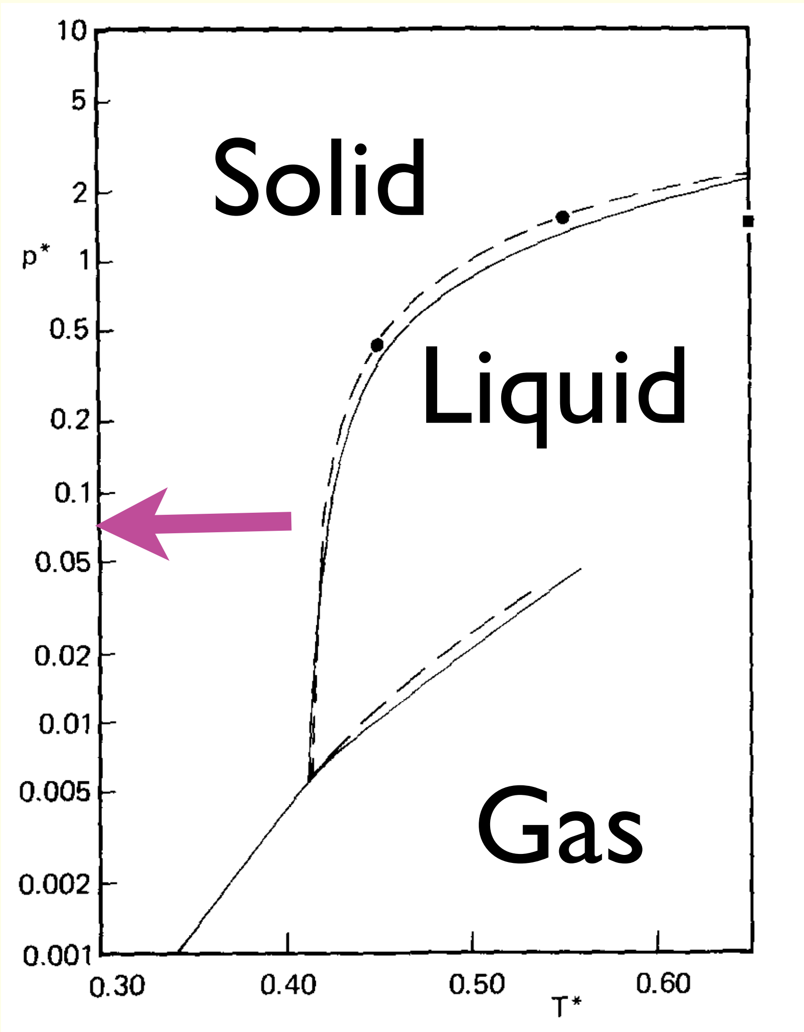


- Structure and dynamics of the critical nucleus.
- Single particle dynamics, dynamical heterogeneities.
- Structure and dynamics of interfaces; growth laws.
- Quench ⇒ glass

  (bidispersity, geometrical frustration)

Barker *et al.* Physica A (1981); ten Wolde *et al.* PRL (1995); Auer *et al.* Nature (2001); Gasser *et al.* Science, (1991); J. Hernandez-Guzman *et al.* PNAS (2009).

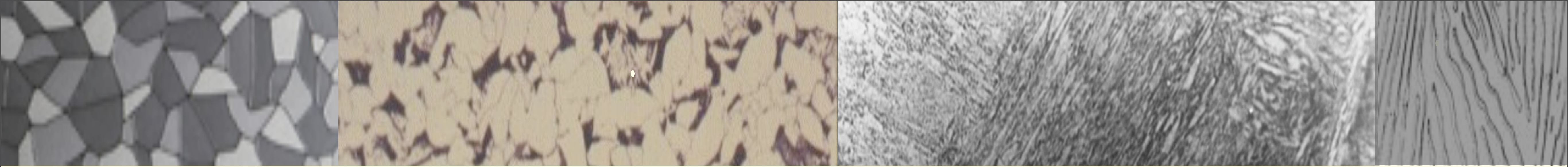


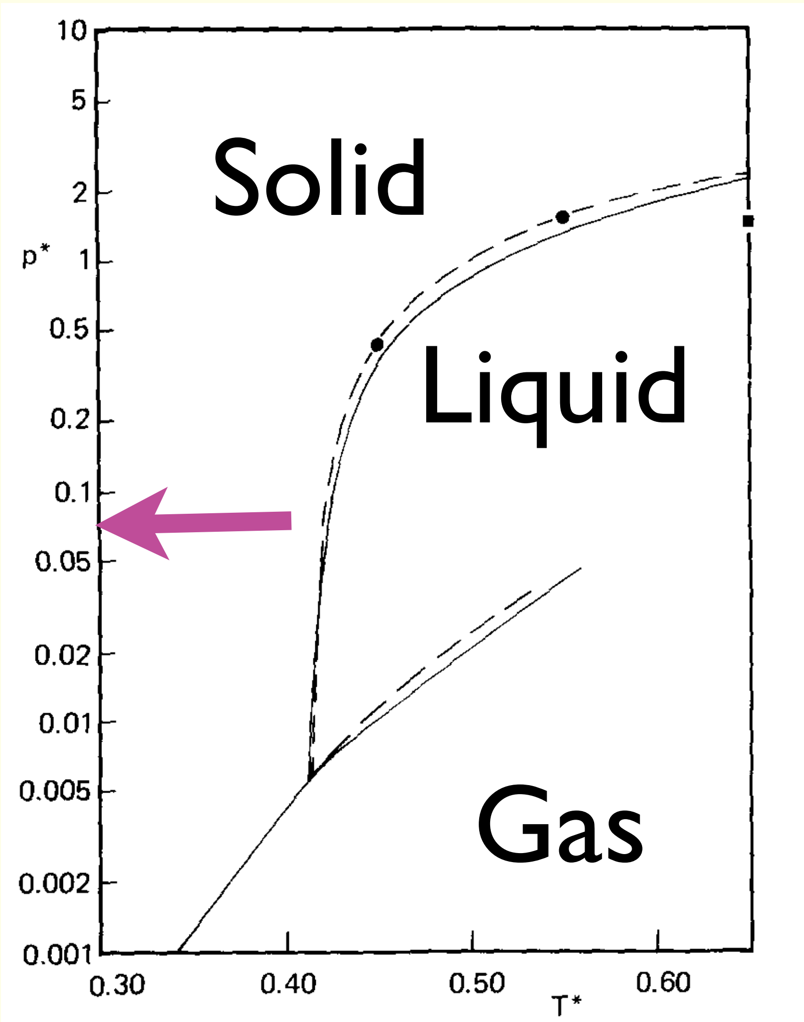


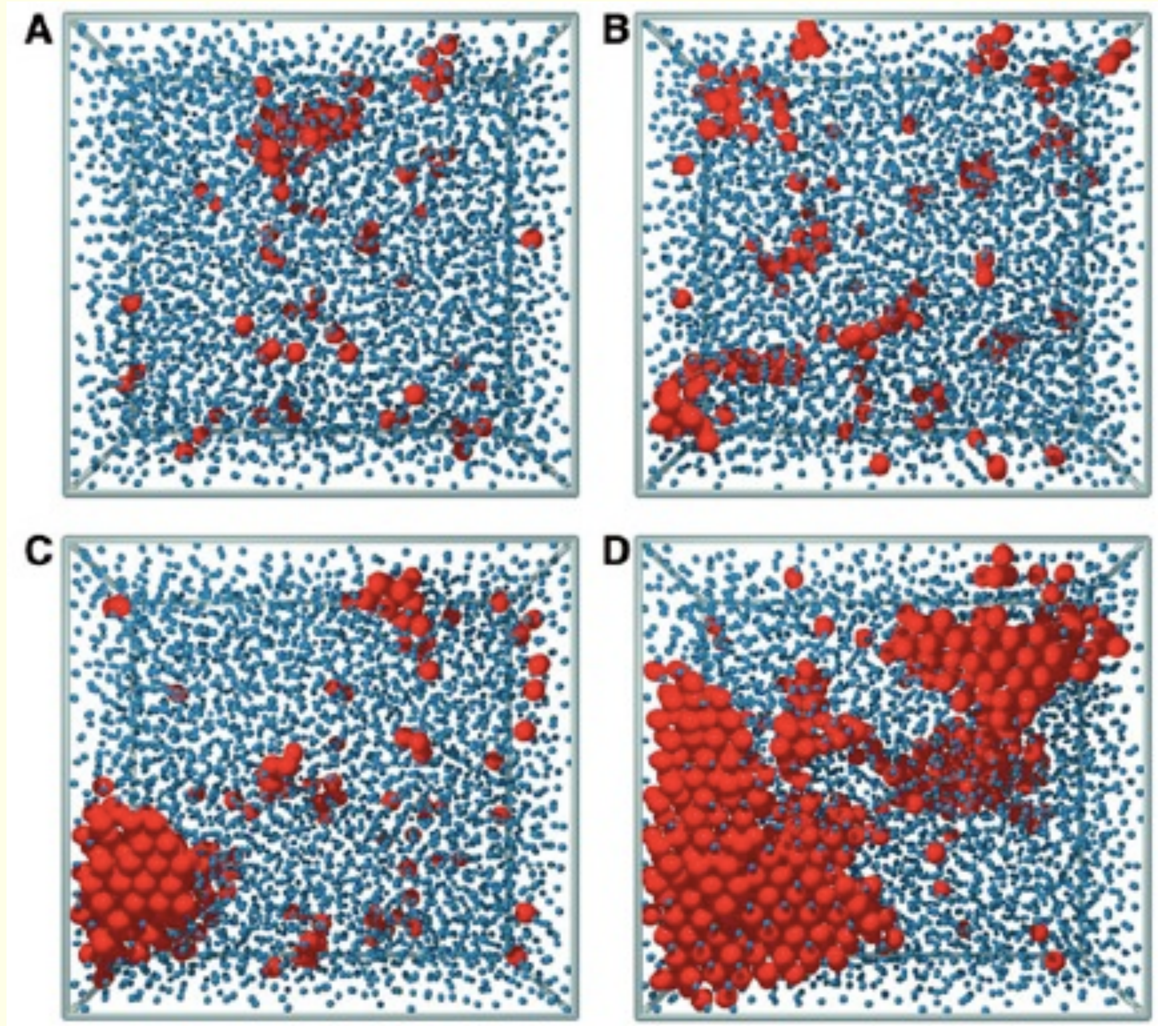
- Structure and dynamics of the critical nucleus.
- Single particle dynamics, dynamical heterogeneities.
- Structure and dynamics of interfaces; growth laws.
- Quench ⇒ glass

  (bidispersity, geometrical frustration)

Barker *et al.* Physica A (1981); ten Wolde *et al.* PRL (1995); Auer *et al.* Nature (2001); Gasser *et al.* Science, (1991); J. Hernandez-Guzman *et al.* PNAS (2009).



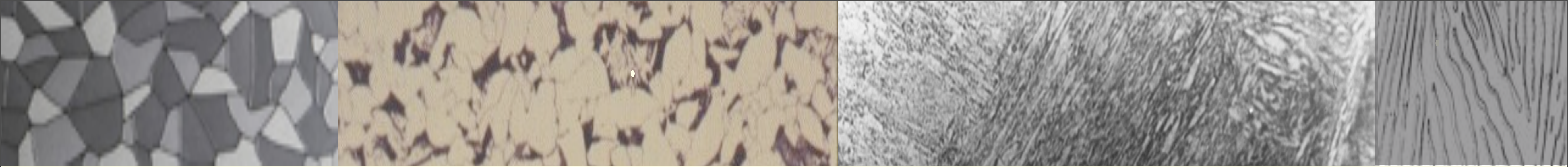


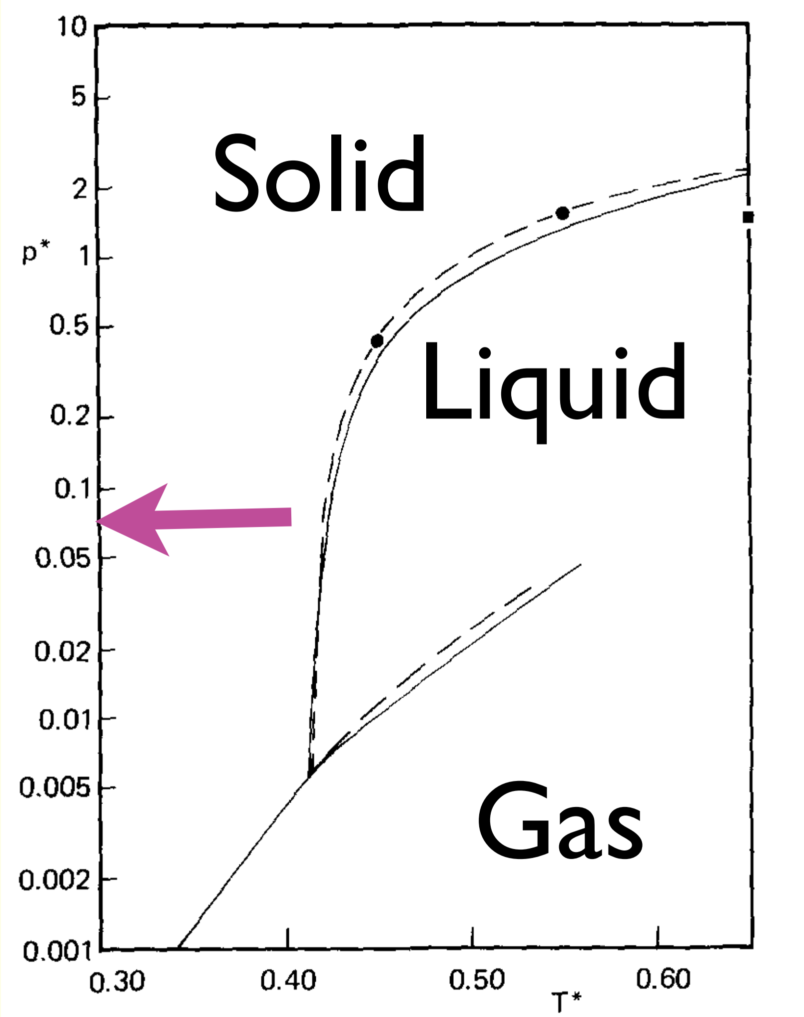


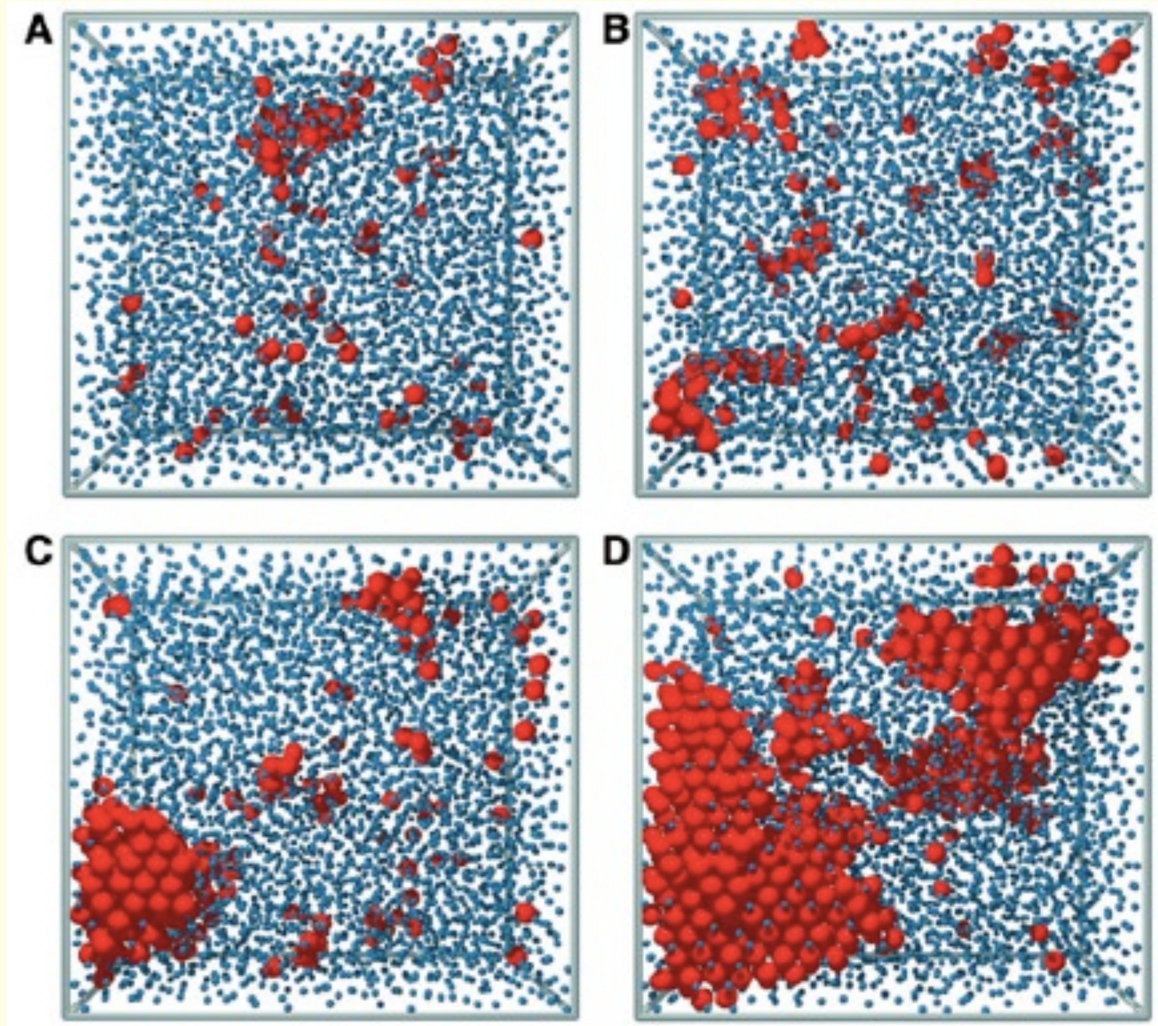
- Structure and dynamics of the critical nucleus.
- Single particle dynamics, dynamical heterogeneities.
- Structure and dynamics of interfaces; growth laws.
- Quench ⇒ glass

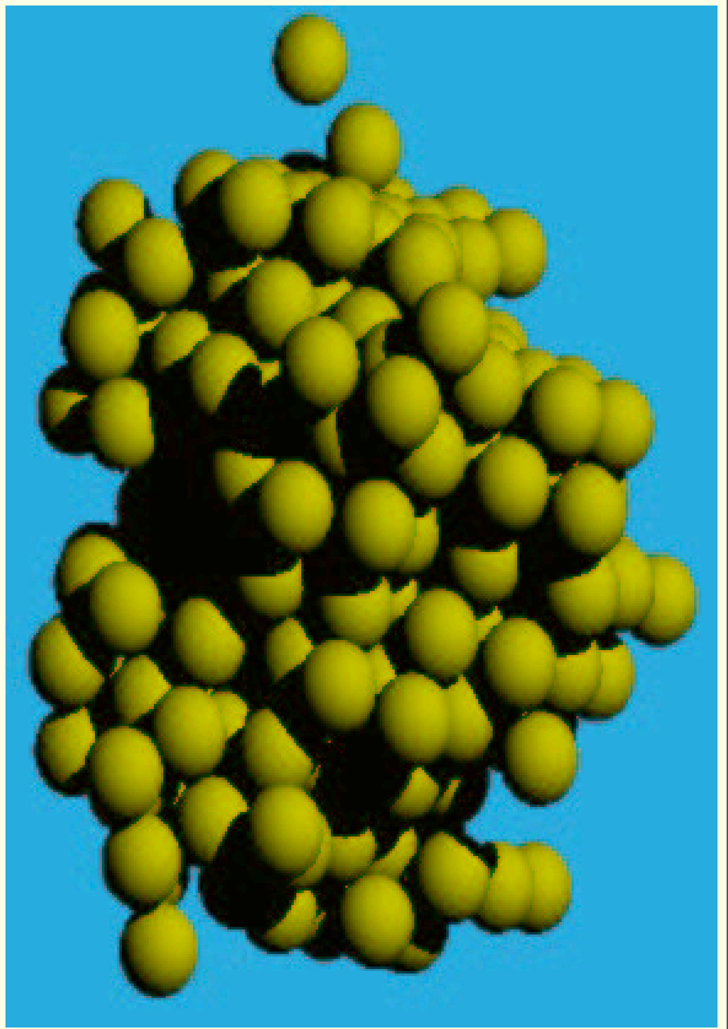
  (bidispersity, geometrical frustration)

Barker *et al.* Physica A (1981); ten Wolde *et al.* PRL (1995); Auer *et al.* Nature (2001); Gasser *et al.* Science, (1991); J. Hernandez-Guzman *et al.* PNAS (2009).





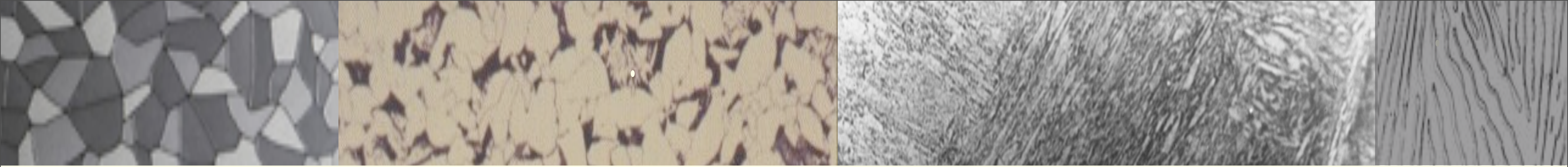


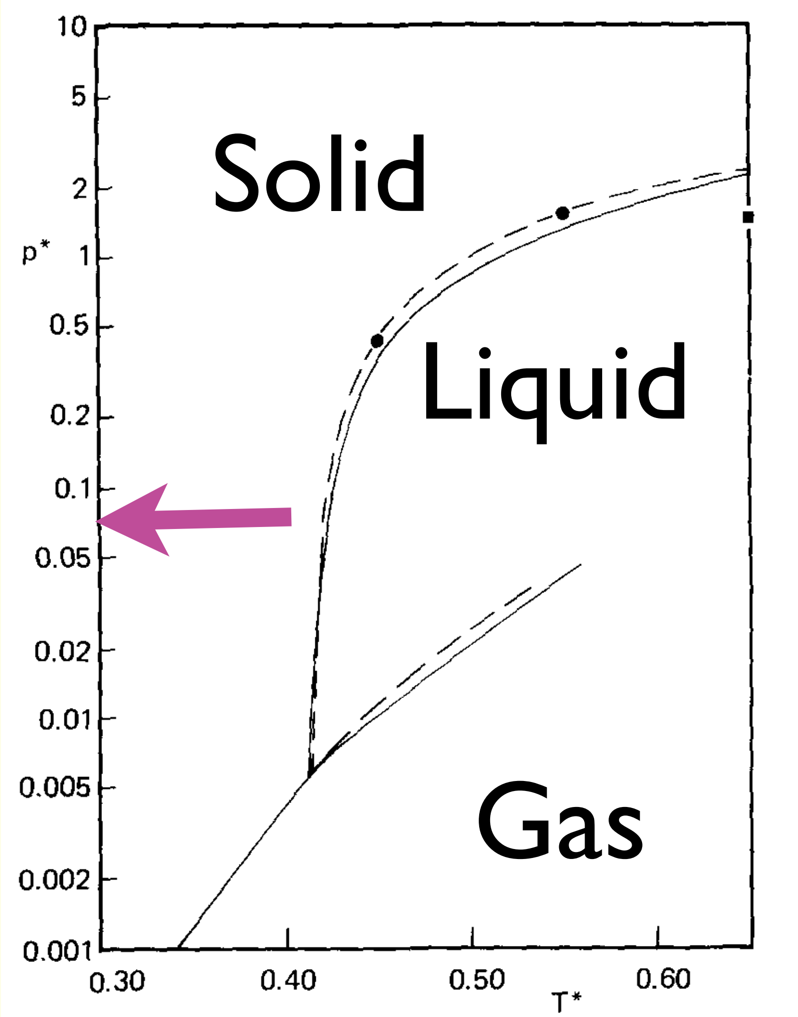


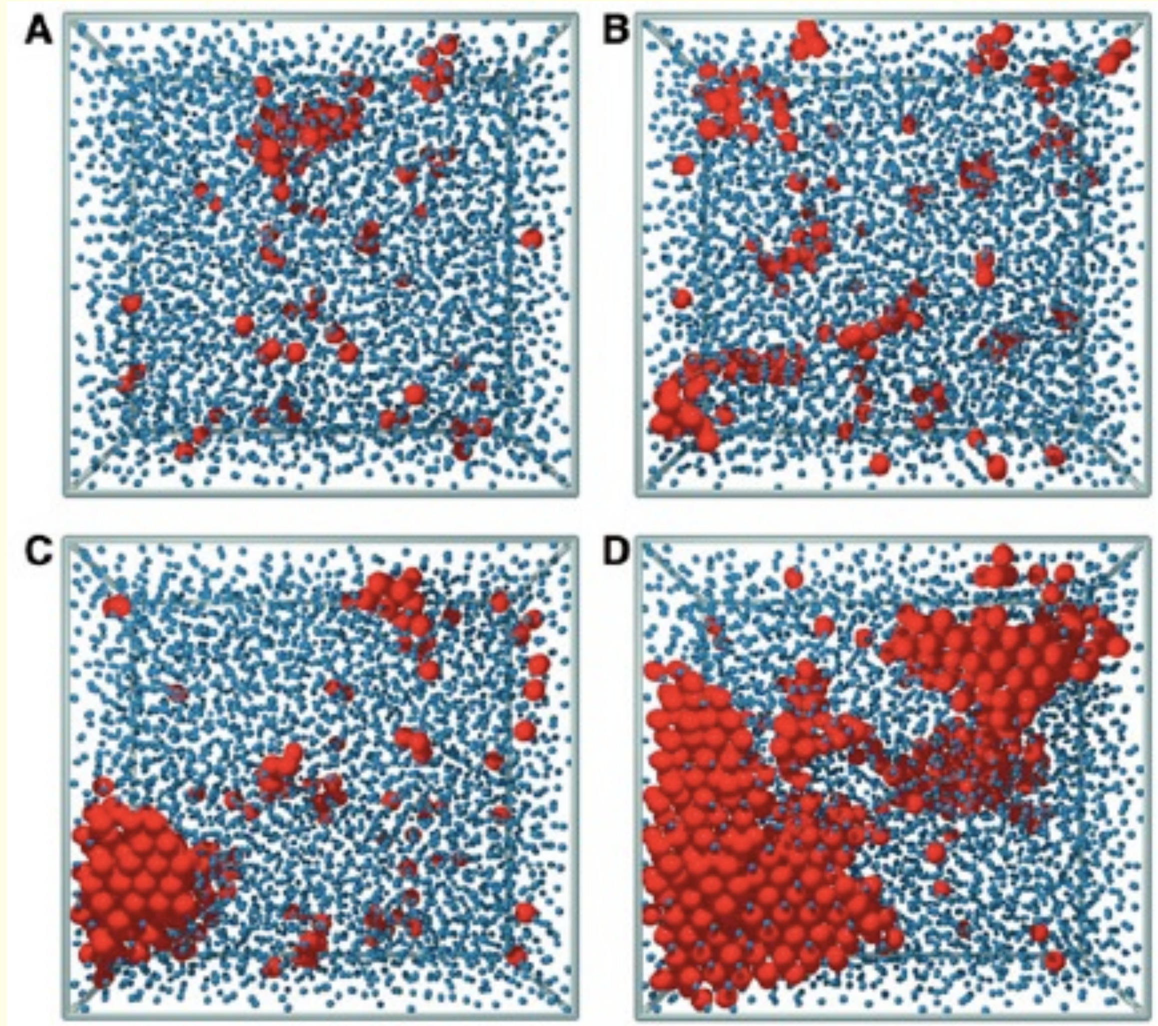
- Structure and dynamics of the critical nucleus.
- Single particle dynamics, dynamical heterogeneities.
- Structure and dynamics of interfaces; growth laws.
- Quench ⇒ glass

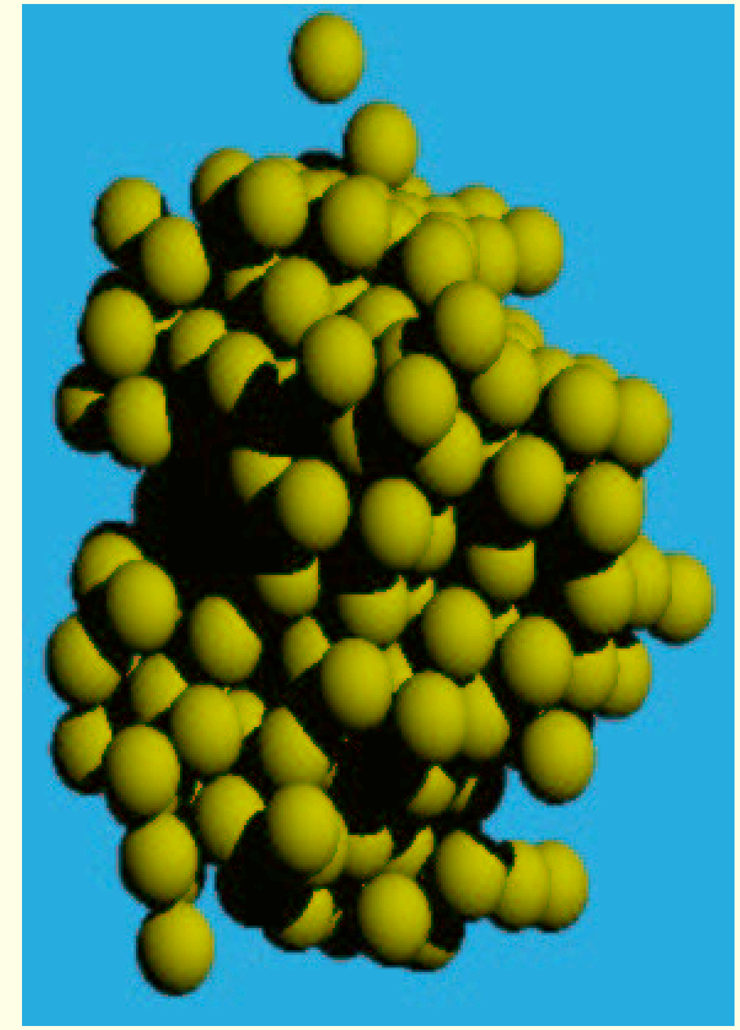
(bidispersity, geometrical frustration)

Barker *et al.* Physica A (1981); ten Wolde *et al.* PRL (1995); Auer *et al.* Nature (2001); Gasser *et al.* Science, (1991); J. Hernandez-Guzman *et al.* PNAS (2009).



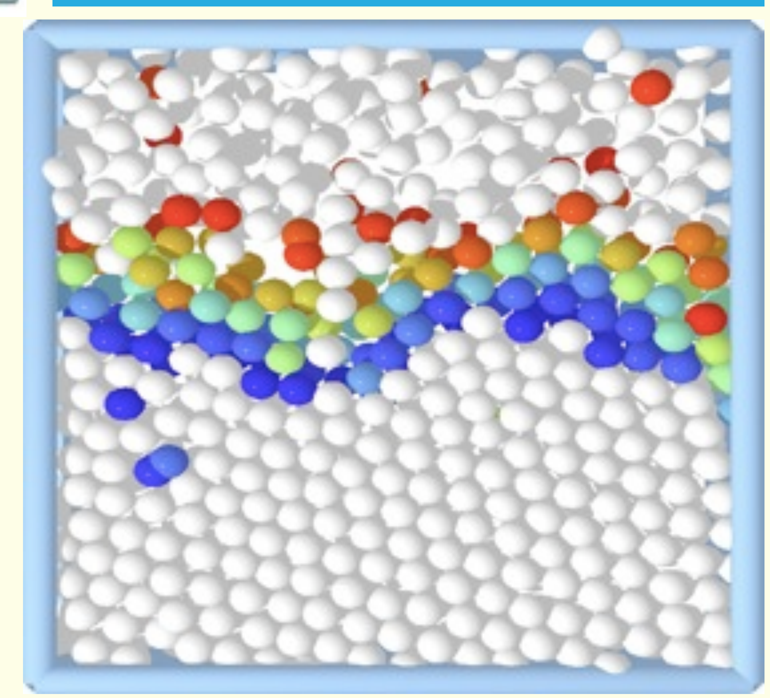




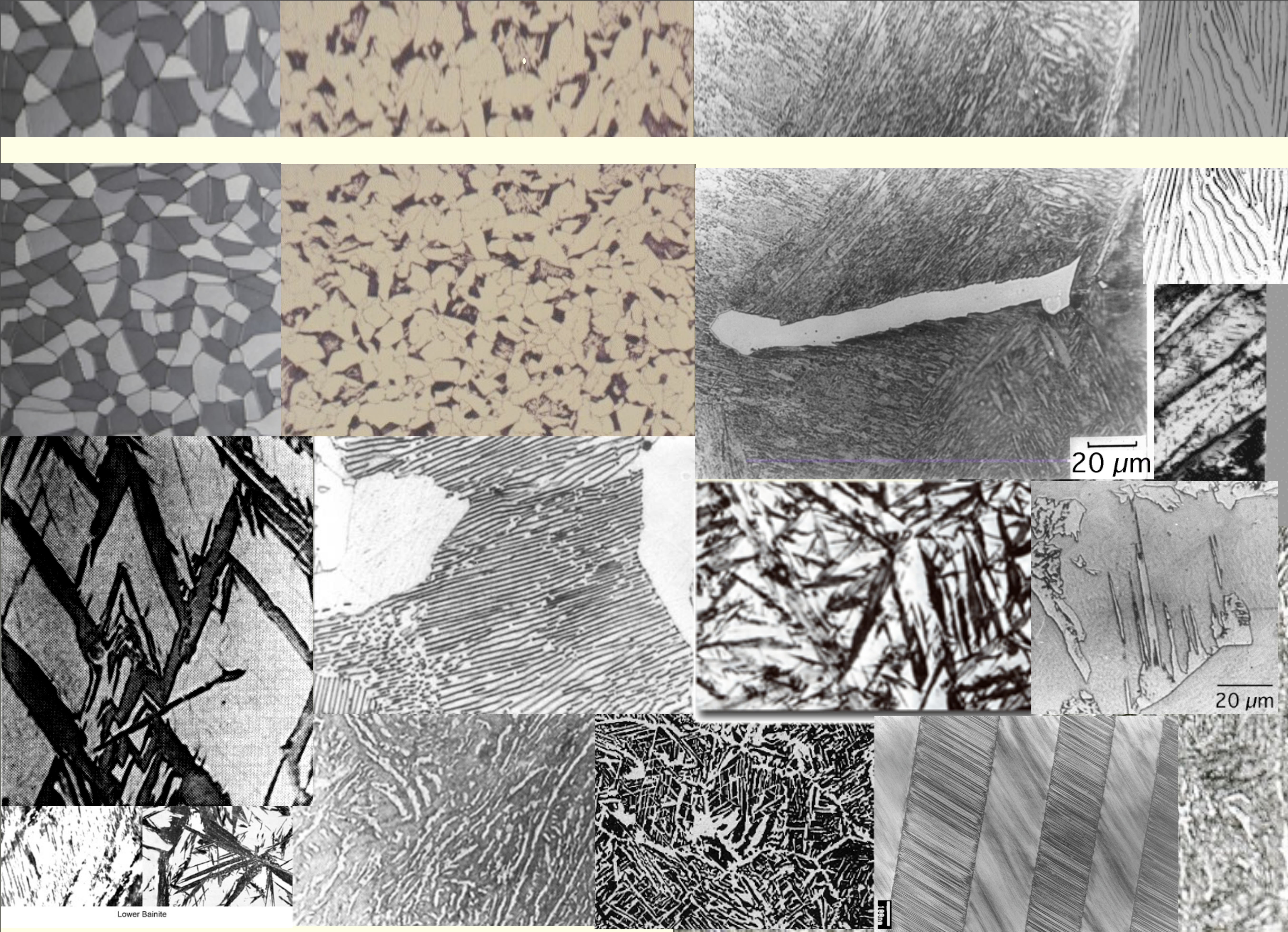


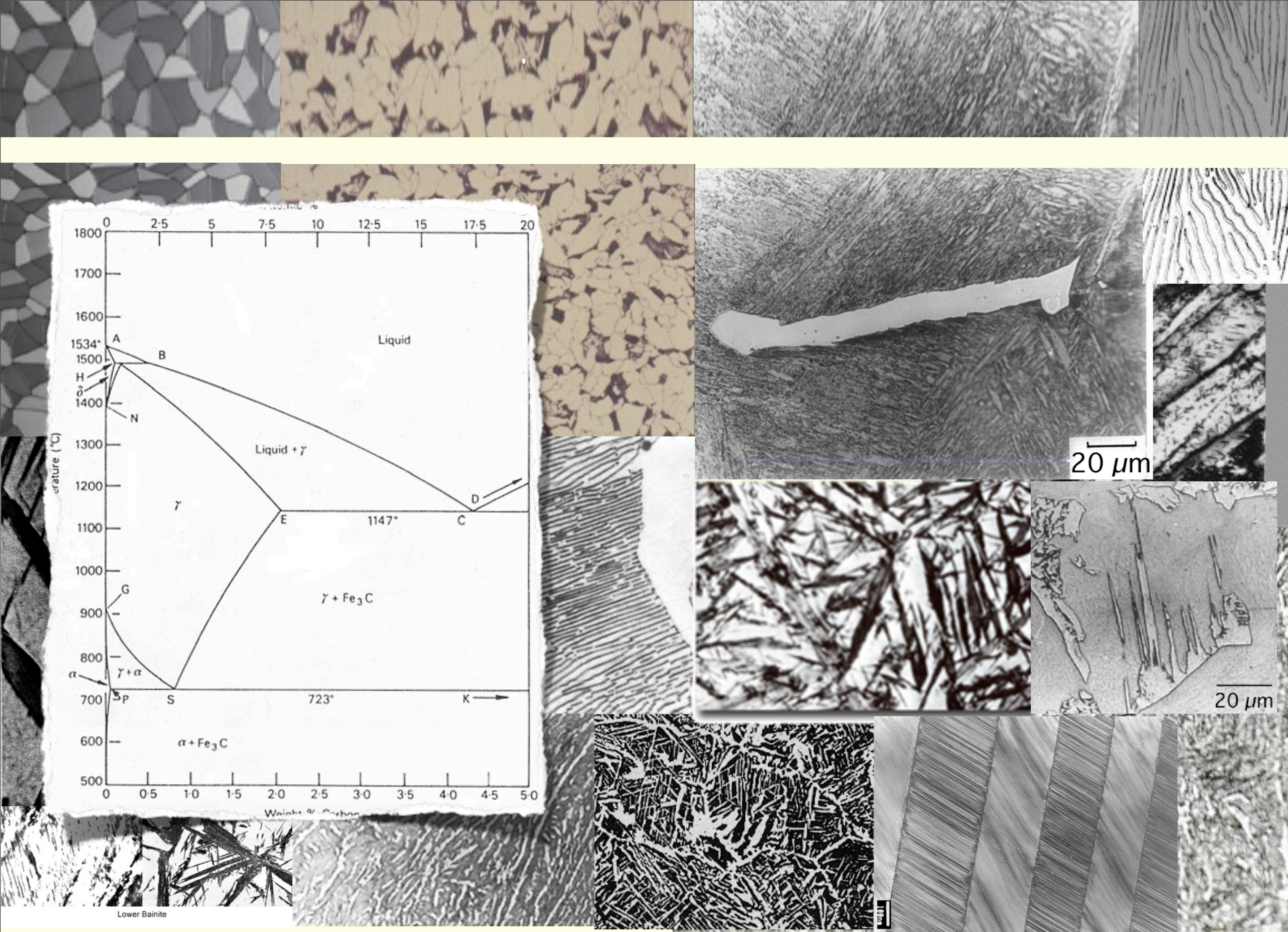
- Structure and dynamics of the critical nucleus.
- Single particle dynamics, dynamical heterogeneities.
- Structure and dynamics of interfaces; growth laws.
- Quench ⇒ glass

  (bidispersity, geometrical frustration)

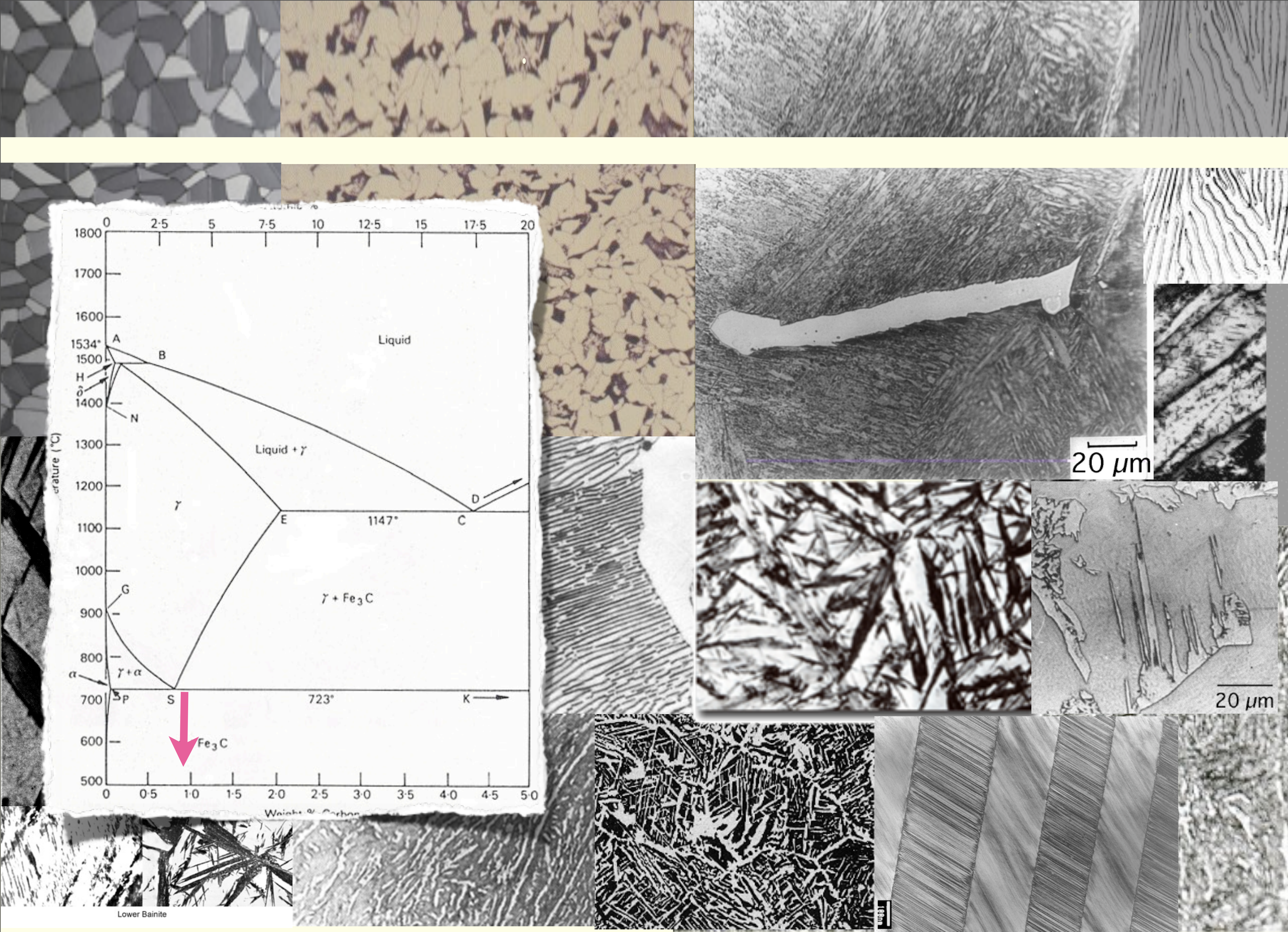


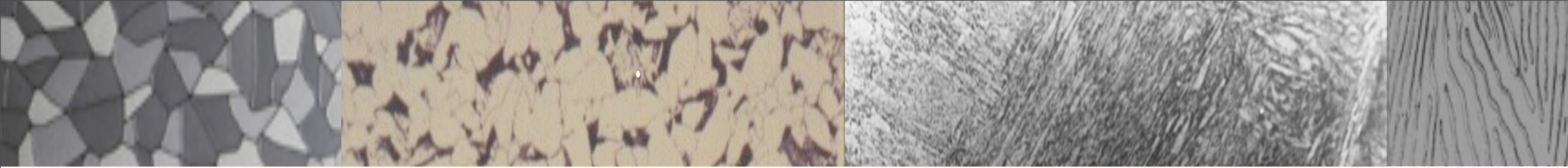
Barker *et al.* Physica A (1981); ten Wolde *et al.* PRL (1995); Auer *et al.* Nature (2001); Gasser *et al.* Science, (1991); J. Hernandez-Guzman *et al.* PNAS (2009).

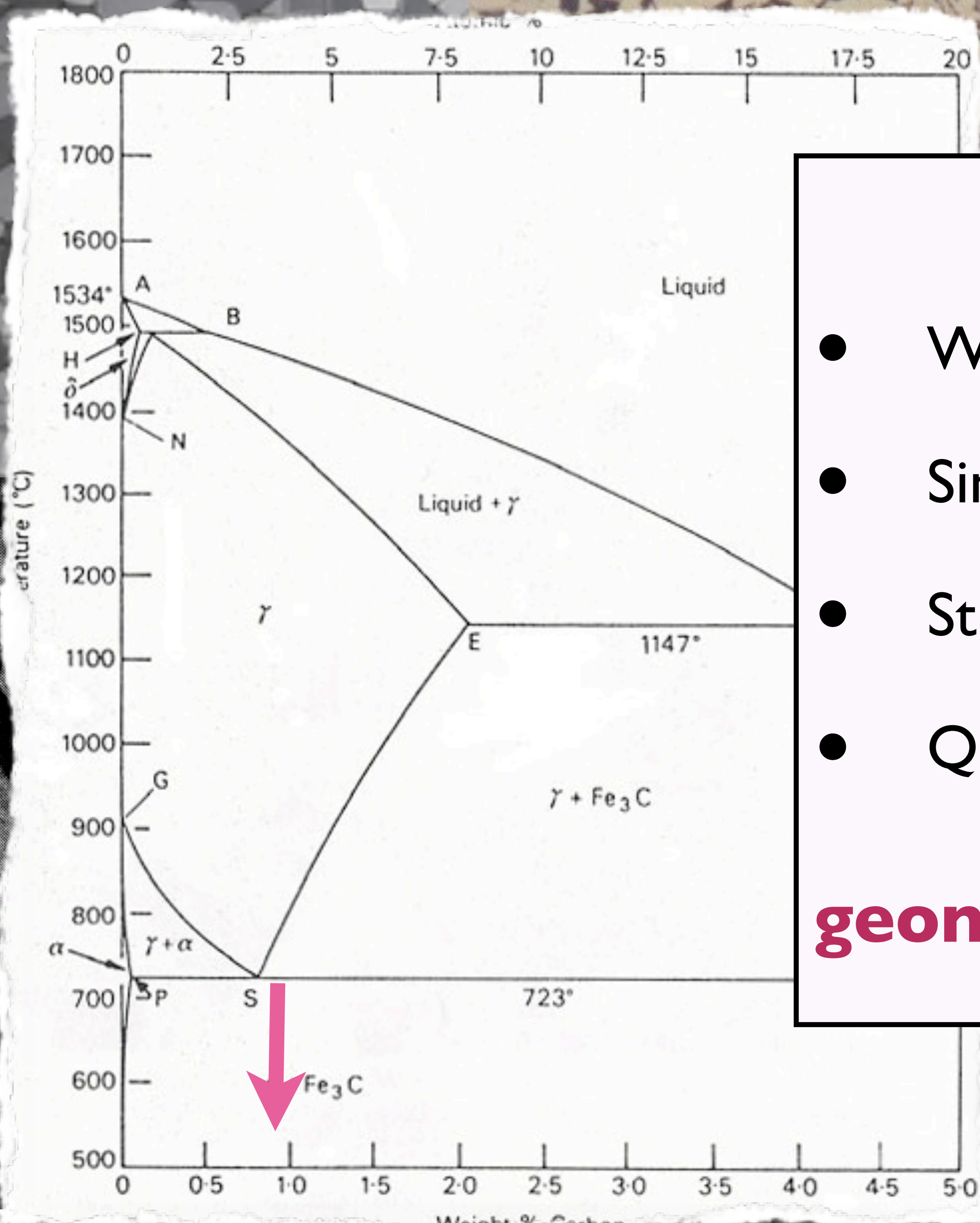

20 μm
20 μm
Lower Bainite



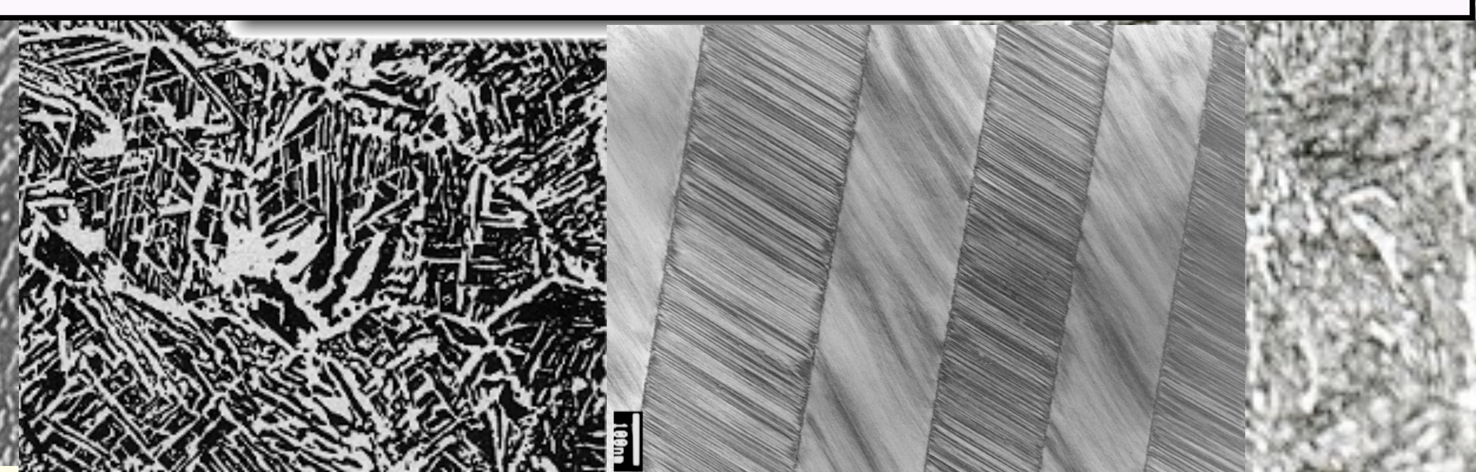
0 2·5 5 7·5 10 12·5 15 17·5 20
1800
1700
1600
1534°
1500
1400
1300
1200
1100
1000
900
800
700
600
500
A
B
H
δ
N
Liquid
Liquid + γ
γ
E
1147°
C
D
G
γ + Fe3C
γ + α
α
P
S
723°
K
α + Fe3C
0 0·5 1·0 1·5 2·0 2·5 3·0 3·5 4·0 4·5 5·0
20 μm
20 μm
Lower Bainite


Liquid
Liquid + γ
γ
γ + Fe₃C
γ + α
Fe₃C
1534°
A
B
H
δ
N
E
1147°
C
D
G
α
P
S
723°
K
Temperature (°C)
Weight % Carbon
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
0
0·5
1·0
1·5
2·0
2·5
3·0
3·5
4·0
4·5
5·0
2·5
5
7·5
10
12·5
15
17·5
20
20 μm
20 μm
Lower Bainite





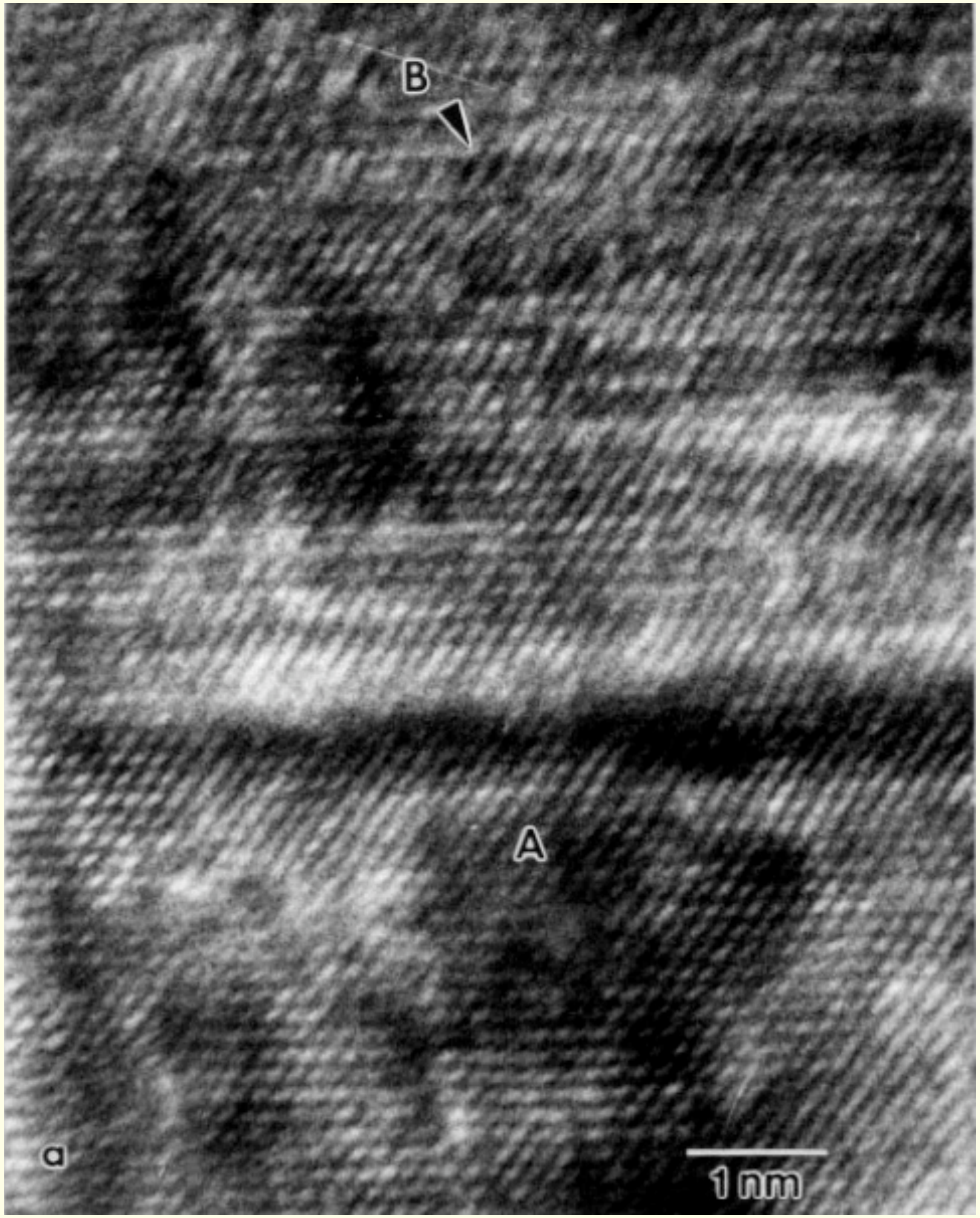

Lower Bainite



- What is the structure and dynamics of the critical nucleus?
- Single particle dynamics, dynamical heterogeneities?
- Structure and dynamics of interfaces; growth laws?
- Quench ⇒ “microstructural” glass?

geometrical frustration in incompatible solids

Compatible solids -Co alloys



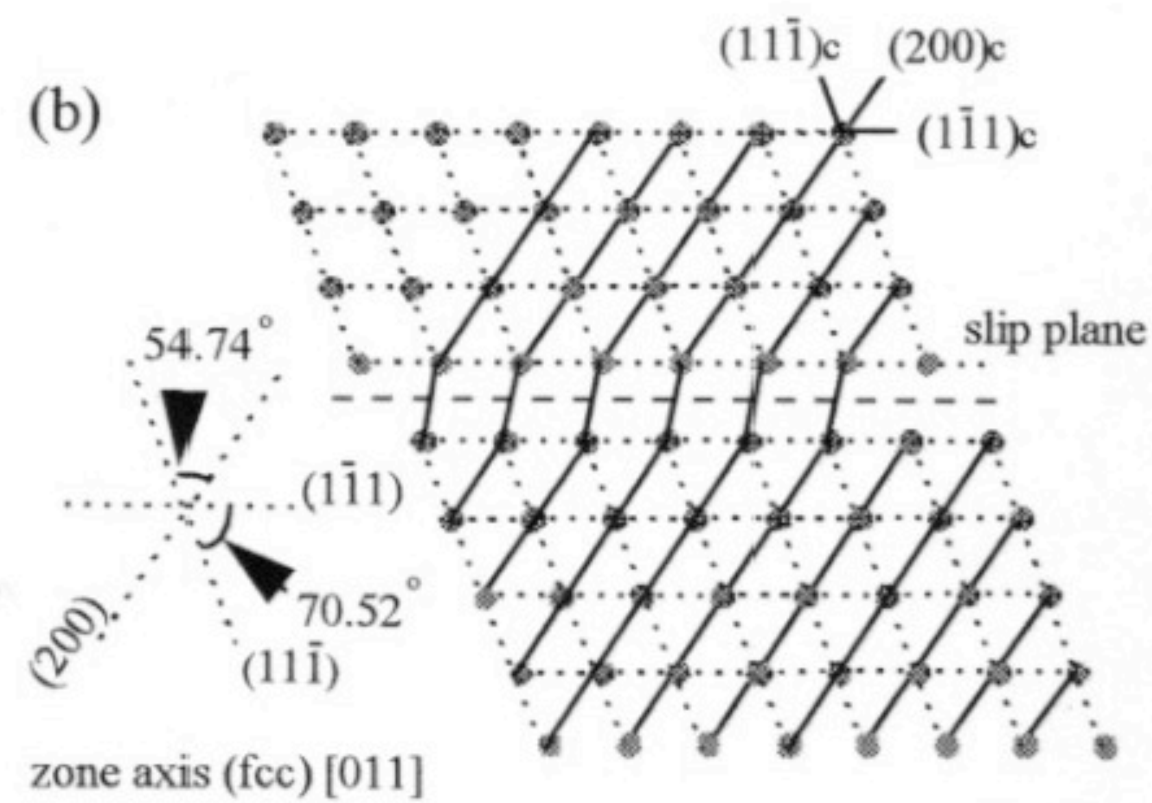
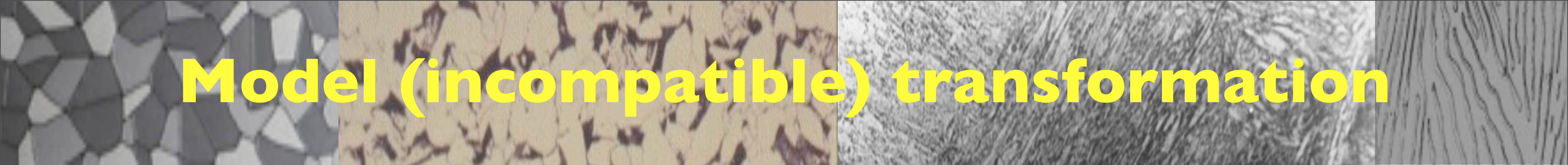
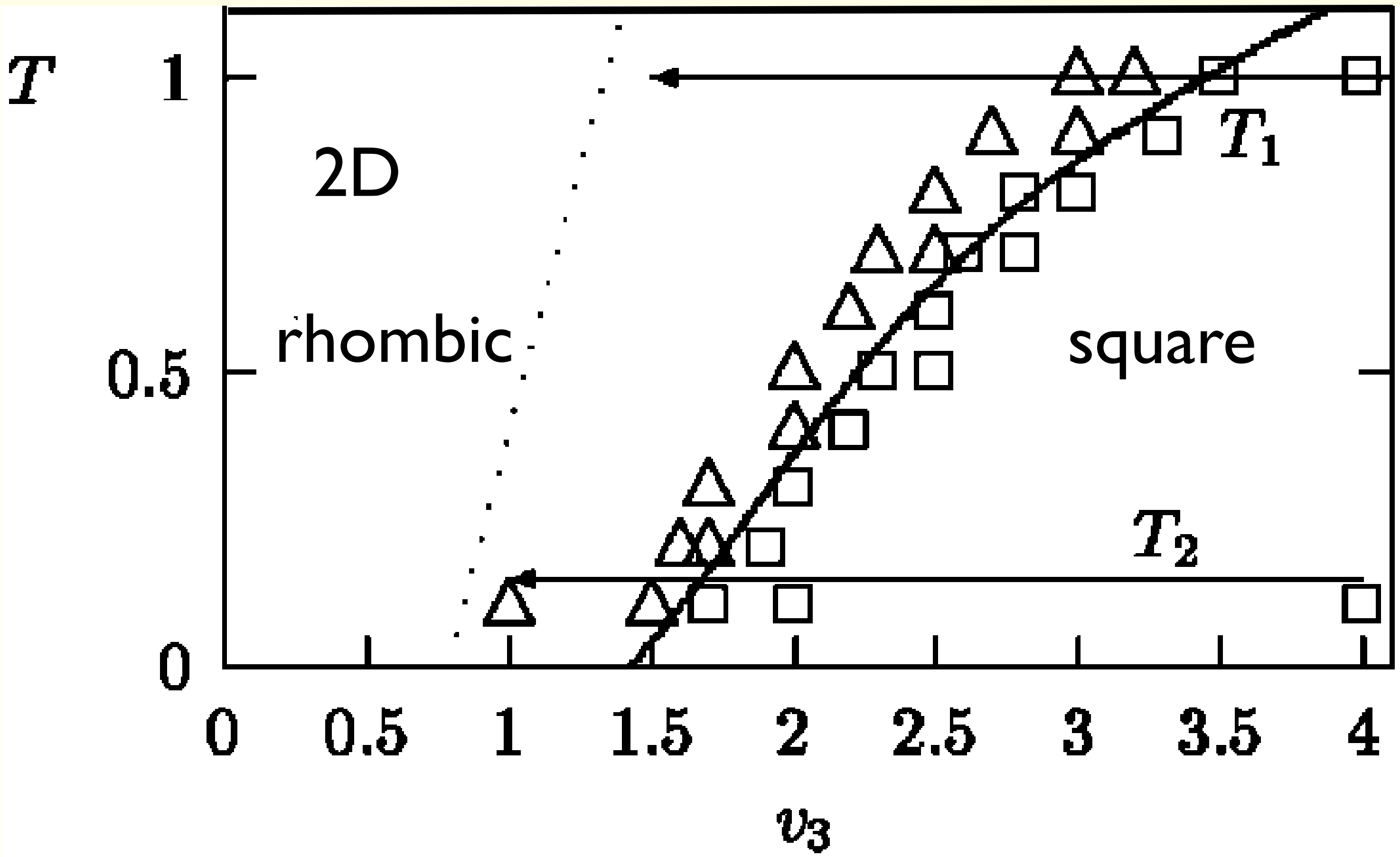
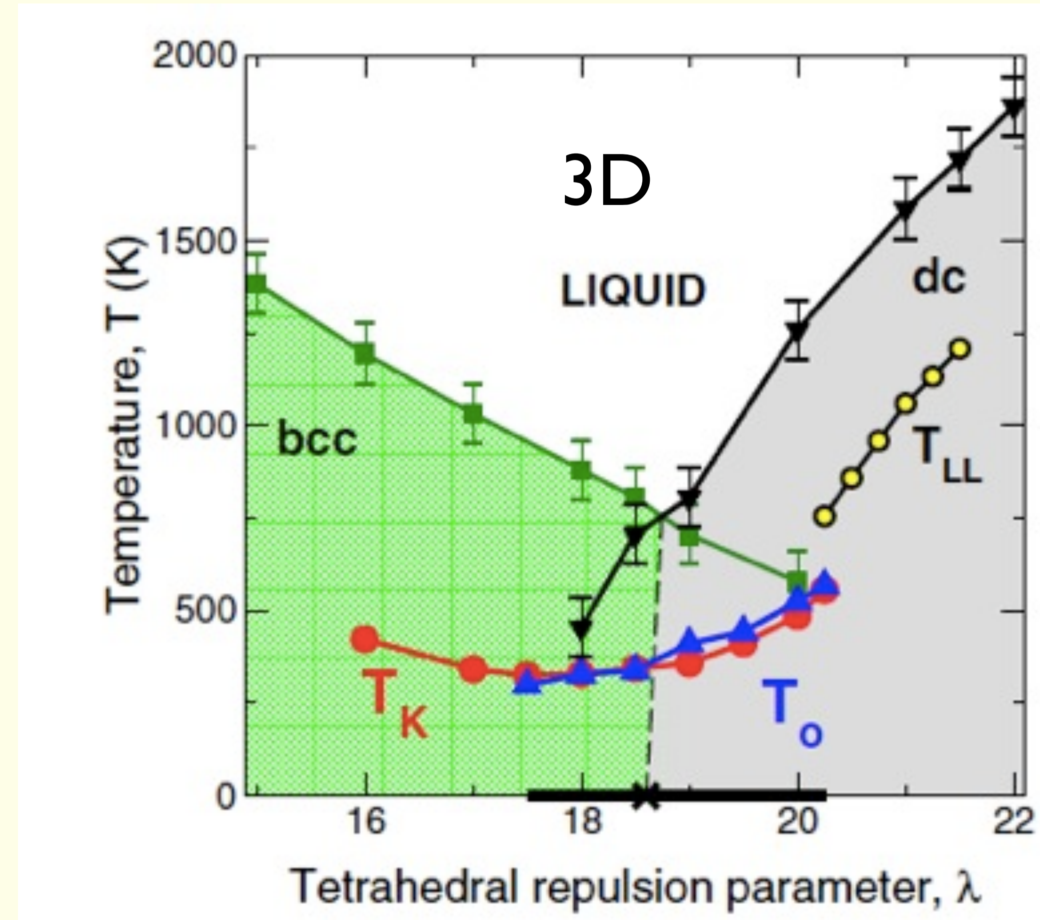


Figure 6. (a) A high-resolution TEM micrograph (plan view) of $Co_{0.75}Pt_{0.25}$ film deposited with IBE 250 eV. Region A is FCC with zone axis [011] and evidence of distortion at B. (b) A schema of areas A and B in the micrograph; this is a projection on the $(011)_c$ plane.



Model (incompatible) transformation

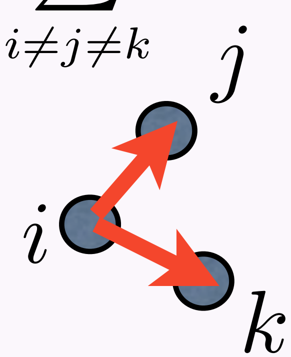




Molinero *et al.* PRL (2006)

$$E = \frac{1}{2}\sum_{i\neq j} V_2(r_{ij}) + \frac{1}{6}\sum_{i\neq j\neq k} V_3(\mathbf{r}_{ij}, \mathbf{r}_{jk}, \mathbf{r}_{ki})$$

$$V_2 = v_2(\frac{\sigma}{r_{ij}})^{12}$$



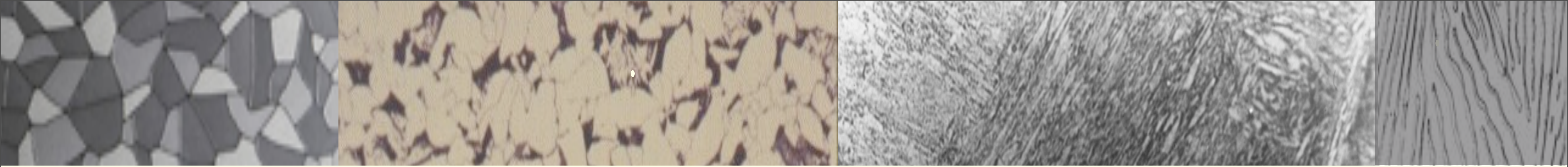
$$V_3 = v_3[f_{ij} f_{ik} sin^2(4\theta_{ijk}) + \cdots]$$

Purely repulsive system

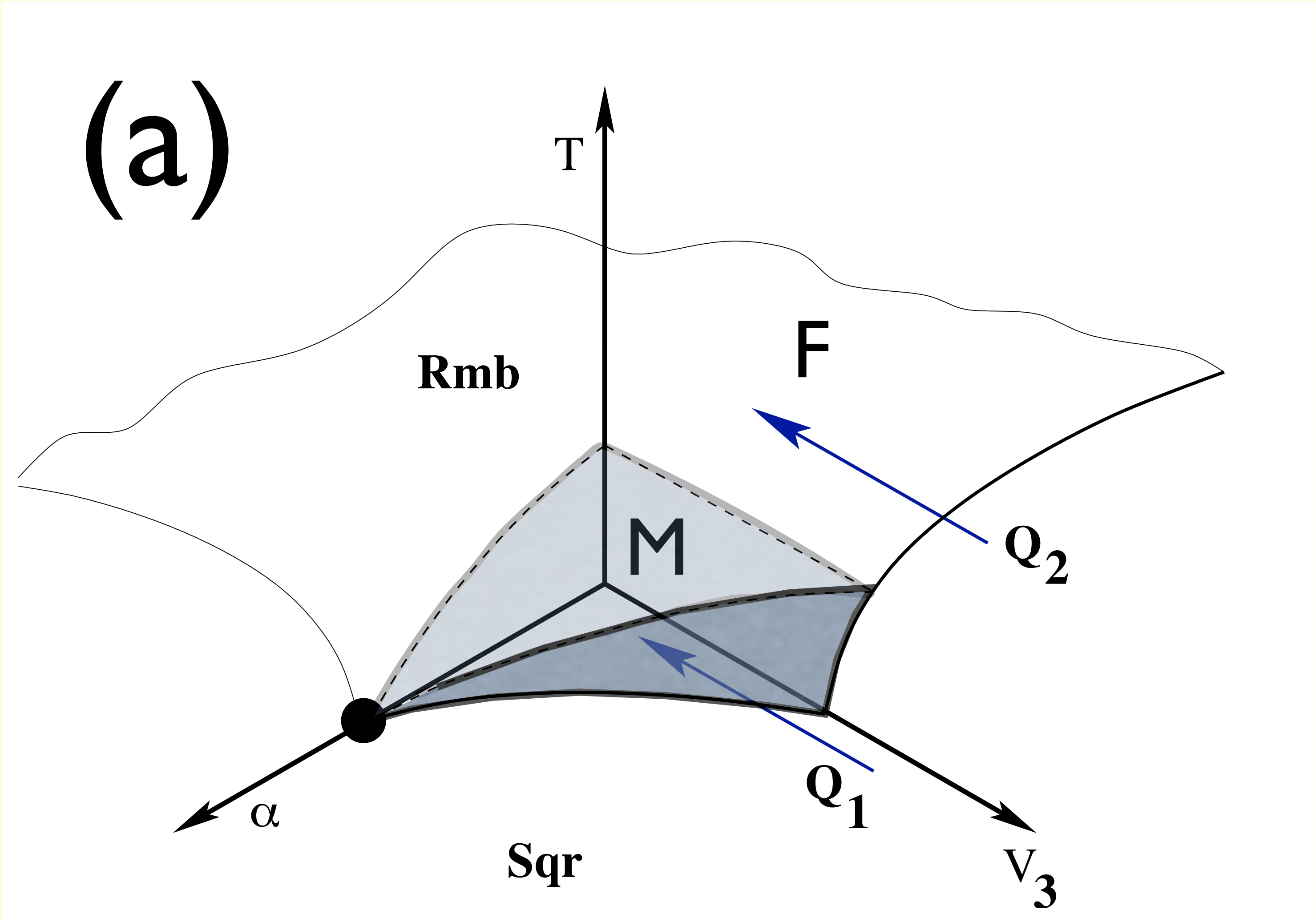
NVT - MD simulations

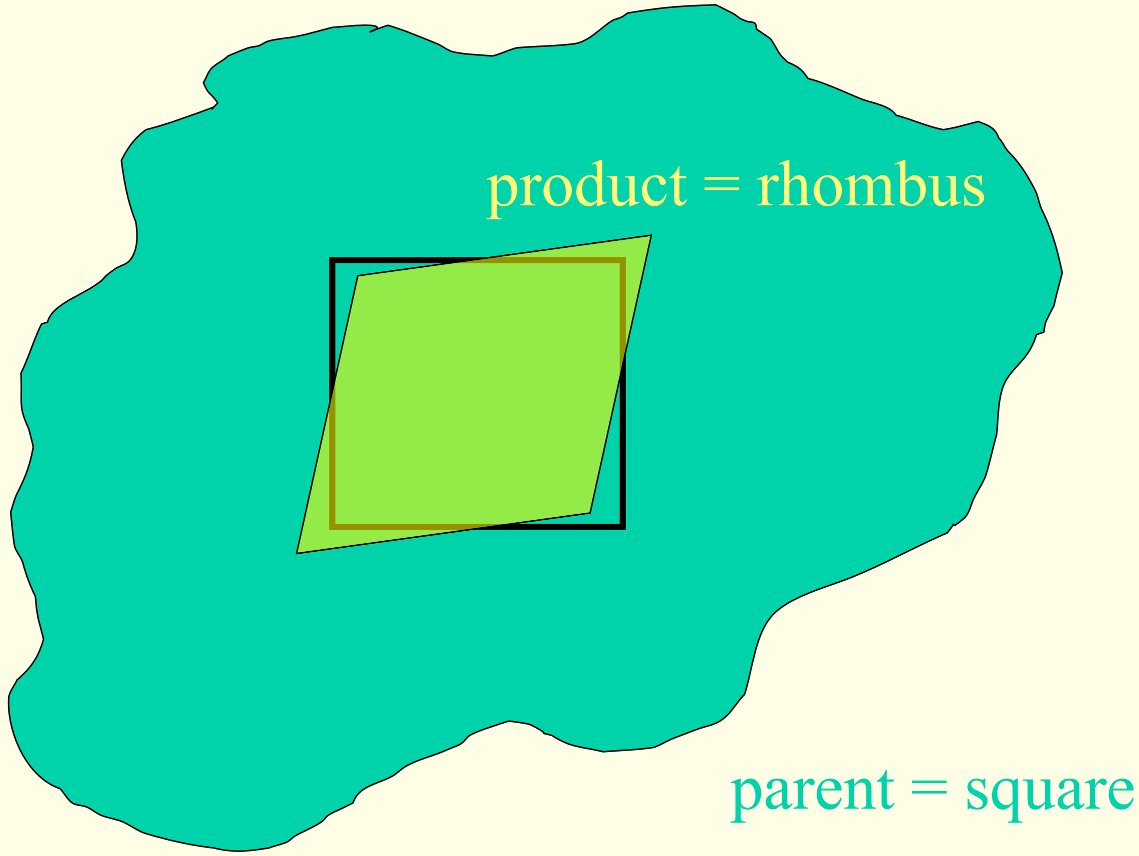
N = 10000-20000

M. Rao S. Sengupta, PRL, (1997), (2003); J. Phys. Condens. Matter (2004)



Tuning incompatibility - frustration

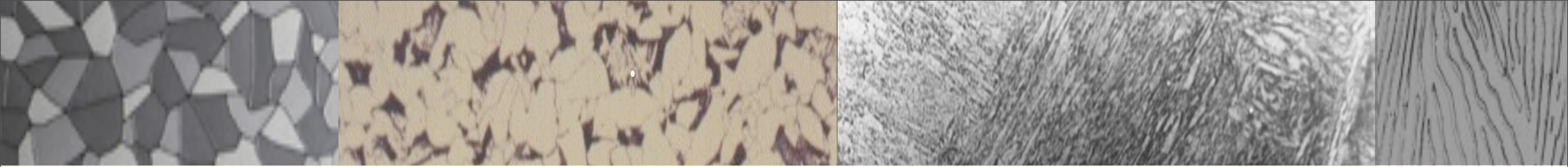




shear strain is the o.p. for the transition

$$e_3 = \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}$$

Rao, Sengupta, PRL, (1997)
J. Bhattacharya et al., J. Phys. Condens. Matt. (2008);

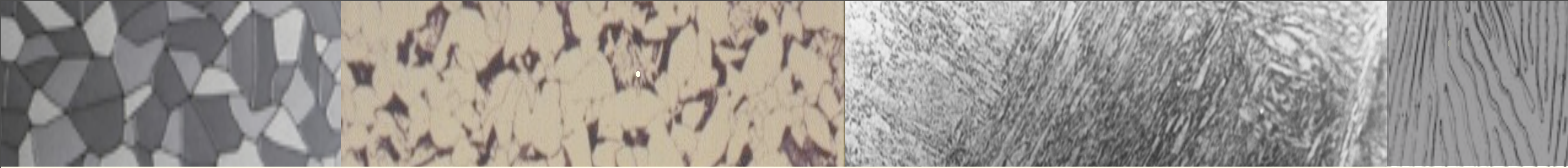


Q1 | Q2
low T | high T

M- phase | F-phase

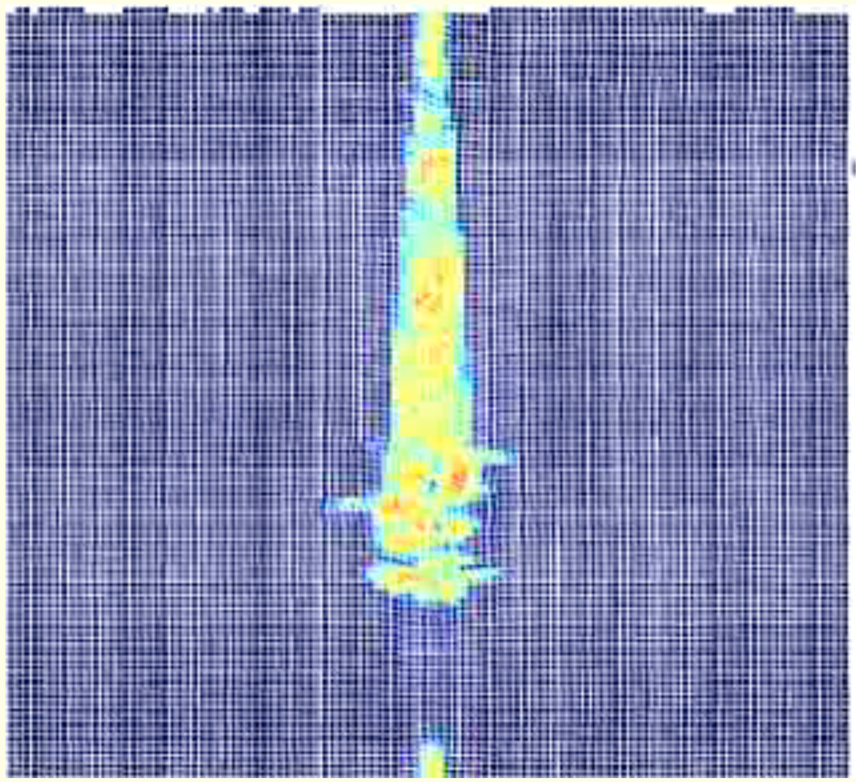
Colors measure local coordination

Blue = 4 Red = 6



Q1

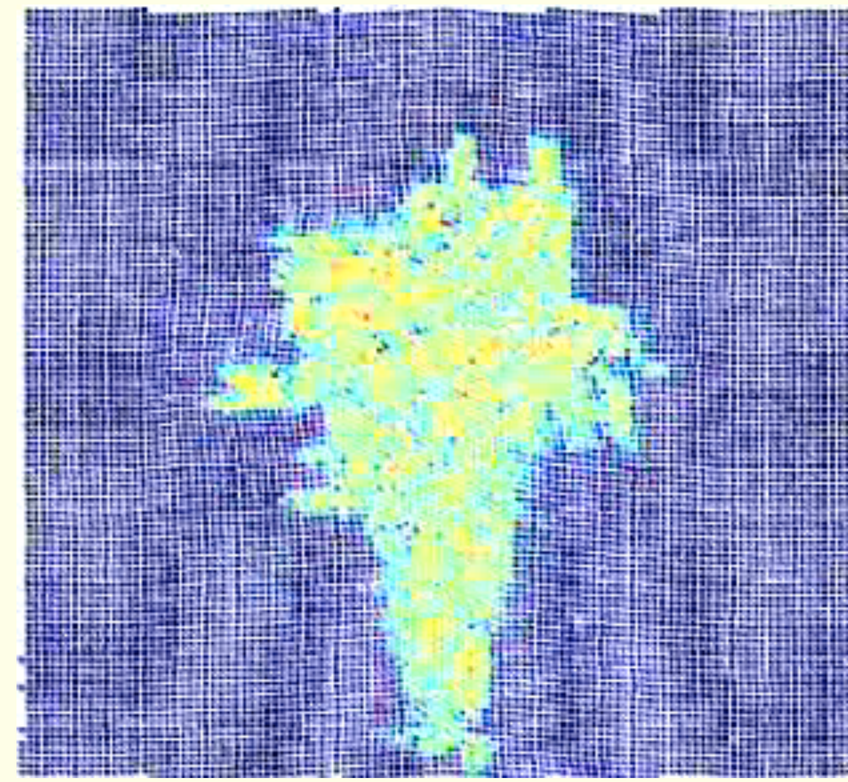
low T



M- phase

Q2

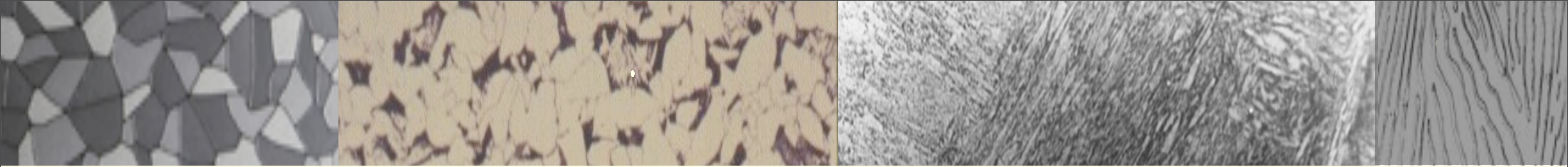
high T



F-phase

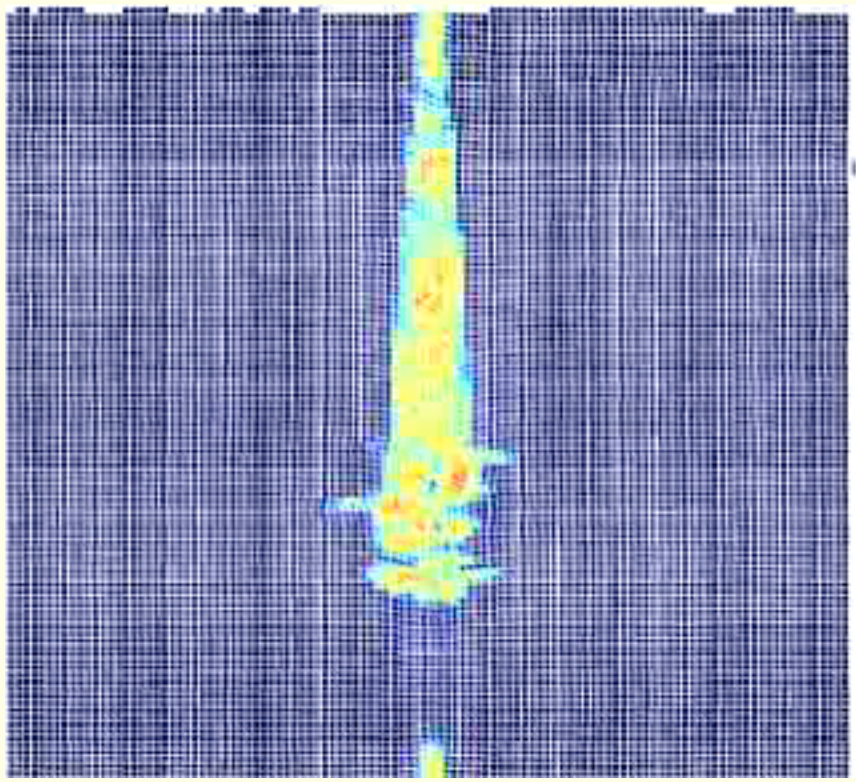
Colors measure local coordination

Blue = 4 Red = 6



Q1

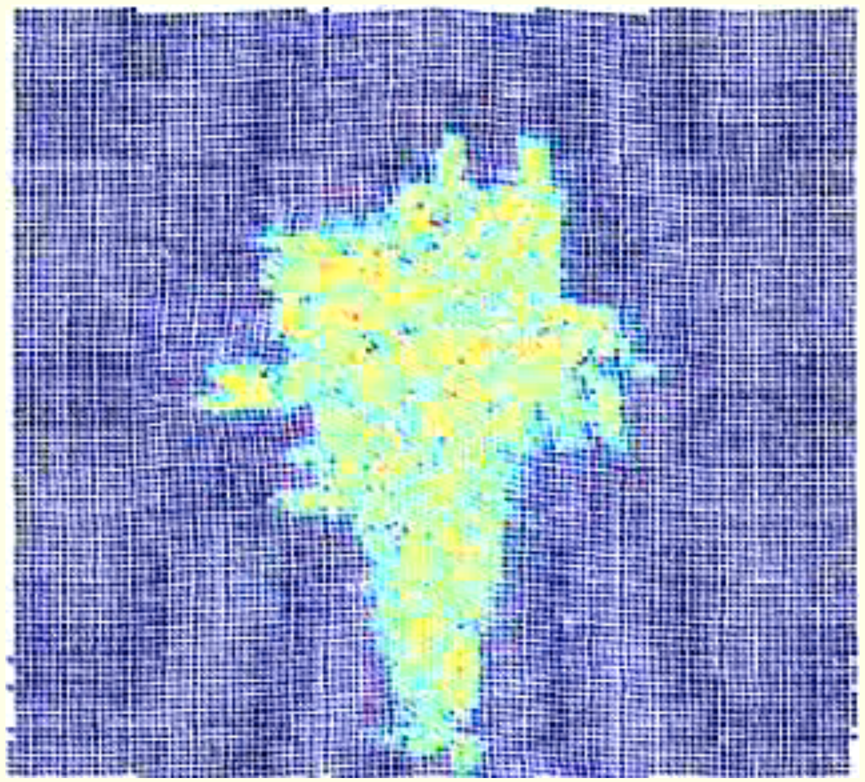
low T



M- phase

Q2

high T

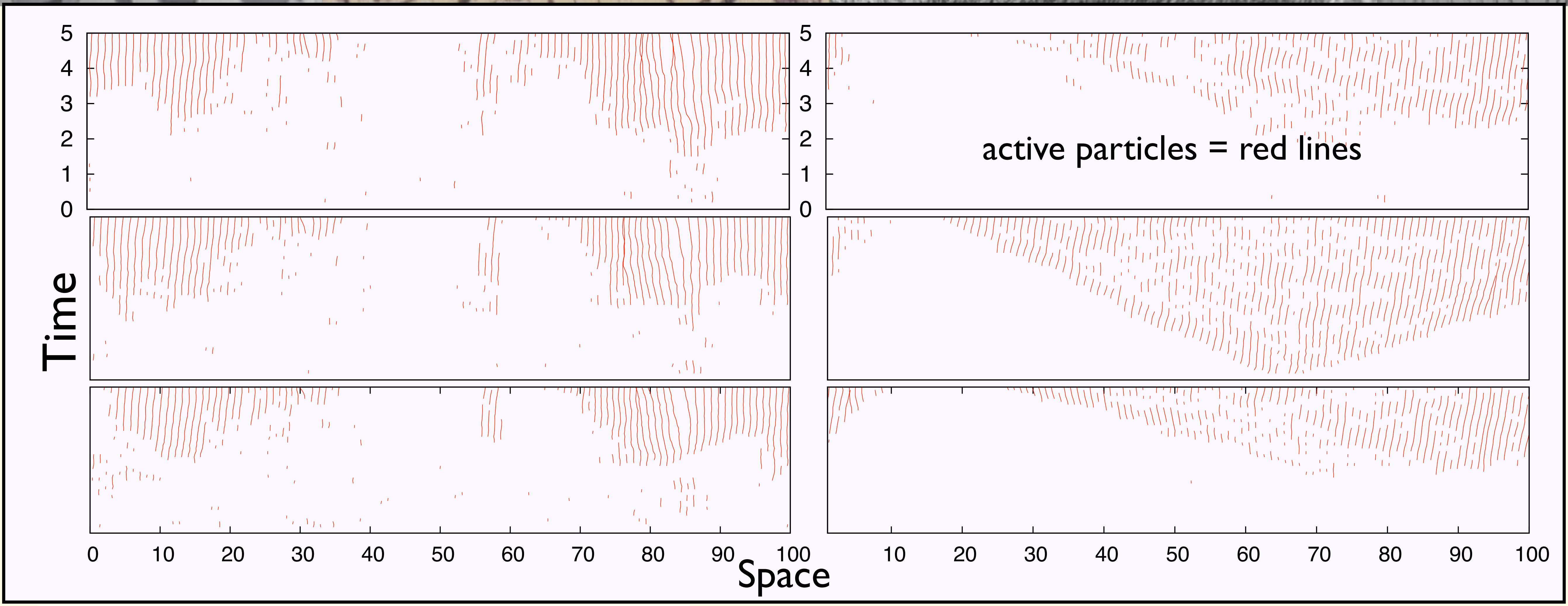


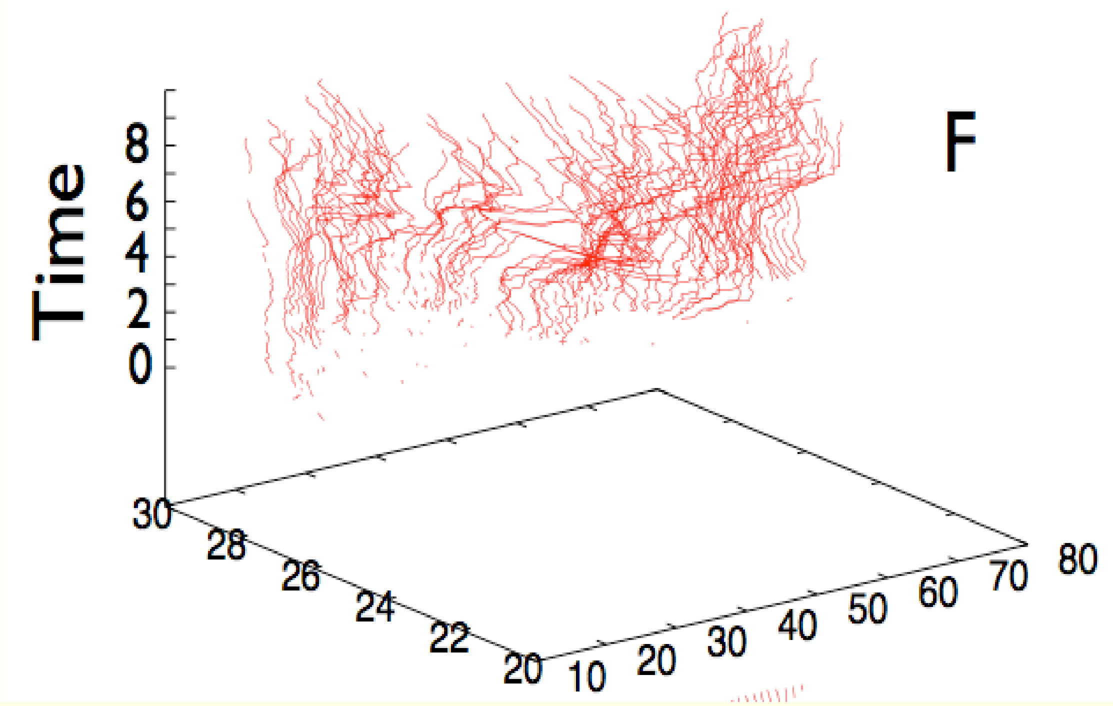
F-phase

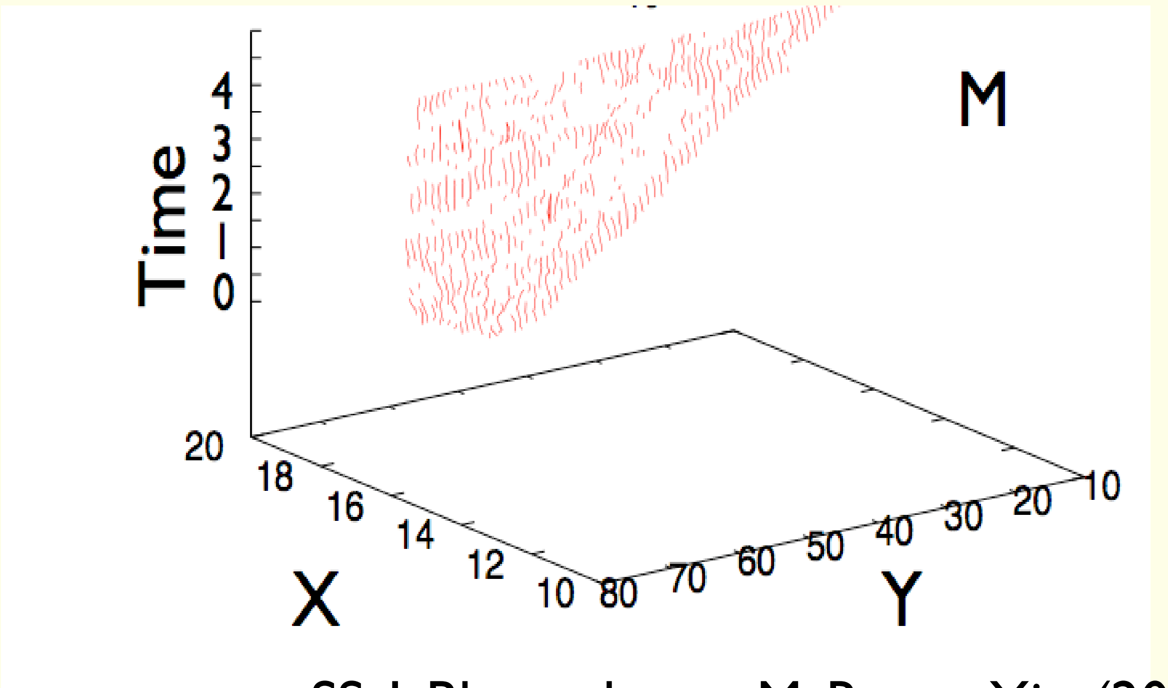
Colors measure local coordination

Blue = 4 Red = 6

Single particle trajectories - “kymographs”

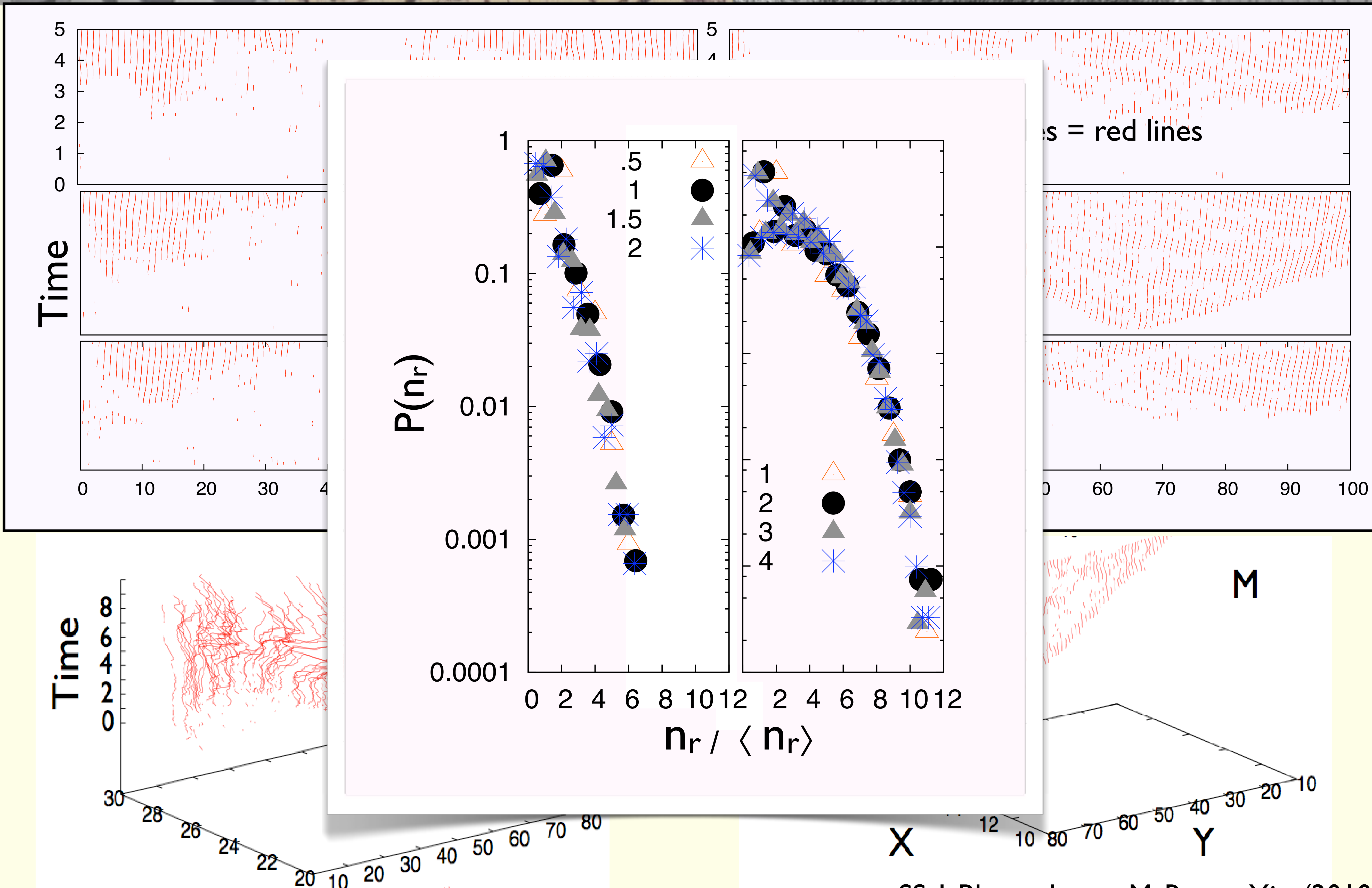






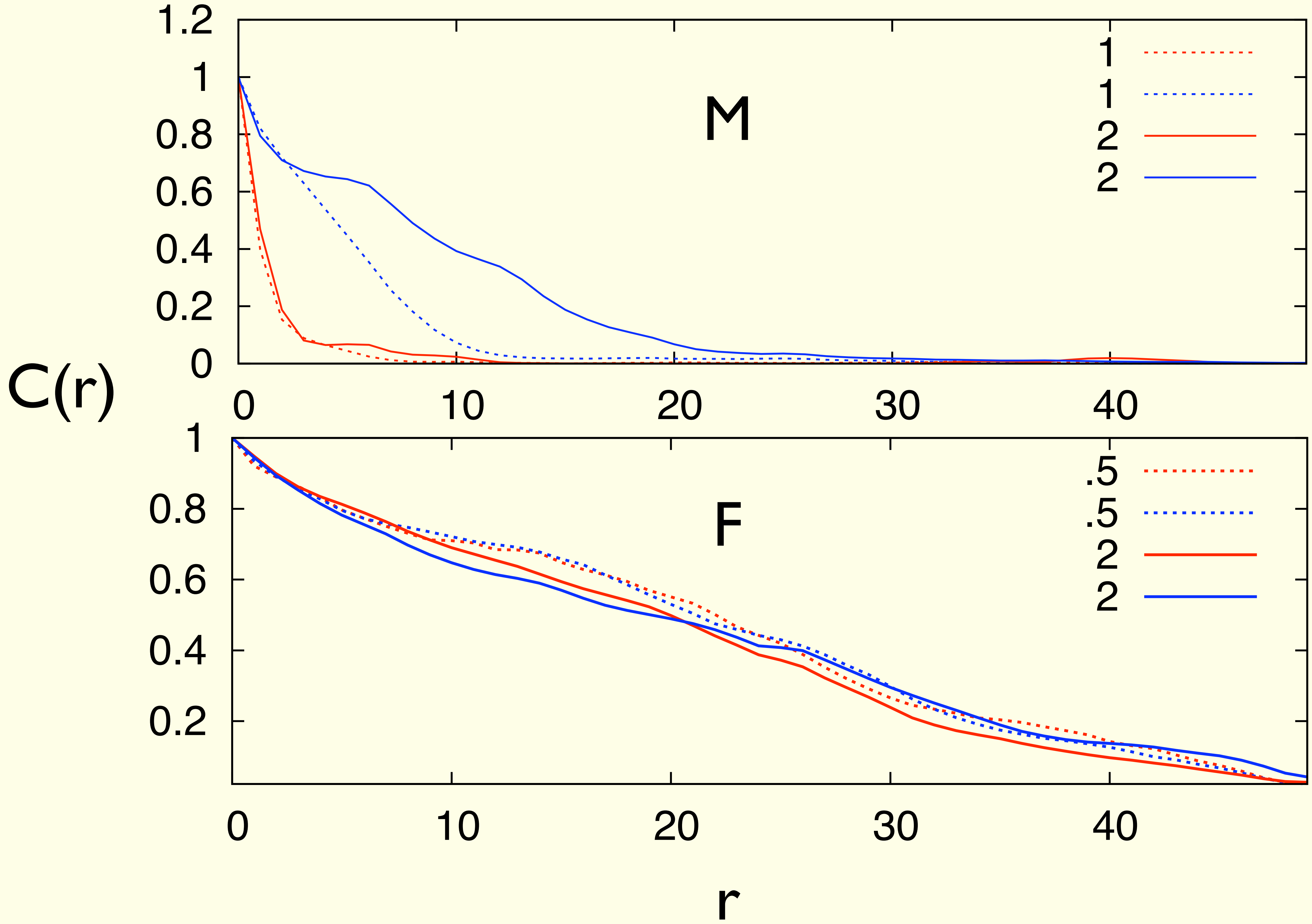
SS, J. Bhattacharya, M. Rao, arXiv: (2010)

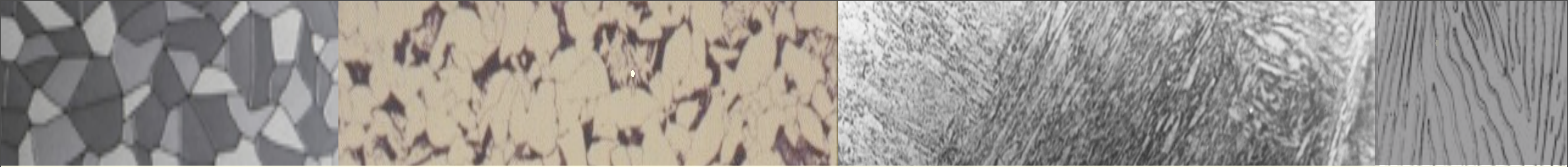
Single particle trajectories - “kymographs”

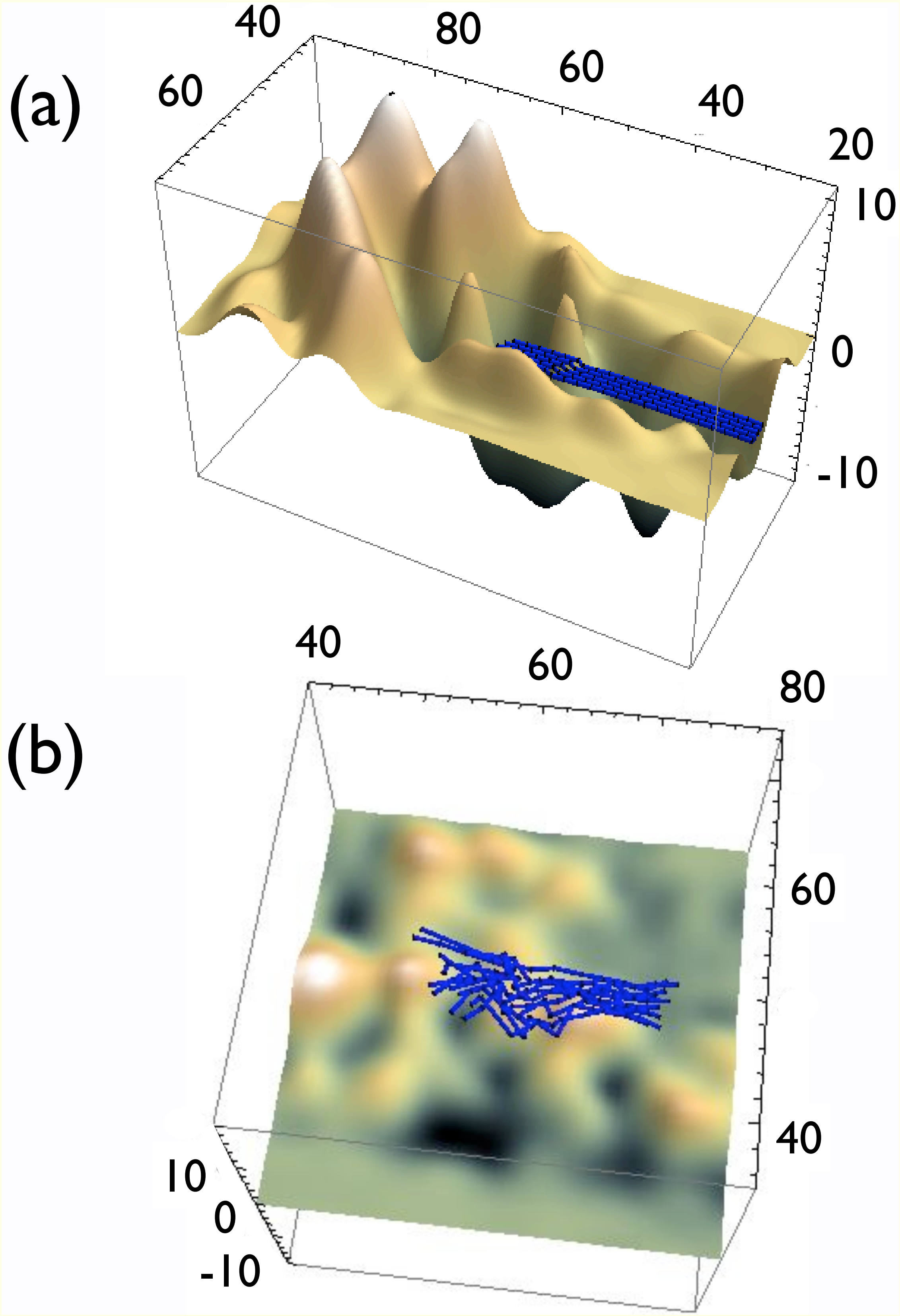


SS, J. Bhattacharya, M. Rao, arXiv: (2010)

Activity correlations







- dynamical heterogeneities localized at the transformation front

- active - inactive transitions.

- active particles flow within channels in the free energy topography shaped by inactive particles.

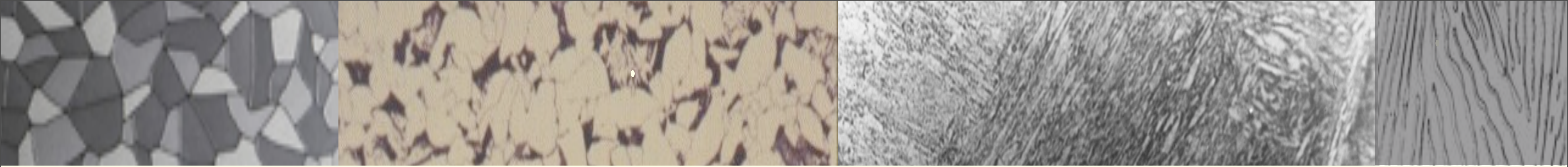
- low temps - few channels - confining potential - ballistic trajectory ⇒ M

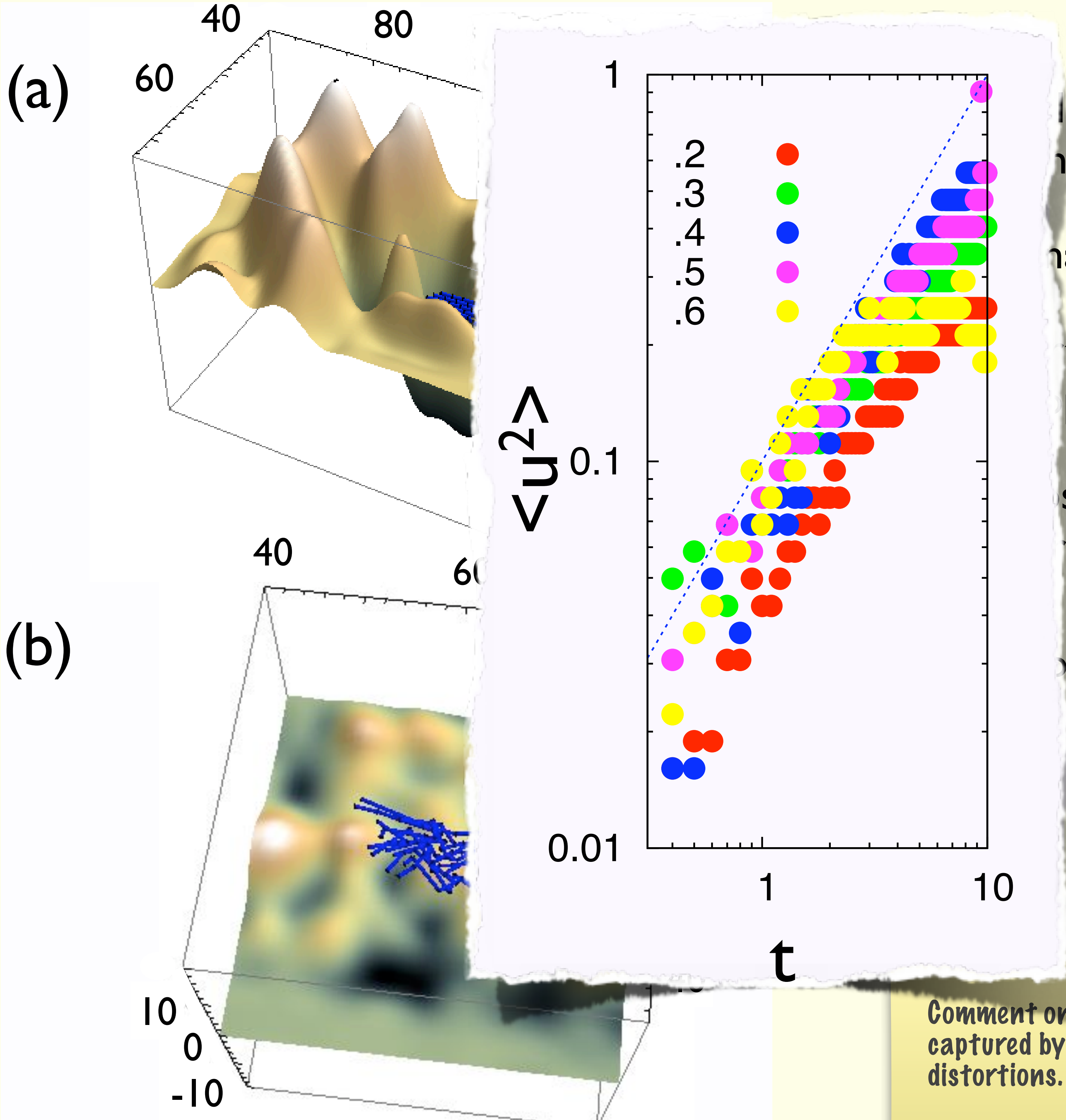
- high temps - many intersecting channels - no confining potential - diffusive trajectories ⇒ F

- **How to characterize these excitations?**

Comment on dynamical matrix. Improbable trajectories are not captured by dynamical matrix which measures the local elastic distortions.

How to characterize these distortions?



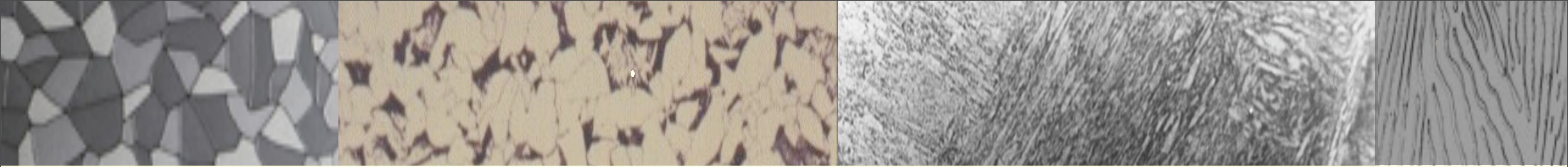


- heterogeneities localized at the ation front
- active transitions.
- ticles flow within channels in the free pography shaped by inactive particles.
- s - few channels - confining potential - ajectory ⇒ M
- s - many intersecting channels - no potential - diffusive trajectories ⇒ F

characterize these excitations?

Comment on dynamical matrix. Improbable trajectories are not captured by dynamical matrix which measures the local elastic distortions.

How to characterize these distortions?



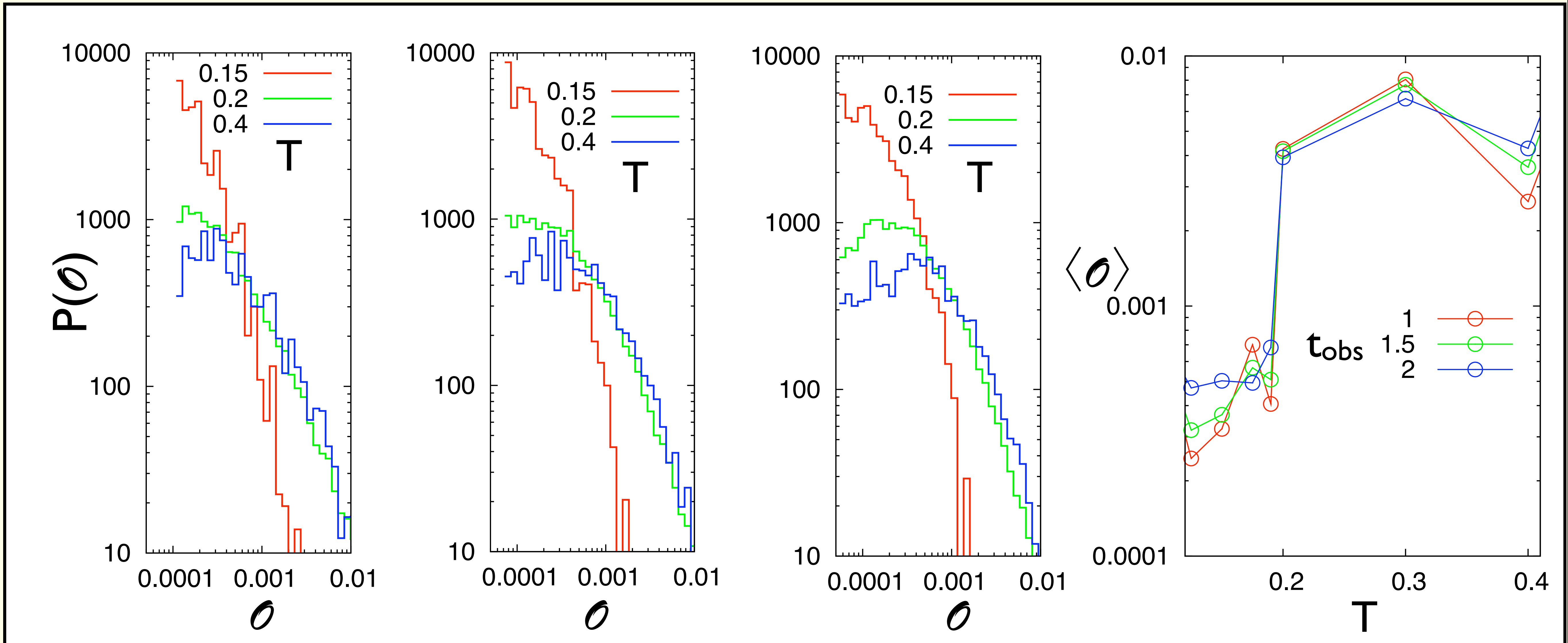
"off-diagonal" order parameter:

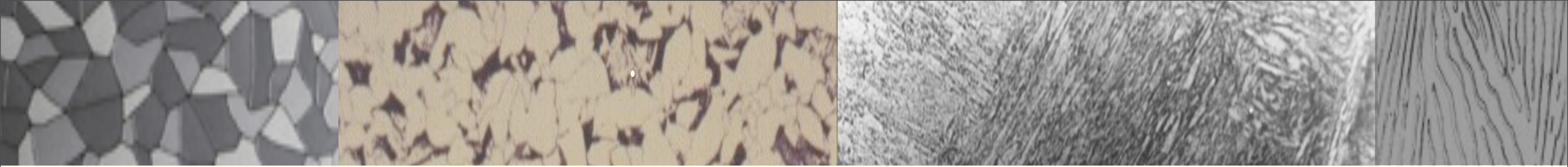
$$\mathcal{O}/N \equiv \frac{1}{t_{obs} N} \int_0^{t_{obs}} dt \sum_i |\Delta^i_{\alpha\beta}(t)|^2$$

with

$$\Delta^i_{\alpha\beta}(t) = u_{i\alpha}(t) u_{i\beta}(t) \ (\alpha \neq \beta) \quad i \in \text{active}$$

$$u_{i\alpha}(t) = r_{i\alpha}(t) - r_{i\alpha}(t - \delta t)$$





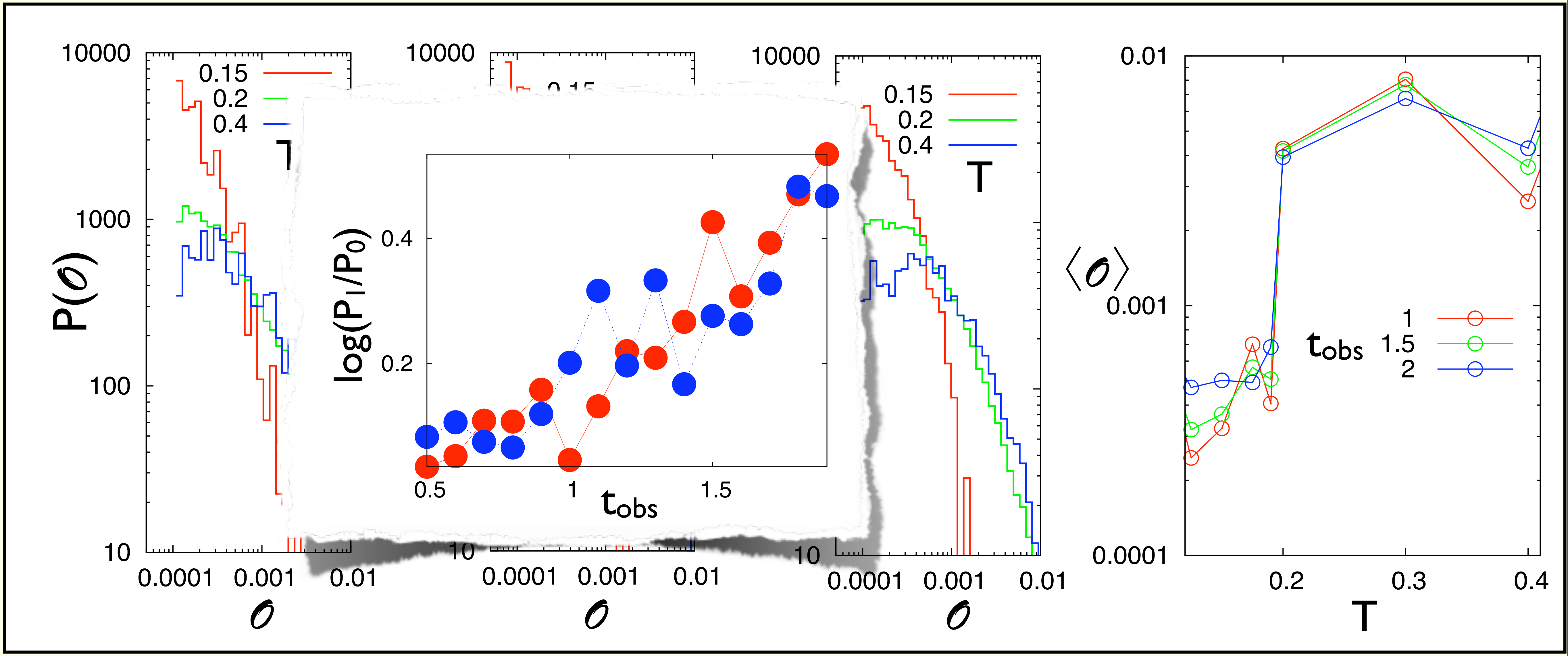
"off-diagonal" order parameter:

$$\mathcal{O}/N \equiv \frac{1}{t_{obs} N} \int_0^{t_{obs}} dt \sum_i |\Delta^i_{\alpha\beta}(t)|^2$$

with

$$\Delta^i_{\alpha\beta}(t) = u_{i\alpha}(t) u_{i\beta}(t) \ (\alpha \neq \beta) \quad i \in \text{active}$$

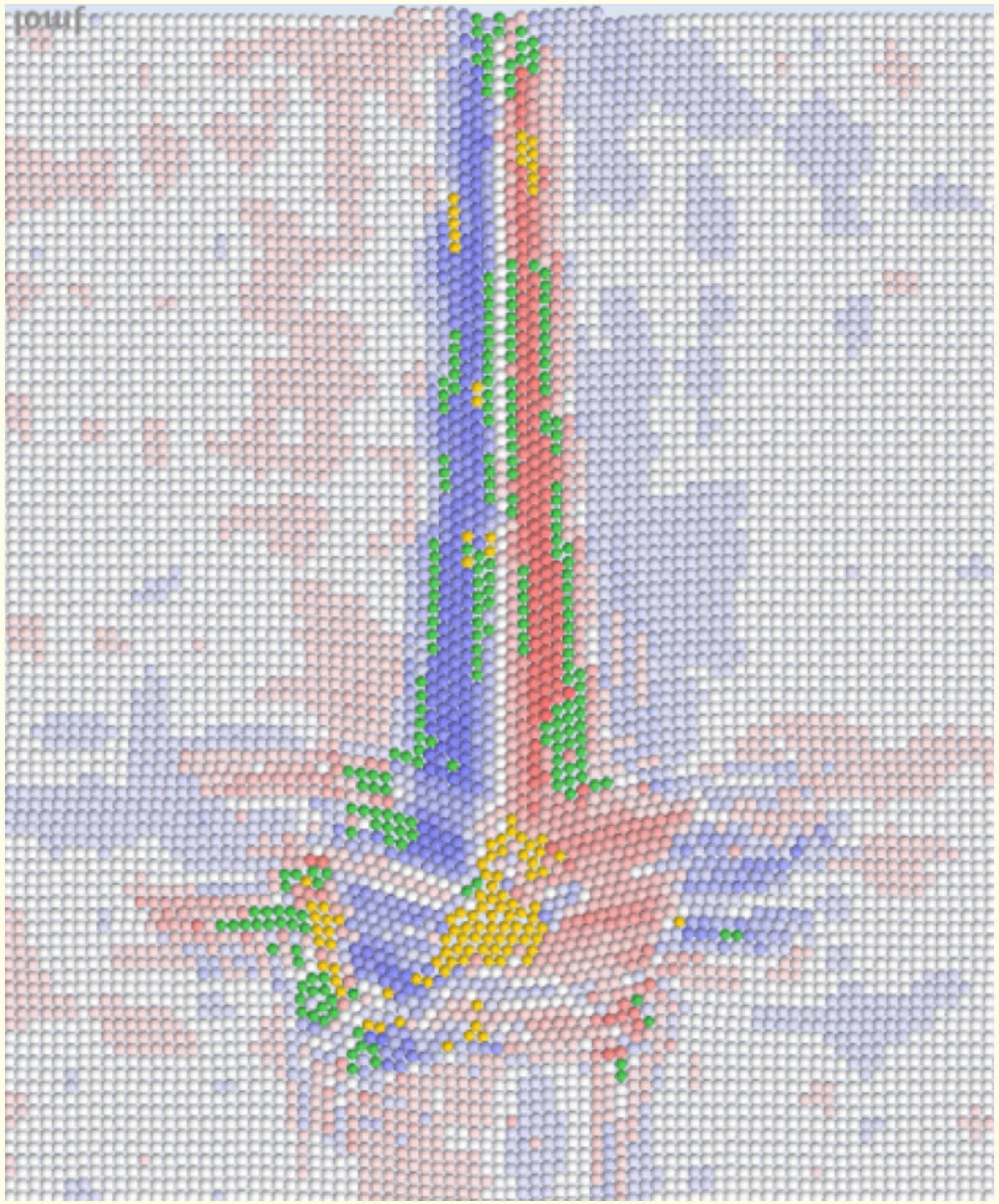
$$u_{i\alpha}(t) = r_{i\alpha}(t) - r_{i\alpha}(t - \delta t)$$



from trajectories to **NAZ**

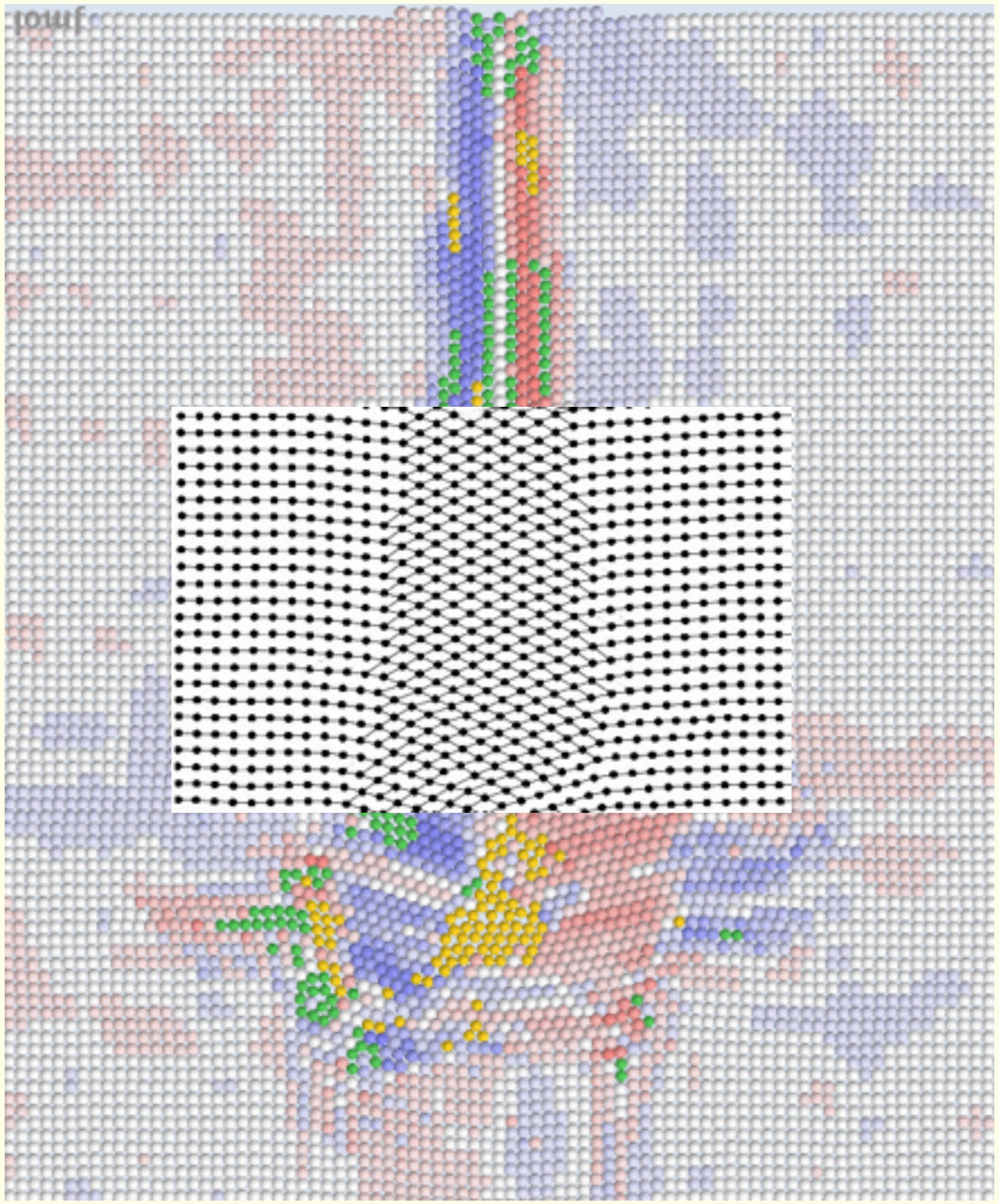
Regions of non-affine ***volume*** strain (NAZ) are automatically produced at the transformation front and are advected by it as transformation proceeds.

from trajectories to **NAZ**



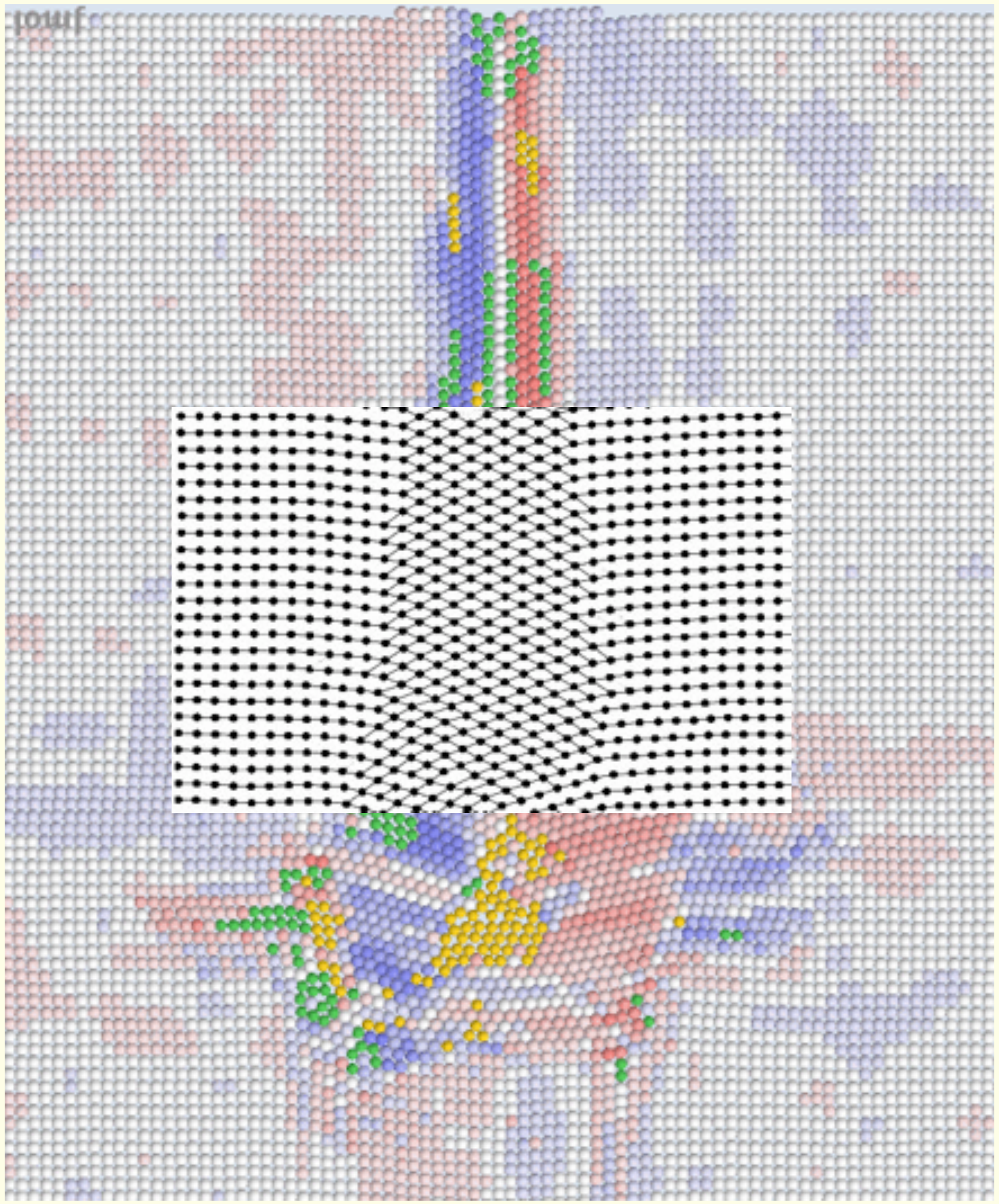
Regions of non-affine ***volume*** strain (NAZ) are automatically produced at the transformation front and are advected by it as transformation proceeds.

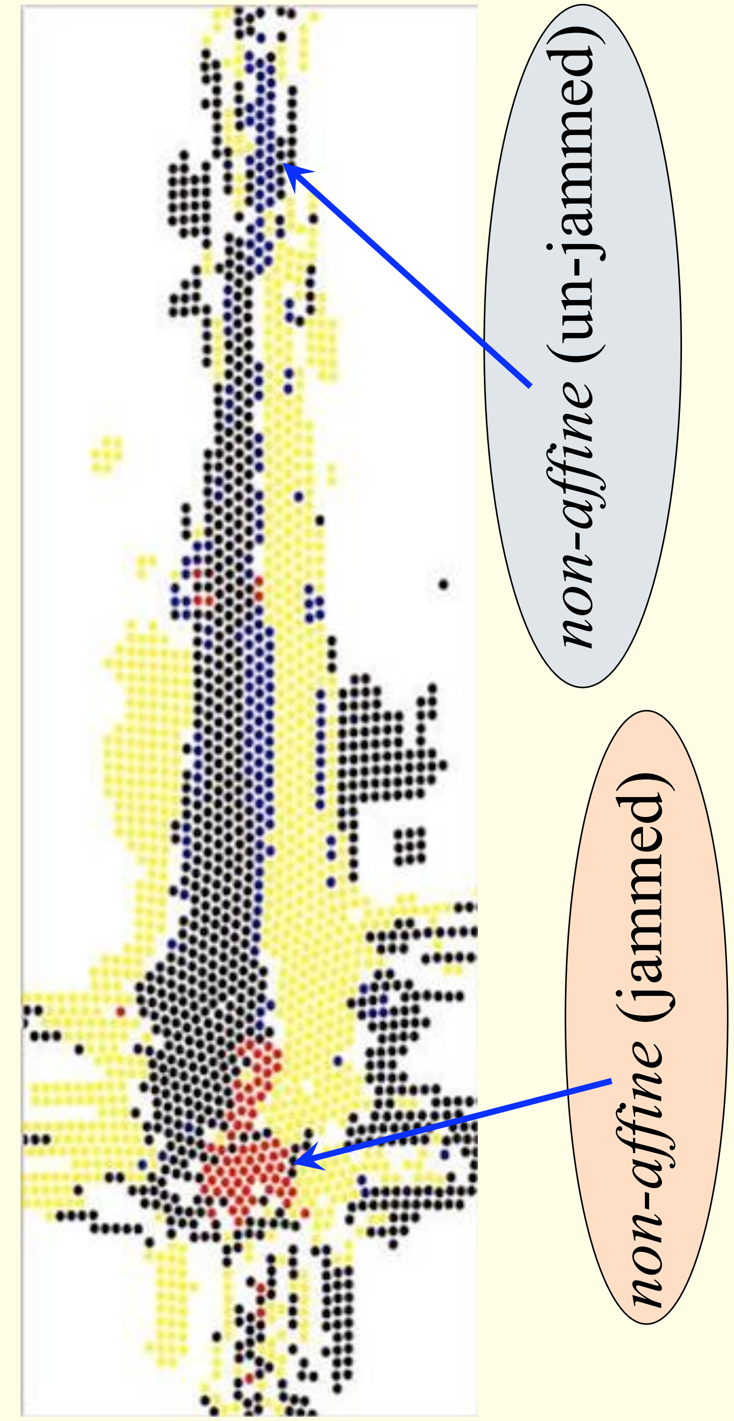
from trajectories to **NAZ**



Regions of non-affine ***volume*** strain (NAZ) are automatically produced at the transformation front and are advected by it as transformation proceeds.

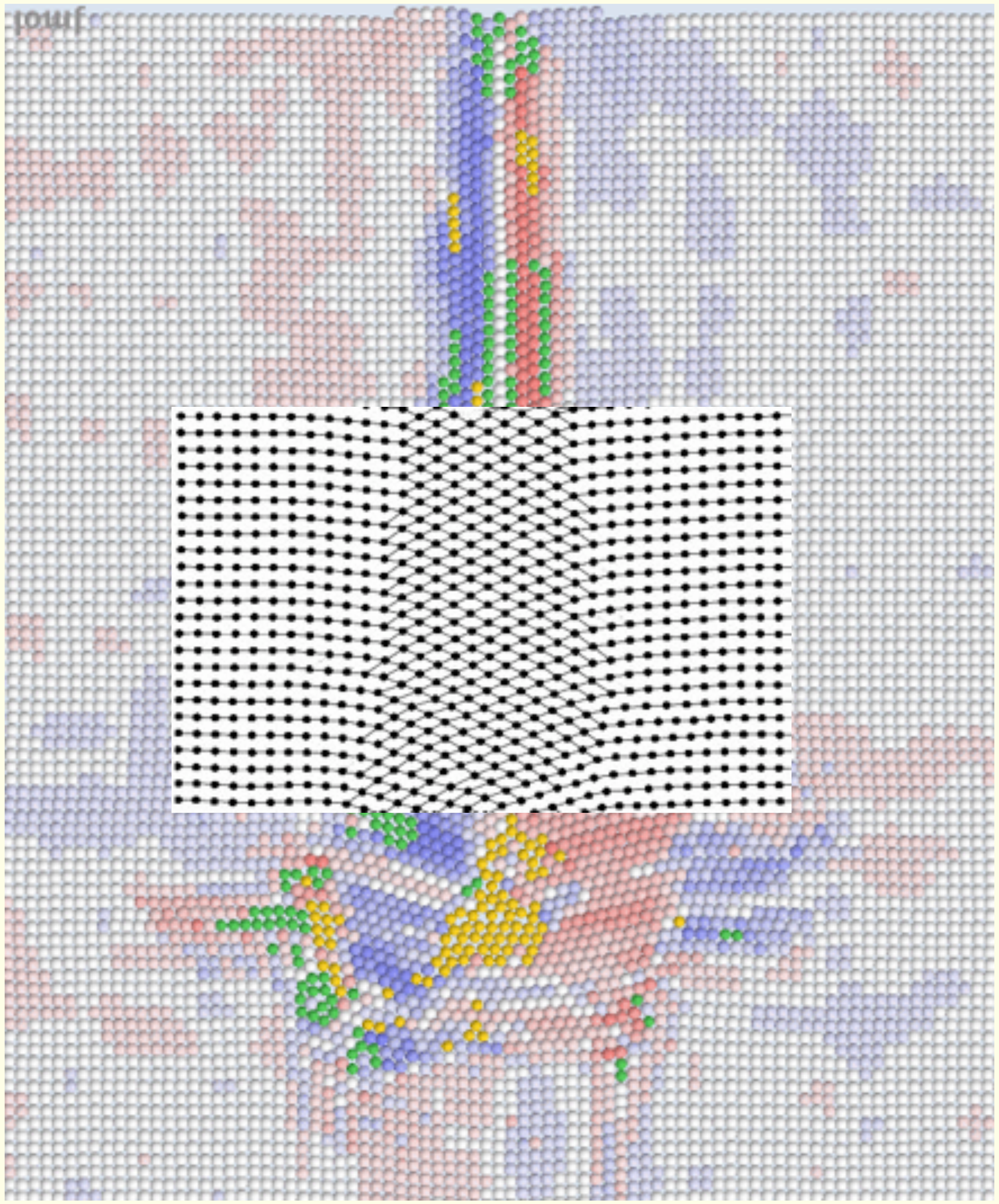
from trajectories to **NAZ**

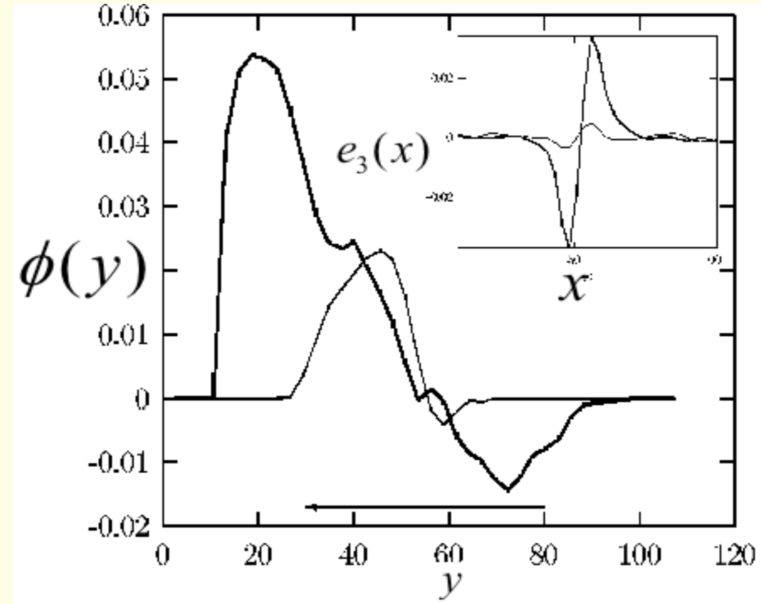


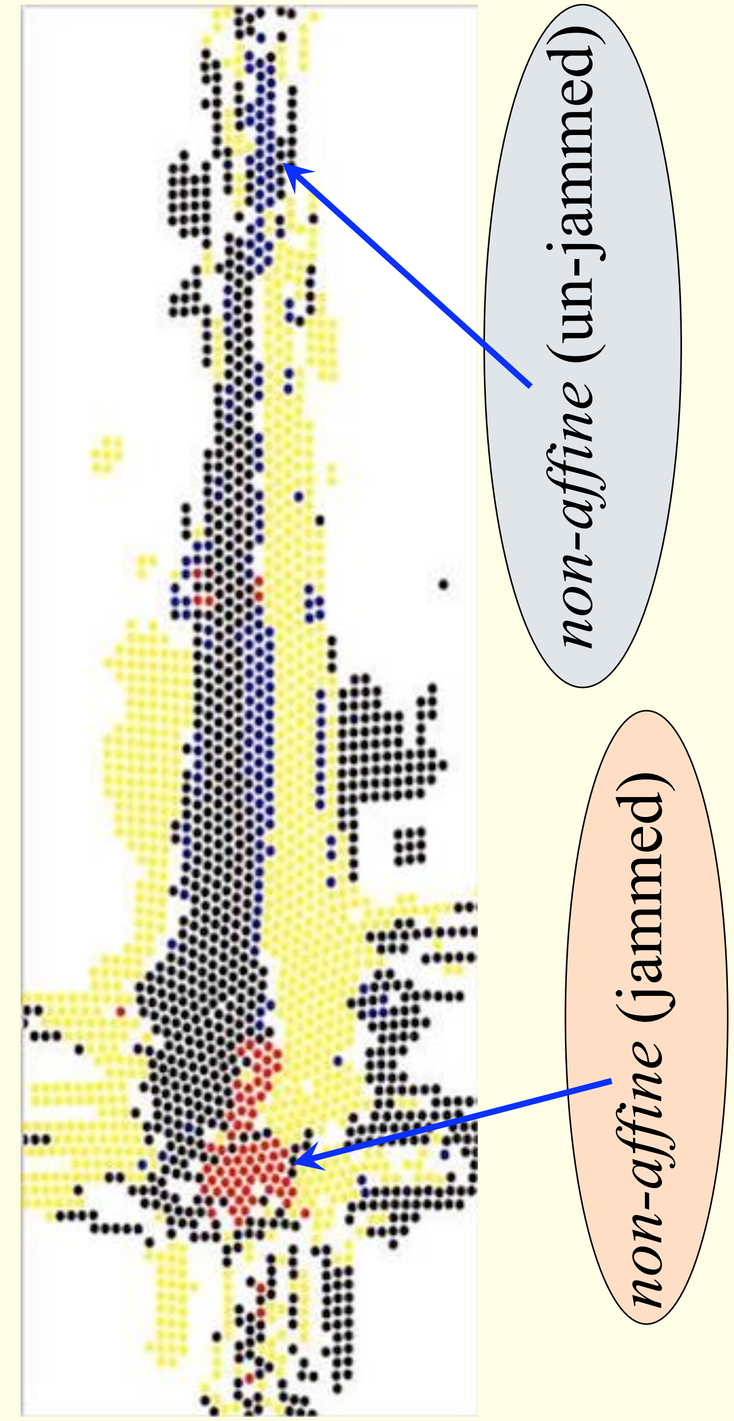


Regions of non-affine ***volume*** strain (NAZ) are automatically produced at the transformation front and are advected by it as transformation proceeds.

from trajectories to **NAZ**

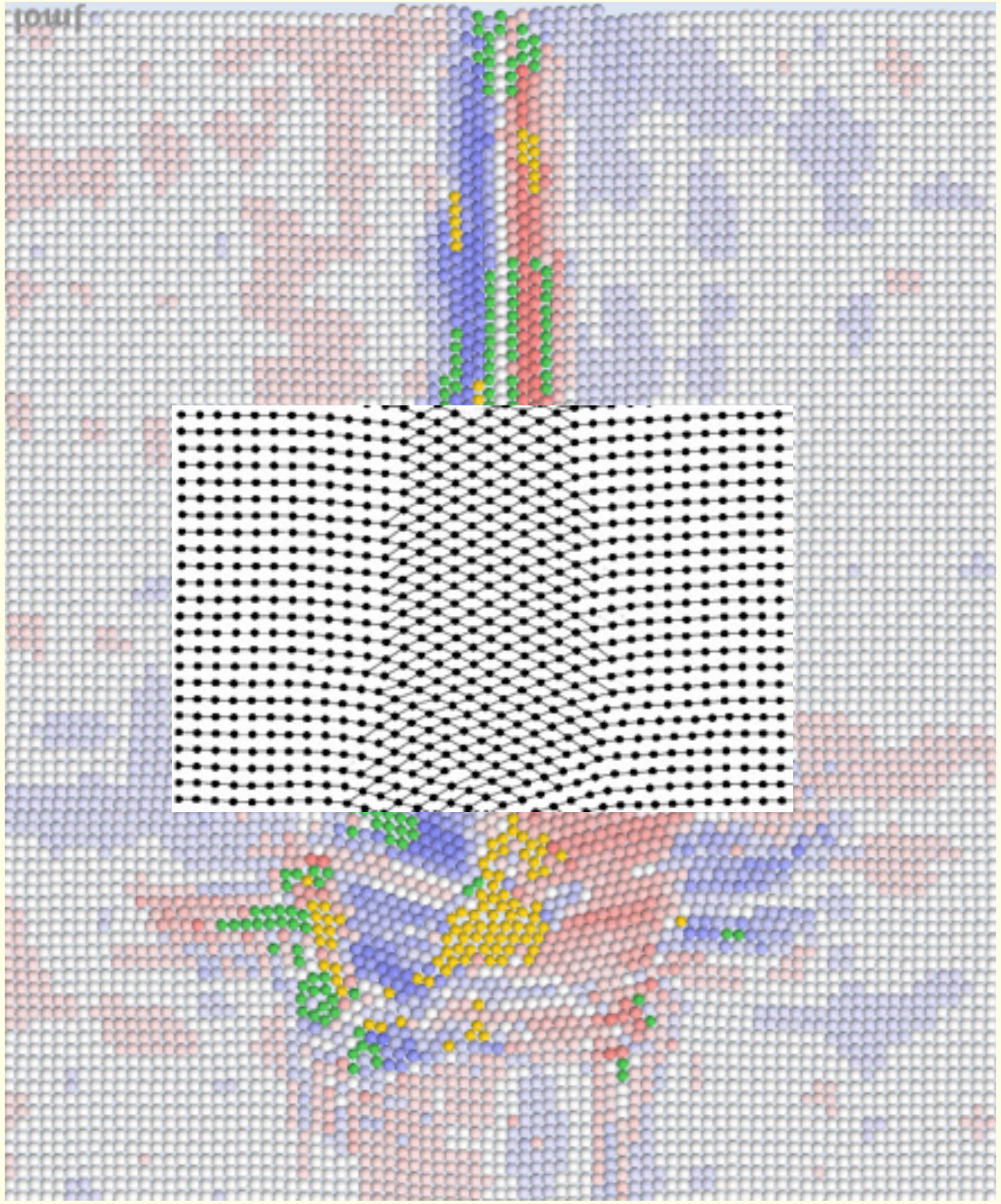


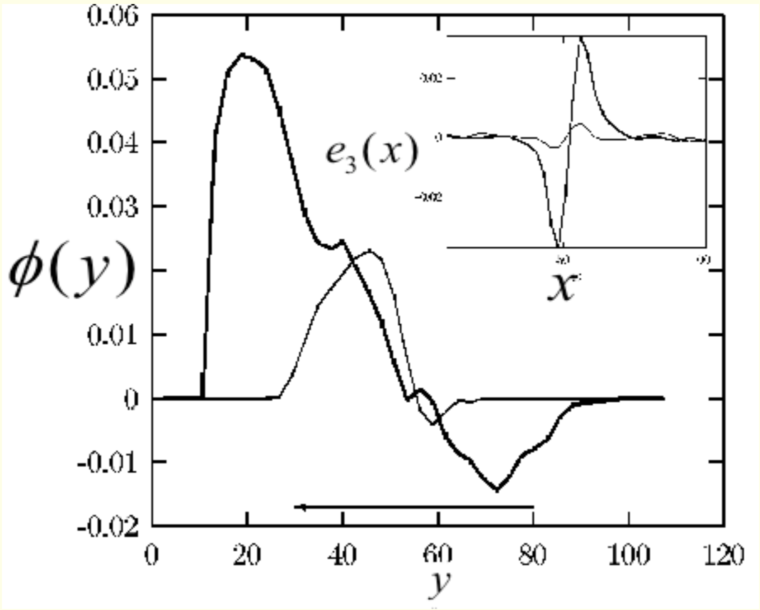


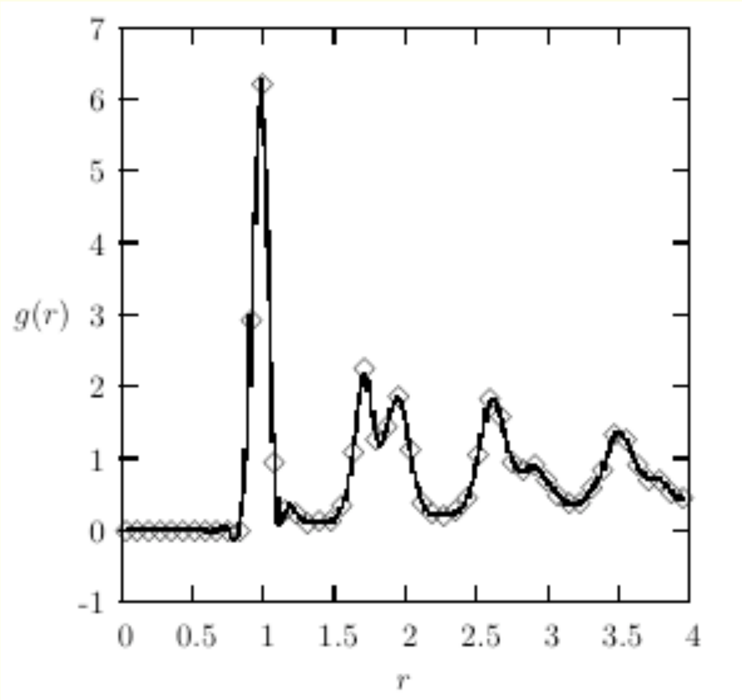


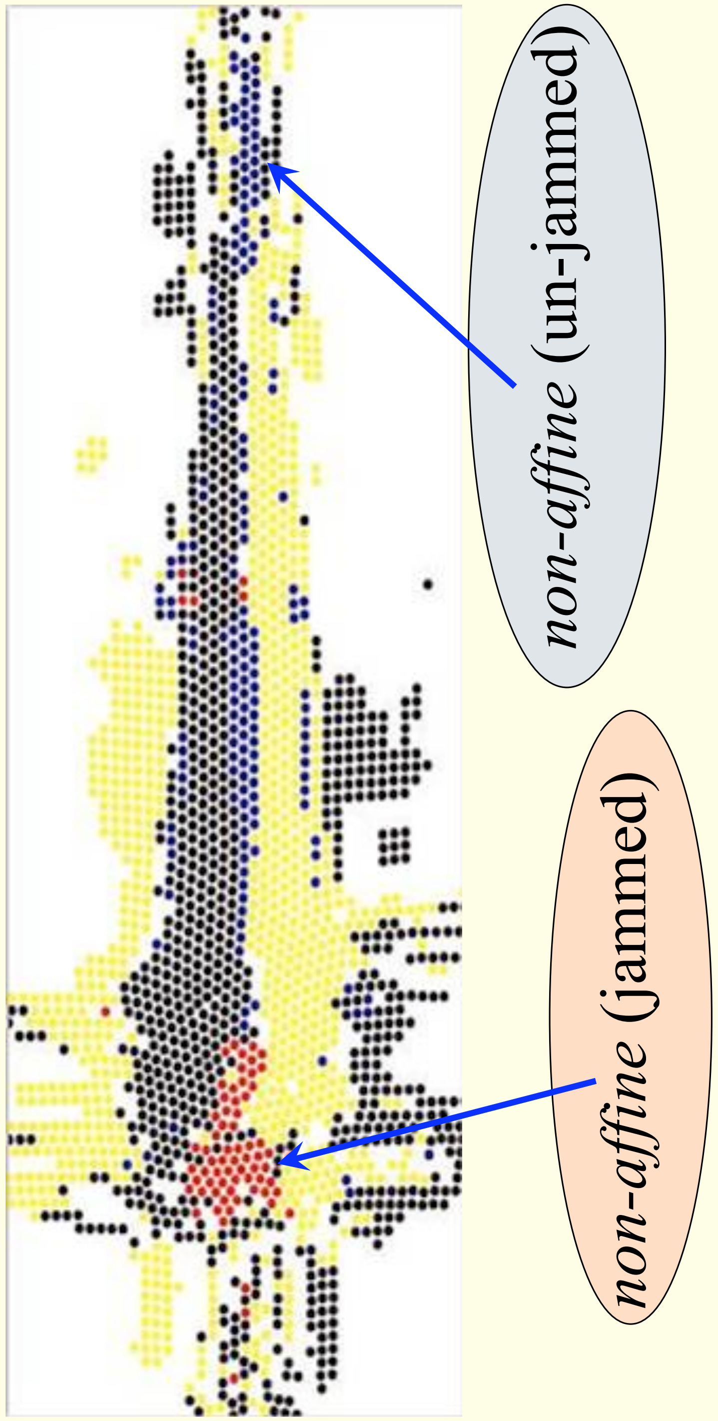
Regions of non-affine ***volume*** strain (NAZ) are automatically produced at the transformation front and are advected by it as transformation proceeds.

from trajectories to NAZ



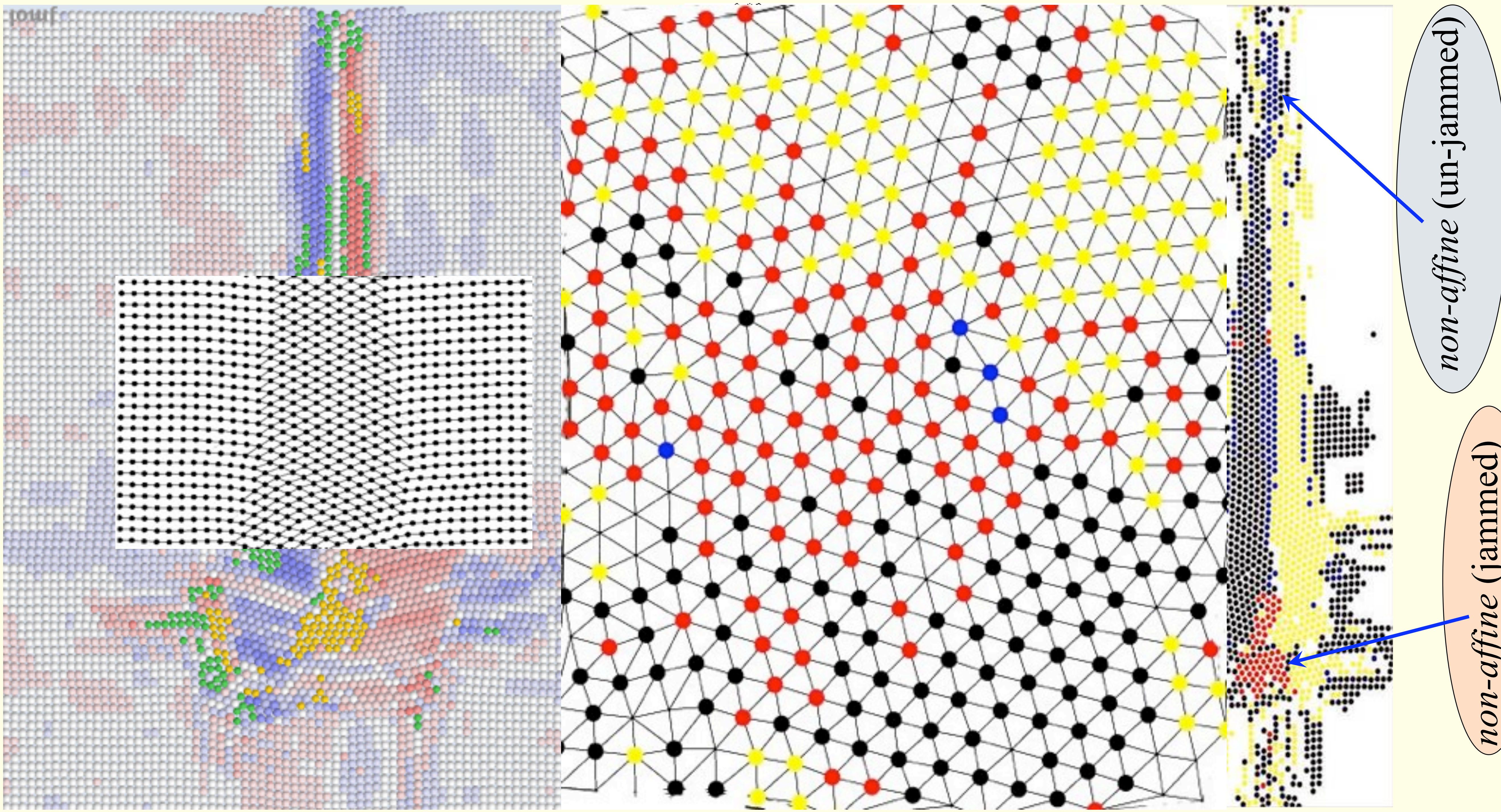




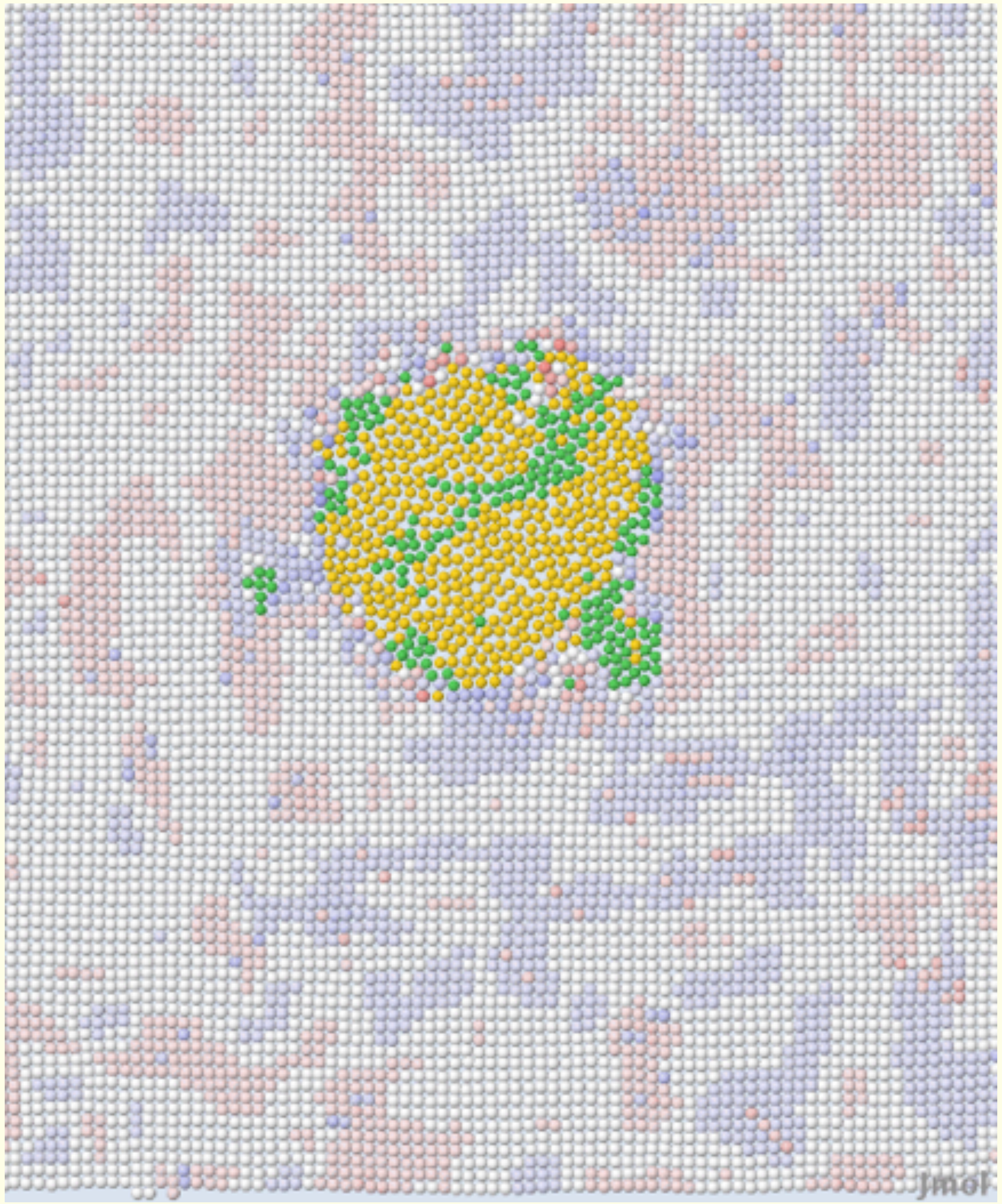


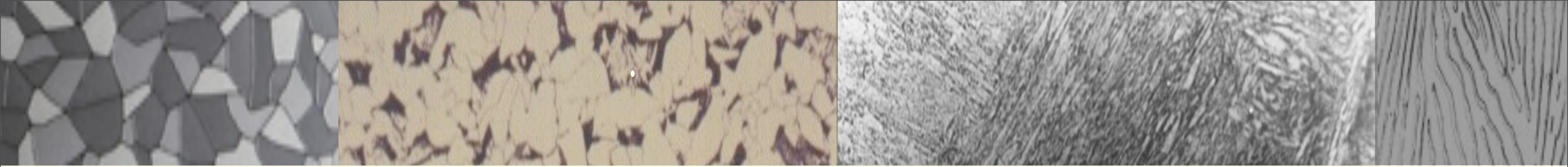
Regions of non-affine ***volume*** strain (NAZ) are automatically produced at the transformation front and are advected by it as transformation proceeds.

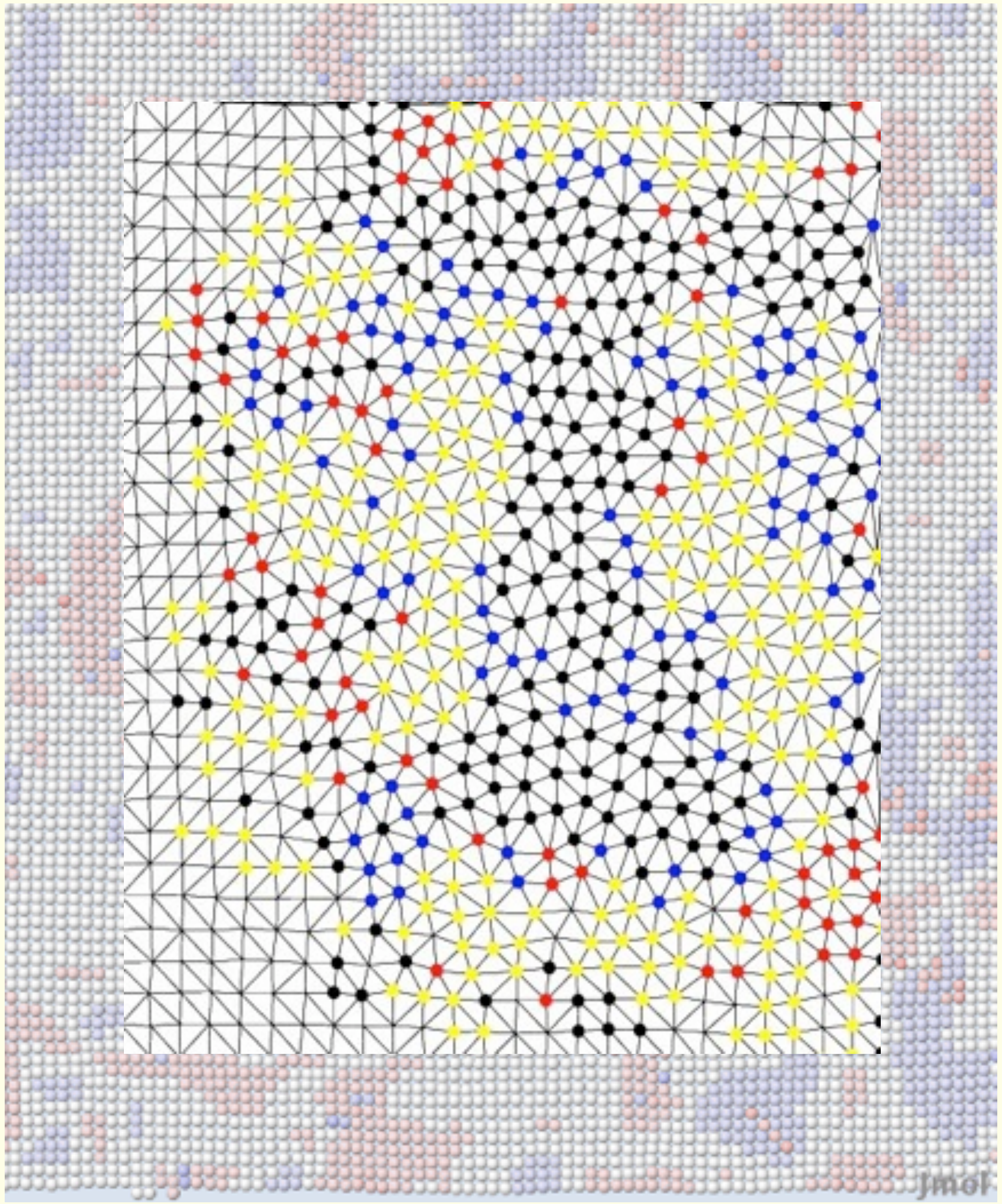
from trajectories to **NAZ**

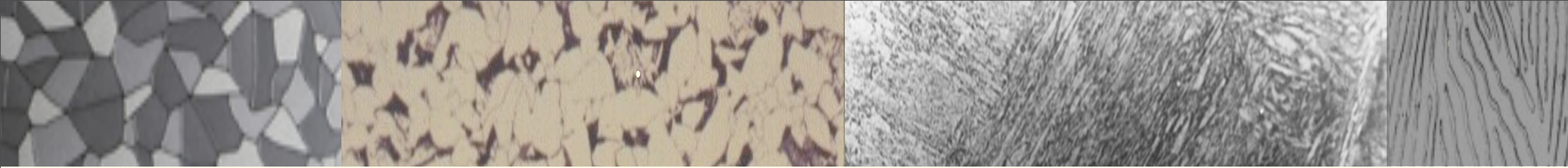


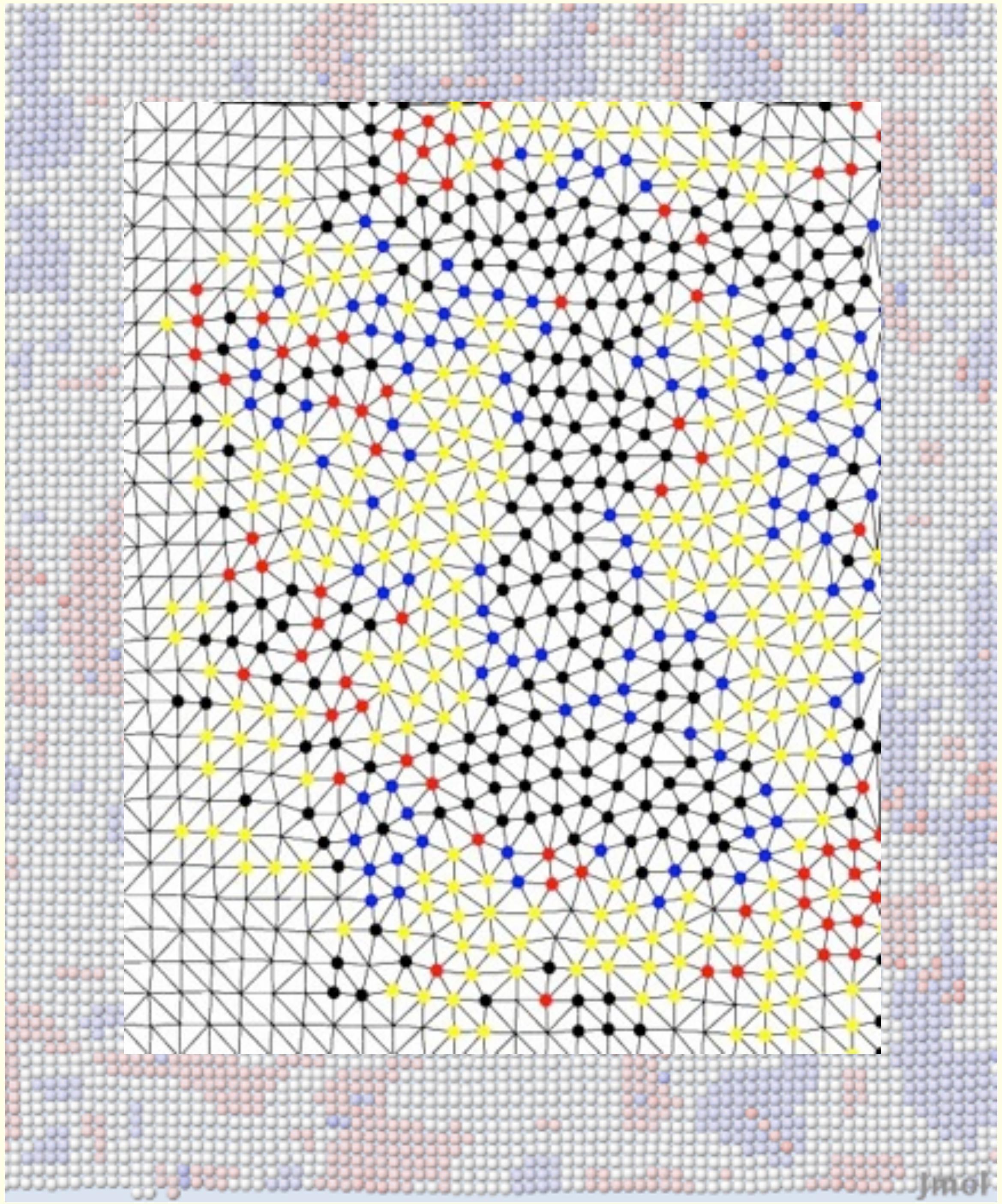
Regions of non-affine ***volume*** strain (NAZ) are automatically produced at the transformation front and are advected by it as transformation proceeds.

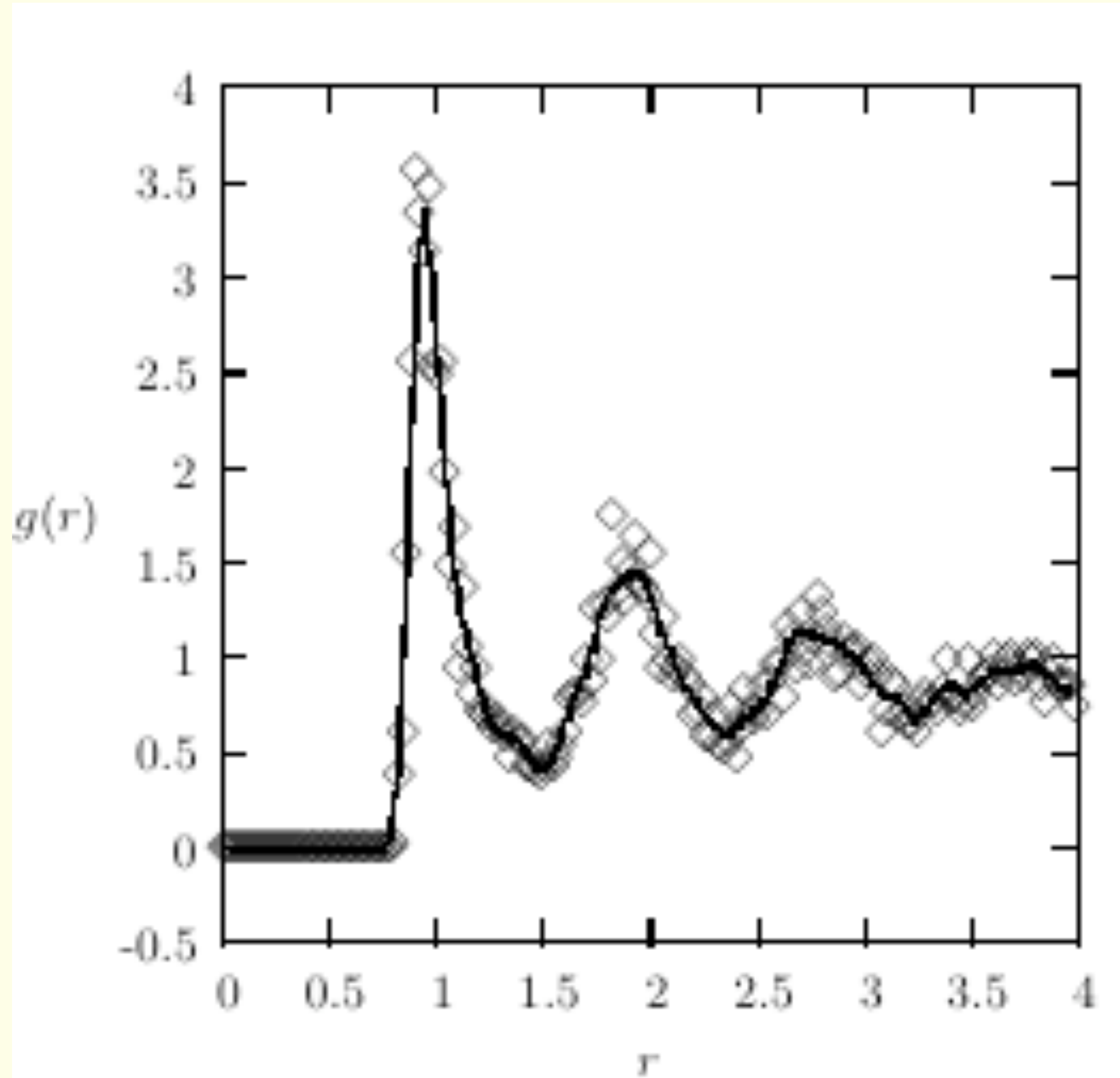

Jmol

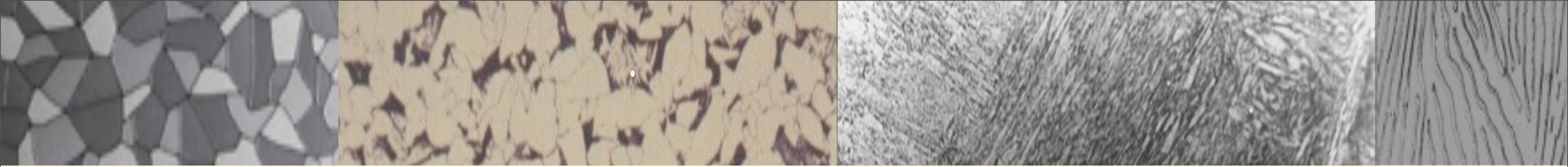


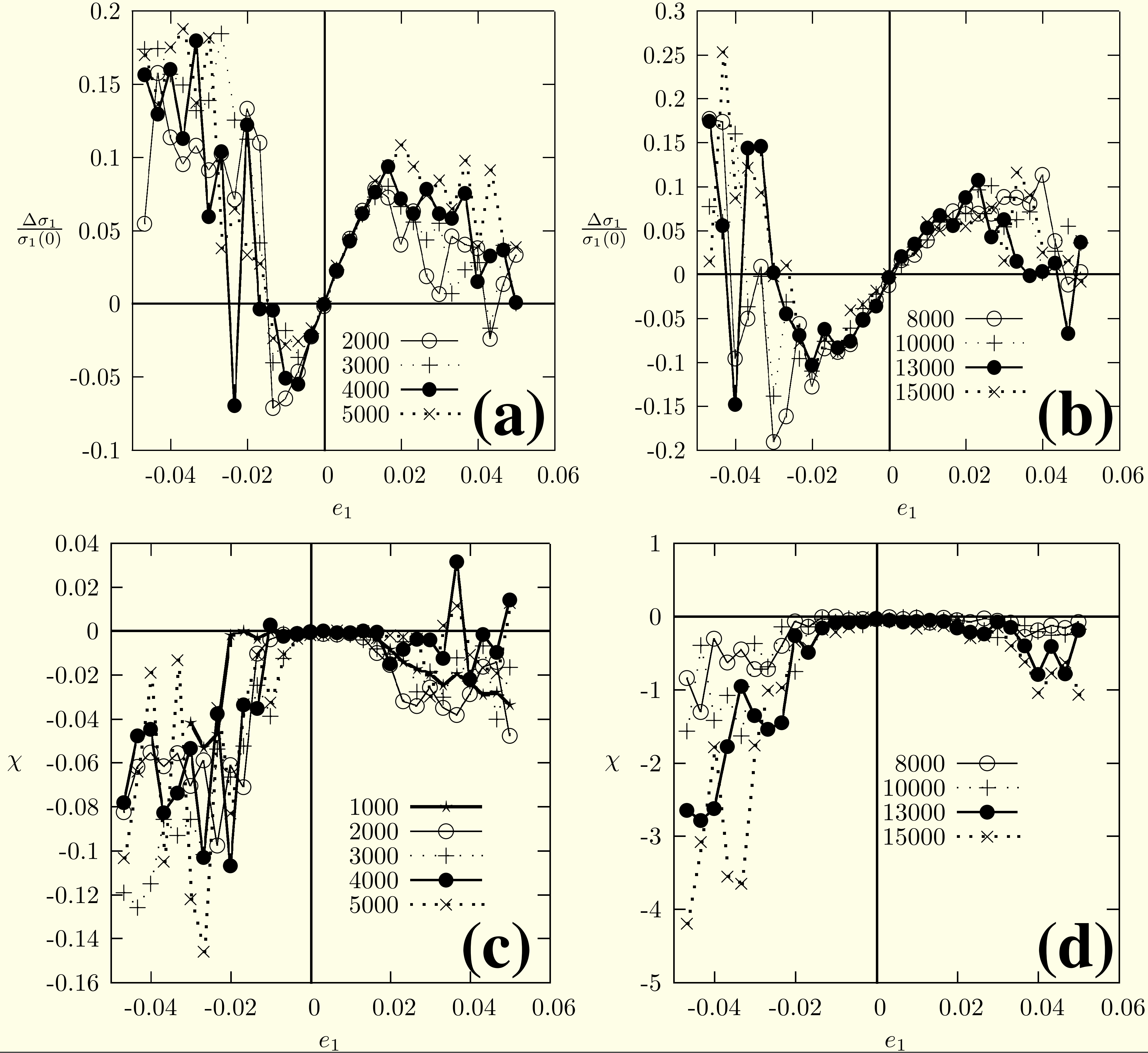

Jmol

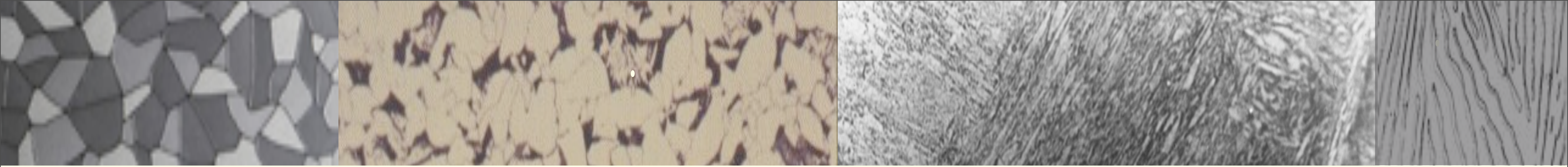


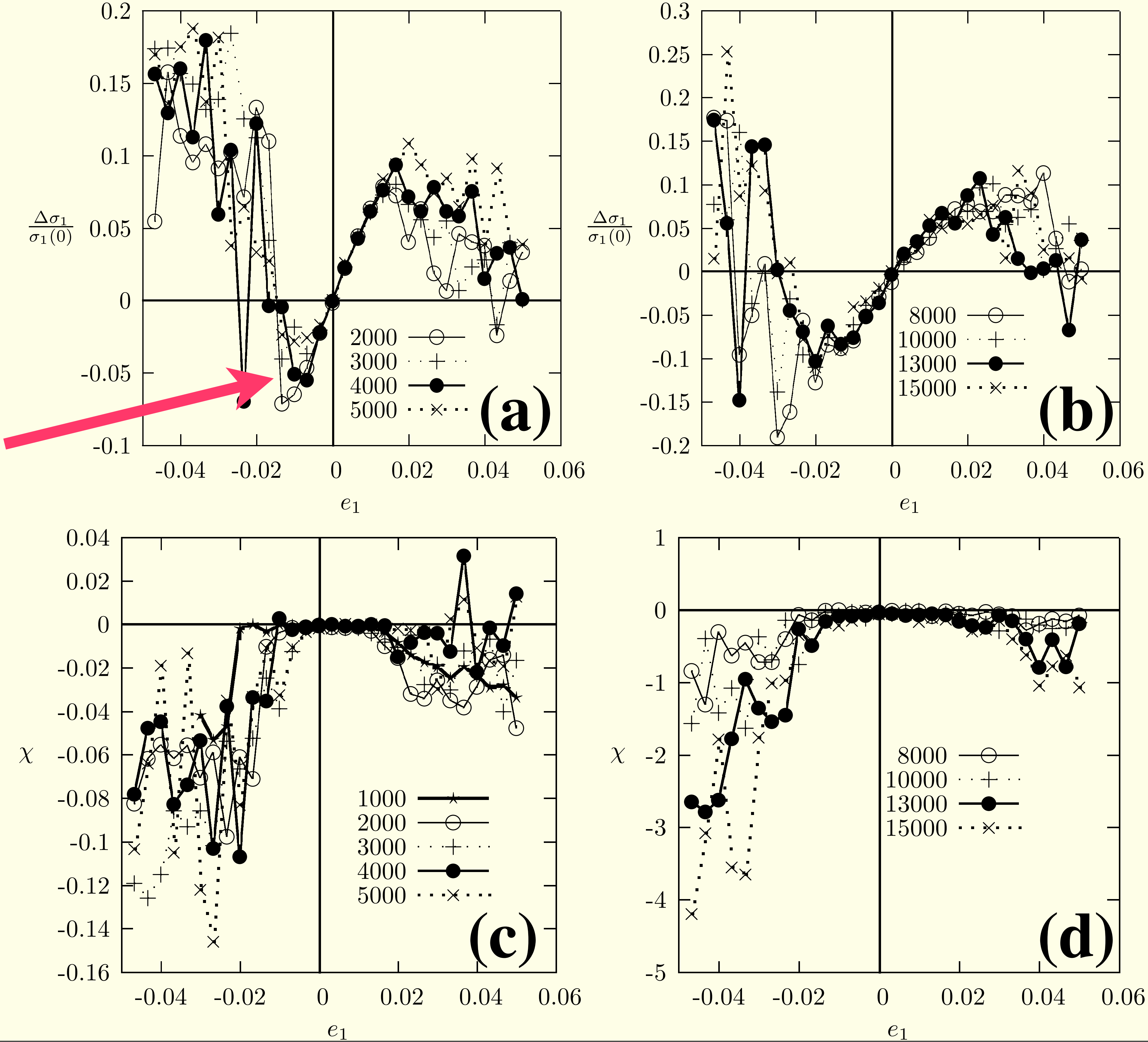



4
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
$g(r)$
0
0.5
1
1.5
2
2.5
3
3.5
4
r

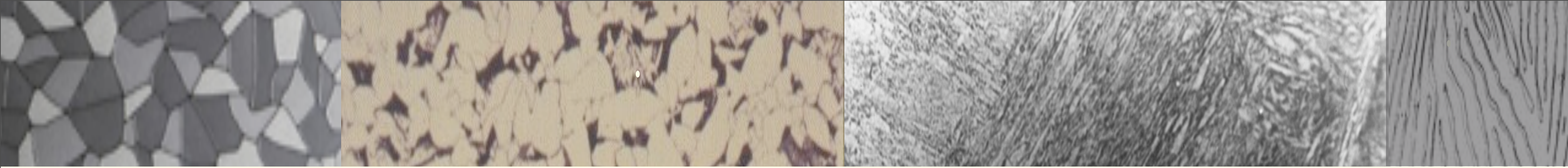



$\frac{\Delta\sigma_1}{\sigma_1(0)}$
χ
e_1
2000
3000
4000
5000
(a)
8000
10000
13000
15000
(b)
1000
2000
3000
4000
5000
(c)
8000
10000
13000
15000
(d)

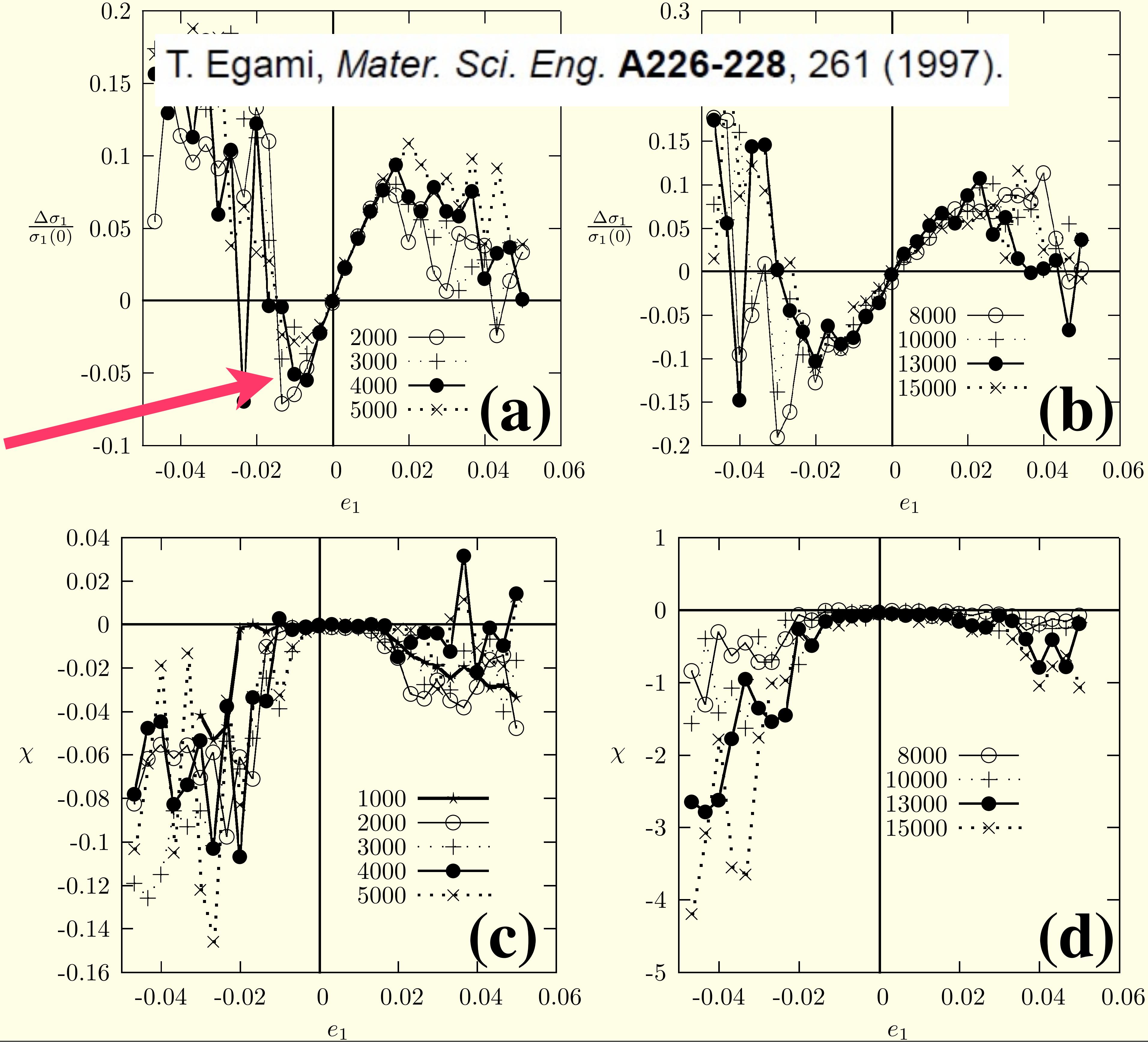




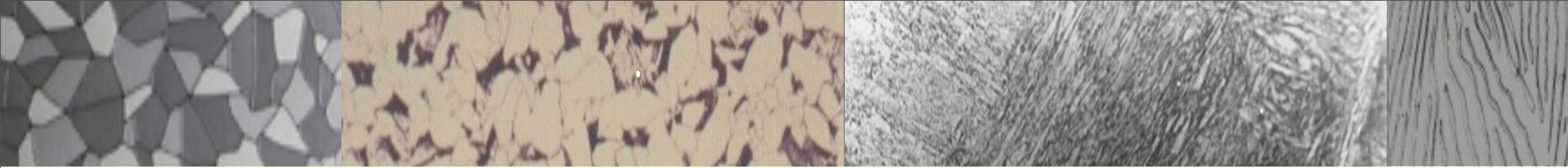
13% = upper bound



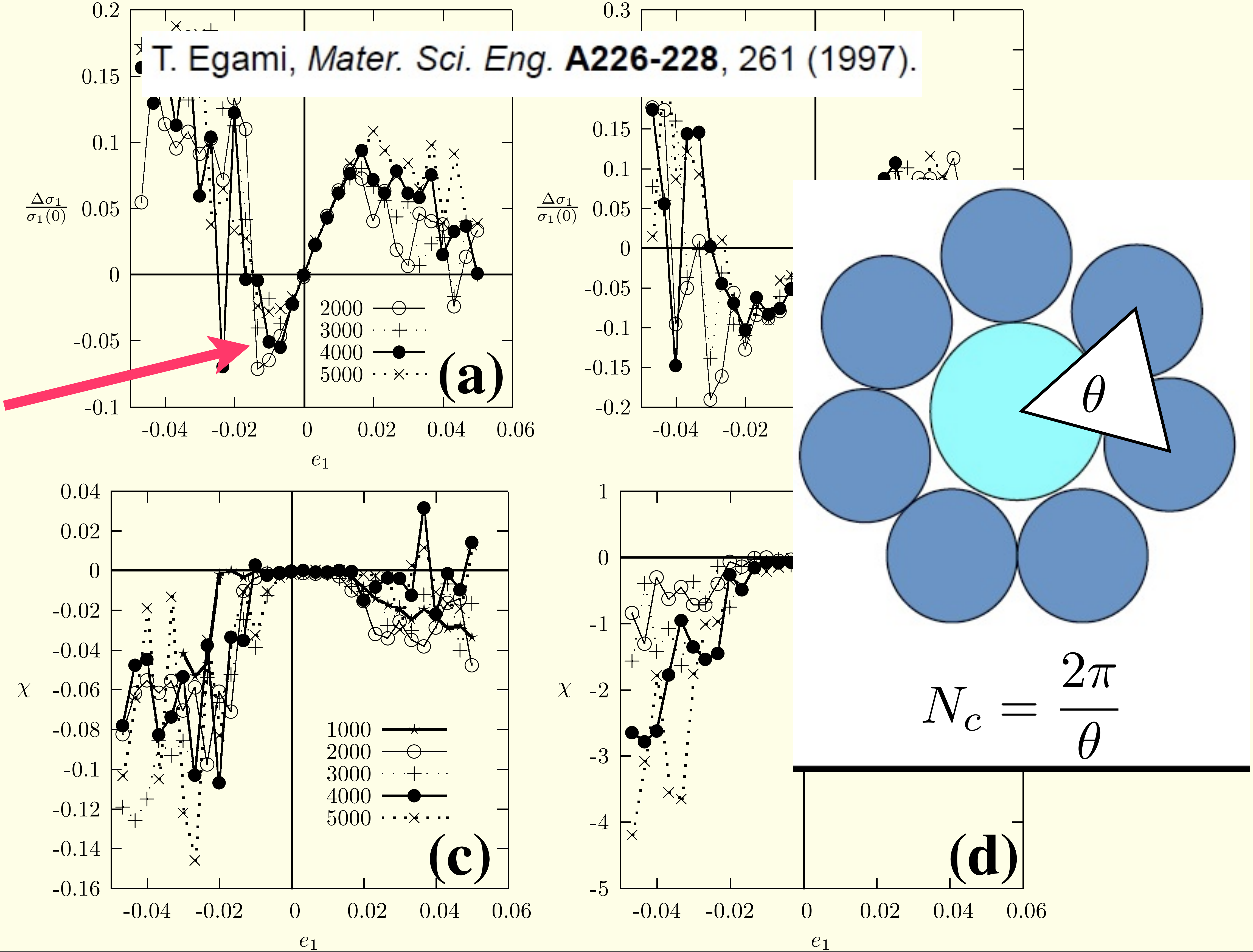
T. Egami, *Mater. Sci. Eng.* **A226-228**, 261 (1997).



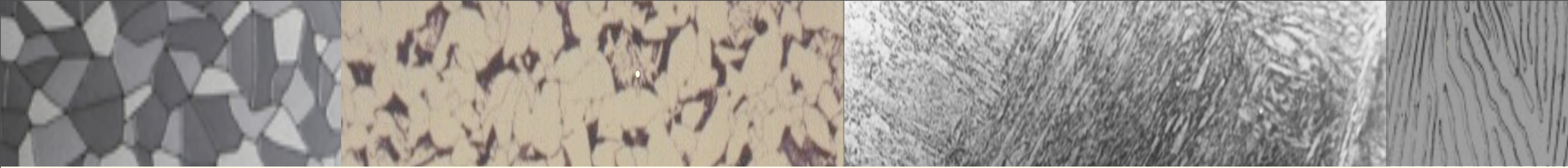
13% = upper bound

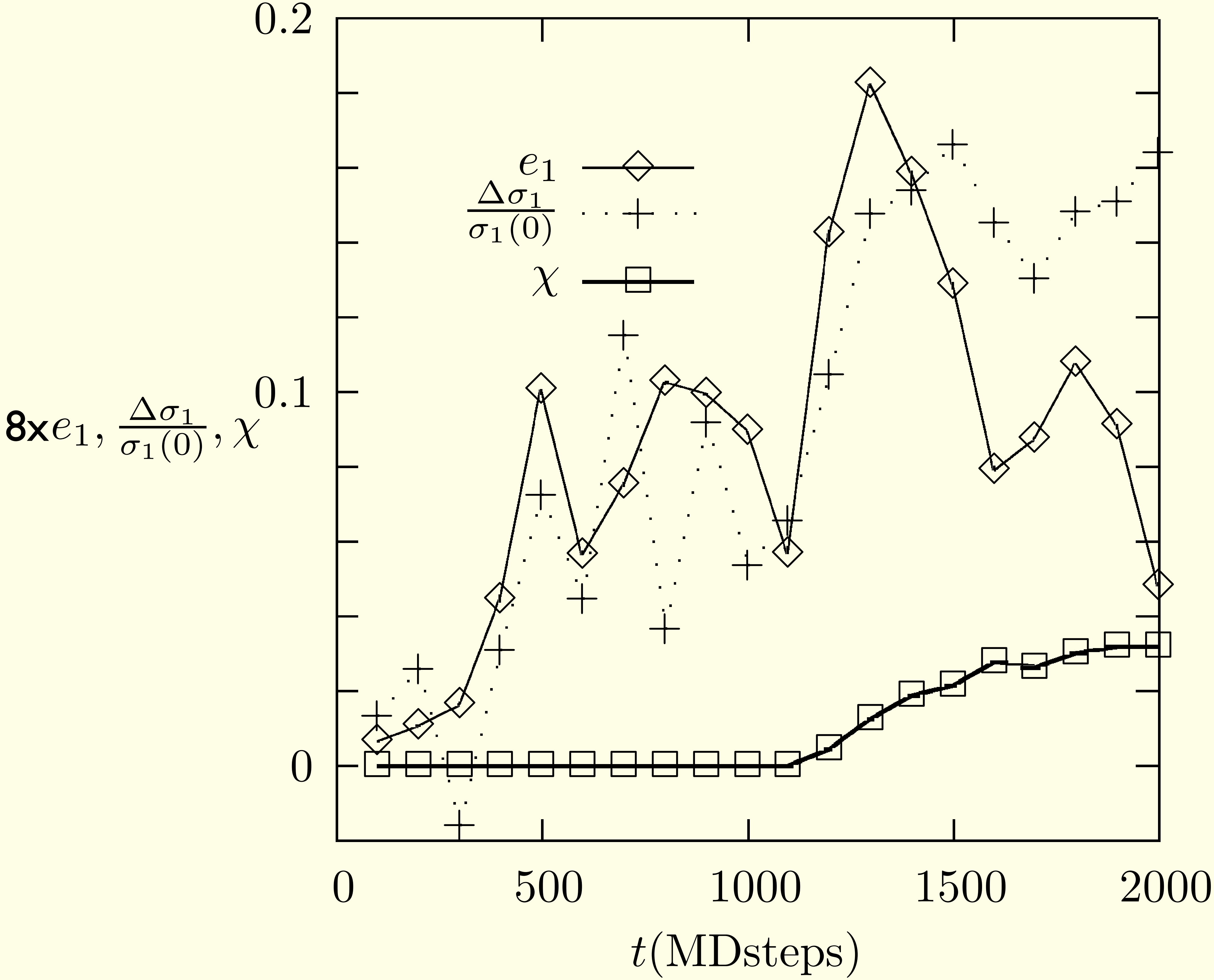


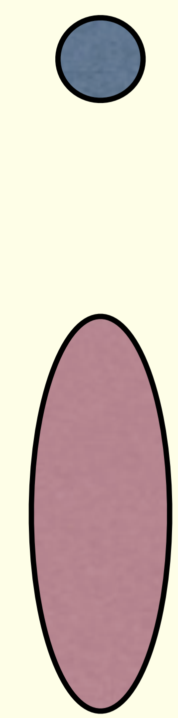
T. Egami, *Mater. Sci. Eng.* **A226-228**, 261 (1997).

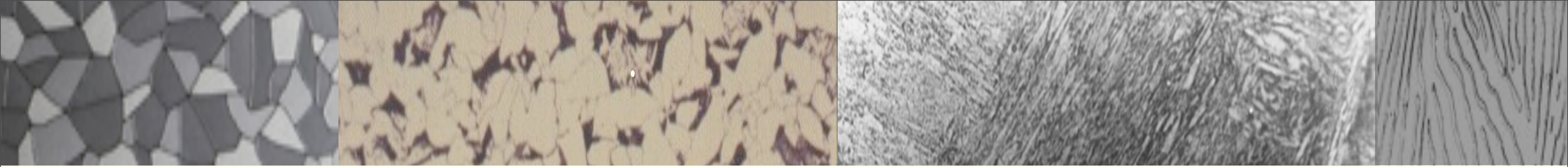


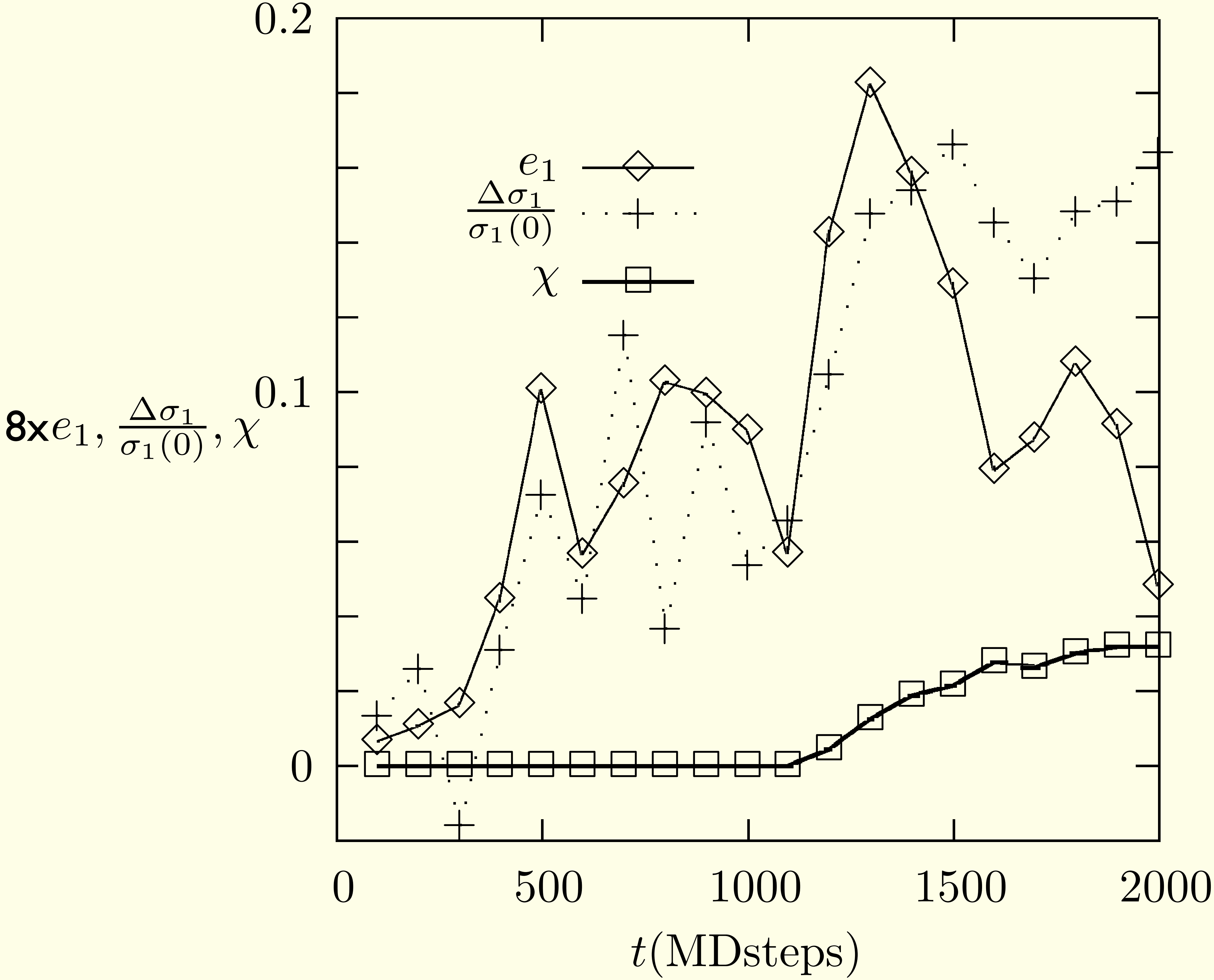
13% = upper bound

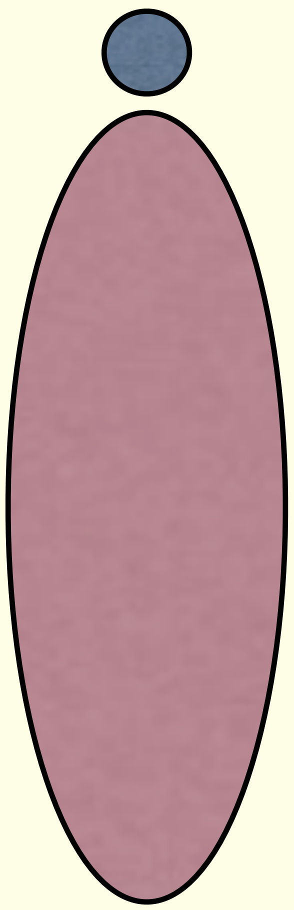


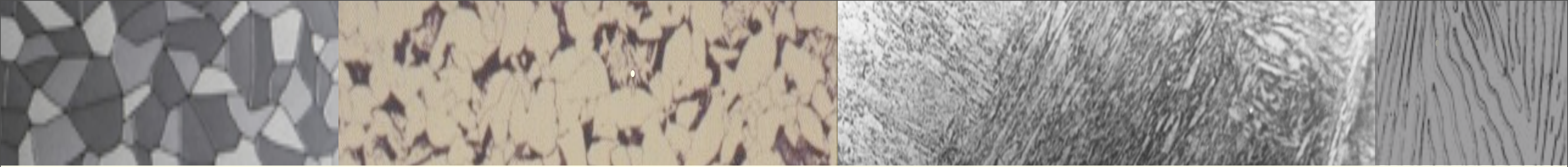

$8\times e_1, \frac{\Delta\sigma_1}{\sigma_1(0)}, \chi$
e_1
$\frac{\Delta\sigma_1}{\sigma_1(0)}$
χ
0.2
0.1
0
0
500
1000
1500
2000
t(MDsteps)

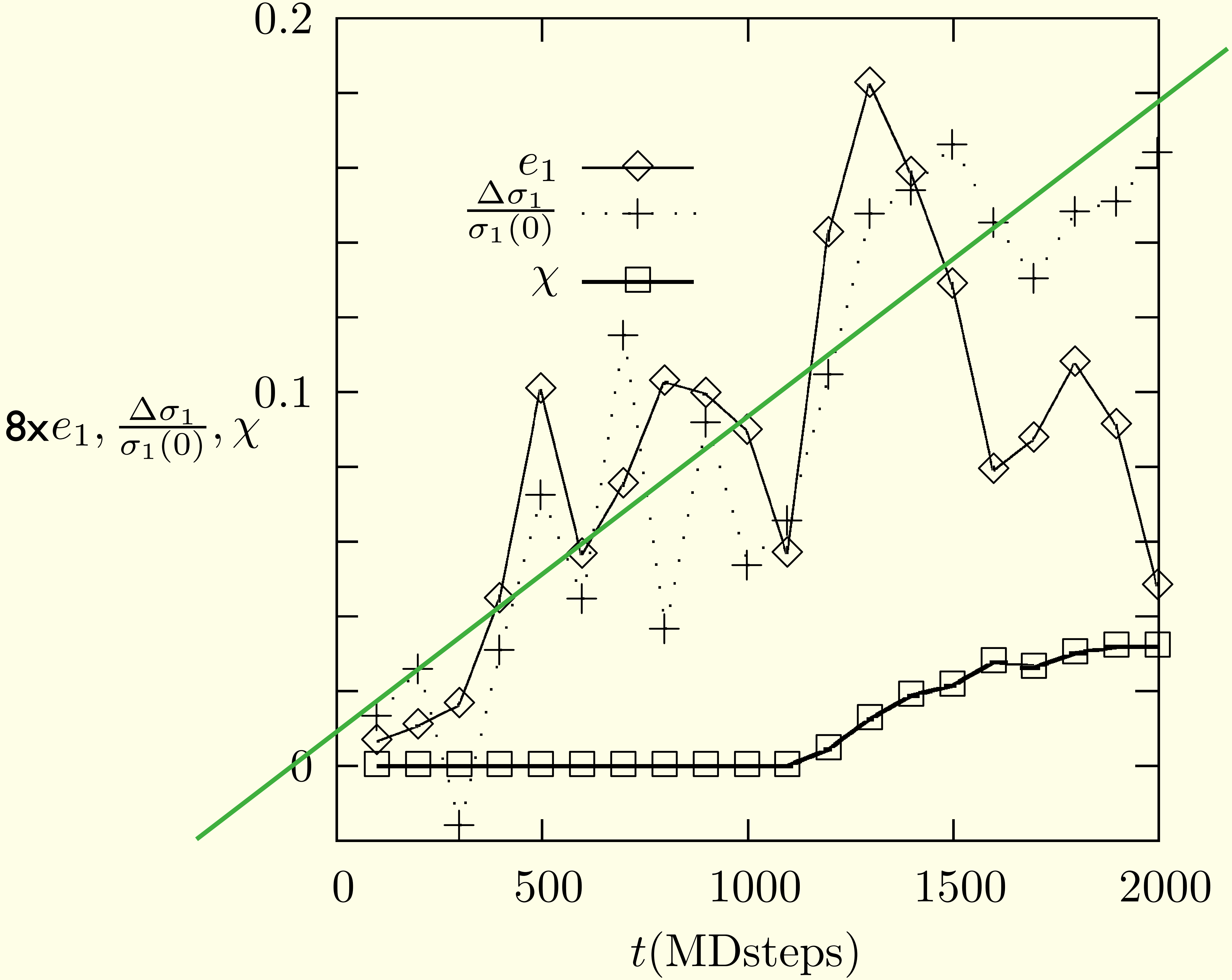




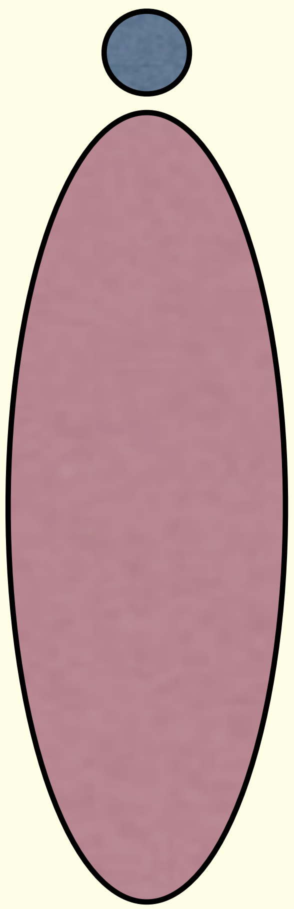

0.2
0.1
0
$8\times e_1, \frac{\Delta\sigma_1}{\sigma_1(0)}, \chi$
e_1
$\frac{\Delta\sigma_1}{\sigma_1(0)}$
χ
0
500
1000
1500
2000
t(MDsteps)

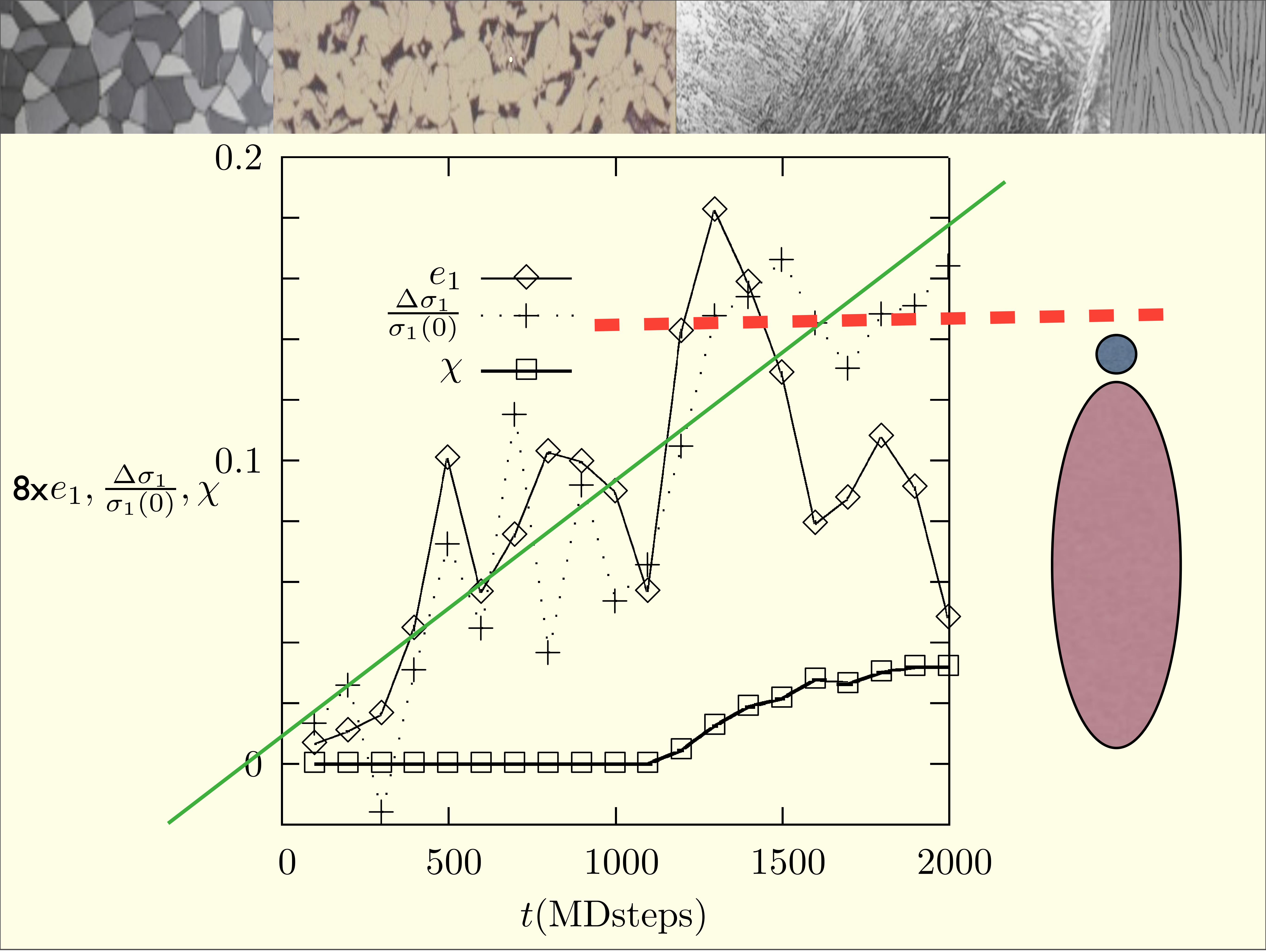


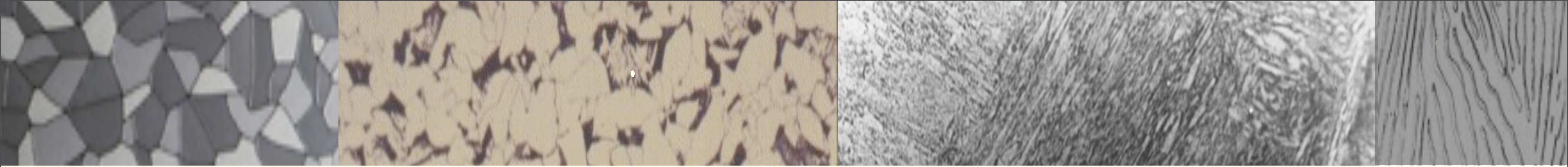




0.2
0.1
0
$8\mathsf{x}e_1, \frac{\Delta\sigma_1}{\sigma_1(0)}, \chi$
e_1
$\frac{\Delta\sigma_1}{\sigma_1(0)}$
χ
0
500
1000
1500
2000
t(MDsteps)




0.2
0.1
0
$8\times e_1, \frac{\Delta\sigma_1}{\sigma_1(0)}, \chi$
e_1
$\frac{\Delta\sigma_1}{\sigma_1(0)}$
χ
0
500
1000
1500
2000
t(MDsteps)



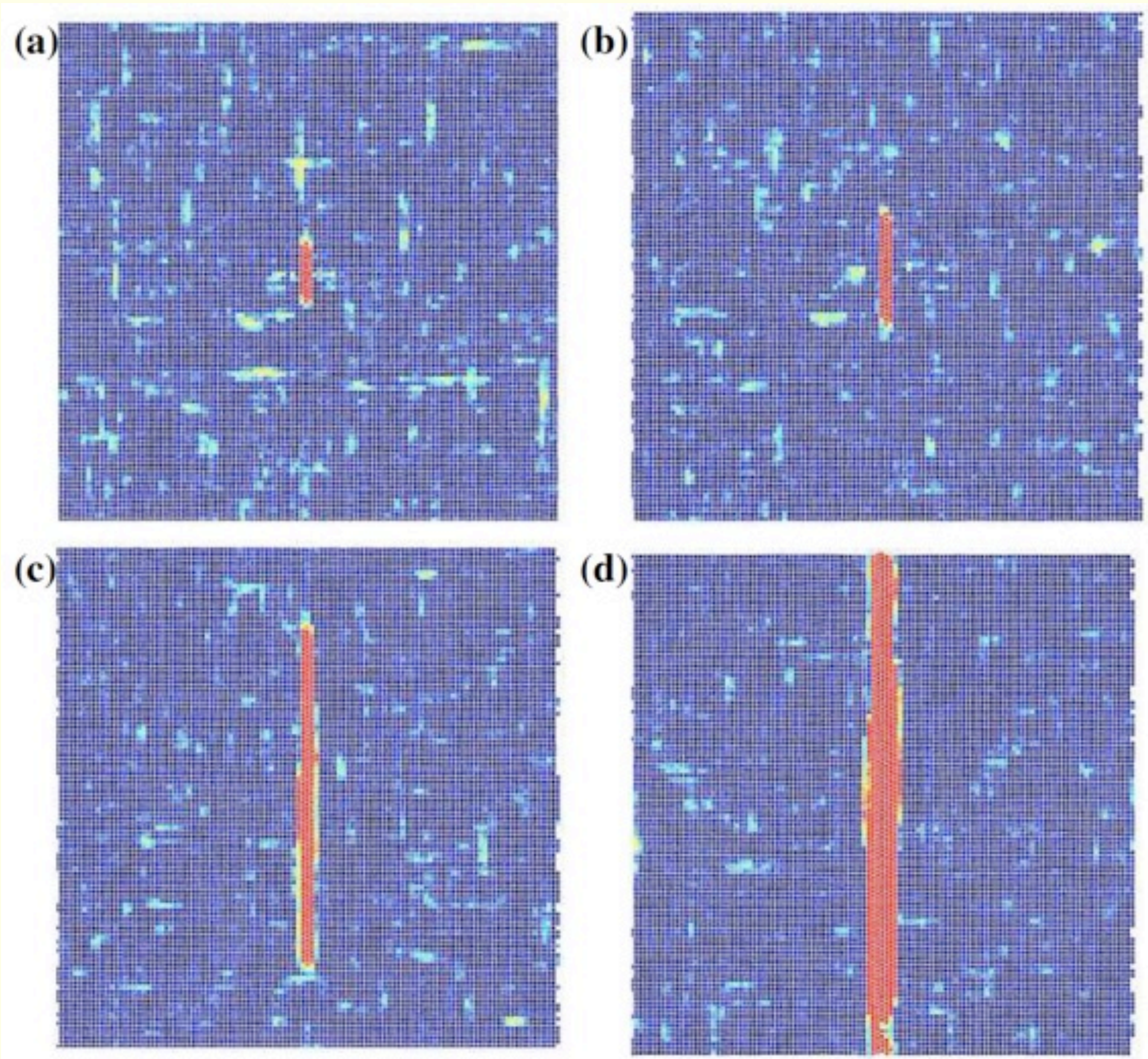


Figure 5.13: Typical molecular dynamics simulation snapshots at (a) 1200 (b) 2000 (c) 5000 and (d) 10000 MD-timesteps showing the growth of a twinned martensite critical nucleus at a low temperature, $T = 0.05$ quenched at $v_3 = 0.3383$. The equilibrated square parent lattice at $\rho = 1.1$ has particles interacting via the anisotropic potential with $\alpha = 1$. The colourscale goes from $\Omega_i = 0$ (blue) representing the untransformed austenite to $\Omega_i = 1$ (red) pertaining to the transformed martensitic microstructure.

Effects of decreasing incompatibility:

- growth velocity increases
- but more fluctuations as TCP is approached - “tweed” like structures

Ingredients for coarse a grained theory

A. Paul et al. J. Phys. Condens. Mat. (2008)

Ingredients for coarse a grained theory

- elasticity is not enough. $\nabla \times (\nabla \times \epsilon)^T = 0$

  Shenoy, Lookman, Saxena, Bishop, PRB, (1997)....etc

A. Paul et al. J. Phys. Condens. Mat. (2008)

Ingredients for coarse a grained theory

- elasticity is not enough. $\nabla \times (\nabla \times \epsilon)^T = 0$

  Shenoy, Lookman, Saxena, Bishop, PRB, (1997)....etc
- *local* plasticity at the growing interface produced when stress reaches a threshold.

A. Paul et al. J. Phys. Condens. Mat. (2008)

Ingredients for coarse a grained theory

- elasticity is not enough. $\nabla \times (\nabla \times \epsilon)^T = 0$
  Shenoy, Lookman, Saxena, Bishop, PRB, (1997)....etc
- *local* plasticity at the growing interface produced when stress reaches a threshold.
- amount of plasticity produced depends on the *incompatibility*.

A. Paul et al. J. Phys. Condens. Mat. (2008)

Ingredients for coarse a grained theory

- elasticity is not enough. $\nabla \times (\nabla \times \epsilon)^T = 0$
  Shenoy, Lookman, Saxena, Bishop, PRB, (1997)....etc
- *local* plasticity at the growing interface produced when stress reaches a threshold.
- amount of plasticity produced depends on the *incompatibility*.
- rate of production of plasticity vs. rate of transformation controls microstructure (*Deborah* number)

A. Paul et al. J. Phys. Condens. Mat. (2008)

Ingredients for coarse a grained theory

- elasticity is not enough. $\nabla \times (\nabla \times \epsilon)^T = 0$
  Shenoy, Lookman, Saxena, Bishop, PRB, (1997)....etc
- *local* plasticity at the growing interface produced when stress reaches a threshold.
- amount of plasticity produced depends on the *incompatibility*.
- rate of production of plasticity vs. rate of transformation controls microstructure (*Deborah* number)
- plasticity relaxes when transformation front moves away.

A. Paul et al. J. Phys. Condens. Mat. (2008)

Elasto-plastic theory

Elasto-plastic theory

$$L[e_i, e_i^p, \dot{u}_x, \dot{u}_y] = \sum_{\mathbf{r}} \left[\frac{m}{2}(\dot{u}_x^2 + \dot{u}_y^2) - F[e_i(\mathbf{r}), e_i^P(\mathbf{r})] \right]$$

Elasto-plastic theory

$$L[e_i, e_i^p, \dot{u}_x, \dot{u}_y] = \sum_{\mathbf{r}} \left[\frac{m}{2} (\dot{u}_x^2 + \dot{u}_y^2) - F[e_i(\mathbf{r}), e_i^P(\mathbf{r})] \right]$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{u}}}\right) = \frac{\partial L}{\partial \mathbf{u}} - \frac{\partial R}{\partial \dot{\mathbf{u}}},$$

Elasto-plastic theory

$$L[e_i, e_i^p, \dot{u}_x, \dot{u}_y] = \sum_{\mathbf{r}} \left[\frac{m}{2}(\dot{u}_x^2 + \dot{u}_y^2) - F[e_i(\mathbf{r}), e_i^P(\mathbf{r})] \right]$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{u}}}\right) = \frac{\partial L}{\partial \mathbf{u}} - \frac{\partial R}{\partial \dot{\mathbf{u}}},$$

$$R[e_i] = \frac{1}{2}\sum_{\mathbf{r}} \left[\gamma_1 \dot{e}_1^2(\mathbf{r}) + \gamma_2 \dot{e}_2^2(\mathbf{r}) + \gamma_3 \dot{e}_3^2(\mathbf{r})\right]$$

$$\begin{aligned}\mathcal{F}[e_i(\mathbf{r}), e_i^P(\mathbf{r})] &= \int [\frac{1}{2}a_1 \underline{(e_1 + e_1^P})^2 + \frac{c_1}{2}(\nabla e_1)^2 + \frac{1}{2}a_2 e_2^2 + \frac{c_2}{2}(\nabla e_2)^2 \\ &\quad \frac{1}{2}a_3 e_3^2 + V(e_i) + \frac{c_3}{2}(\nabla e_3)^2] d\mathbf{r}.\end{aligned}$$

$$\begin{aligned} e_1(\mathbf{r}) &= \frac{\partial u_x(\mathbf{r})}{\partial x} + \frac{\partial u_y(\mathbf{r})}{\partial y}, \\ e_2(\mathbf{r}) &= \frac{\partial u_x(\mathbf{r})}{\partial x} - \frac{\partial u_y(\mathbf{r})}{\partial y}, \\ e_3(\mathbf{r}) &= \frac{\partial u_x(\mathbf{r})}{\partial y} + \frac{\partial u_y(\mathbf{r})}{\partial x}. \end{aligned}$$

Elasto-plastic theory

$$L[e_i, e_i^p, \dot{u}_x, \dot{u}_y] = \sum_{\mathbf{r}} \left[\frac{m}{2}(\dot{u}_x^2 + \dot{u}_y^2) - F[e_i(\mathbf{r}), e_i^P(\mathbf{r})] \right]$$

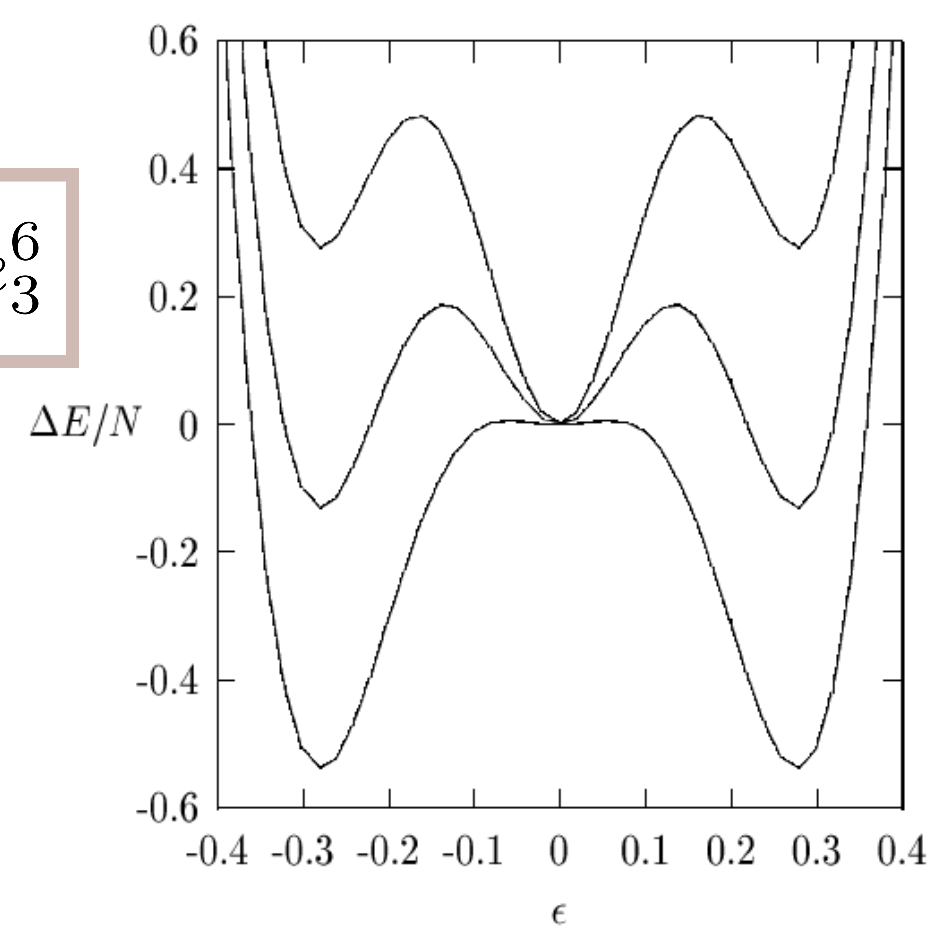
$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{u}}}\right) = \frac{\partial L}{\partial \mathbf{u}} - \frac{\partial R}{\partial \dot{\mathbf{u}}},$$

$$R[e_i] = \frac{1}{2}\sum_{\mathbf{r}} \left[\gamma_1 \dot{e}_1^2(\mathbf{r}) + \gamma_2 \dot{e}_2^2(\mathbf{r}) + \gamma_3 \dot{e}_3^2(\mathbf{r})\right]$$

$$\begin{aligned} \mathcal{F}[e_i(\mathbf{r}), e_i^P(\mathbf{r})] &= \int [\frac{1}{2}a_1(\underline{e_1 + e_1^P})^2 + \frac{c_1}{2}(\nabla e_1)^2 + \frac{1}{2}a_2 e_2^2 + \frac{c_2}{2}(\nabla e_2)^2 \\ &\quad \frac{1}{2}a_3 e_3^2 + V(e_i) + \frac{c_3}{2}(\nabla e_3)^2] d\mathbf{r}. \end{aligned}$$

$$\begin{aligned} e_1(\mathbf{r}) &= \frac{\partial u_x(\mathbf{r})}{\partial x} + \frac{\partial u_y(\mathbf{r})}{\partial y} \\ e_2(\mathbf{r}) &= \frac{\partial u_x(\mathbf{r})}{\partial x} - \frac{\partial u_y(\mathbf{r})}{\partial y}, \\ e_3(\mathbf{r}) &= \frac{\partial u_x(\mathbf{r})}{\partial y} + \frac{\partial u_y(\mathbf{r})}{\partial x}. \end{aligned}$$

$$V(e_i) = \frac{1}{4}b_3 e_3^4 + \frac{1}{6}d_3 e_3^6$$

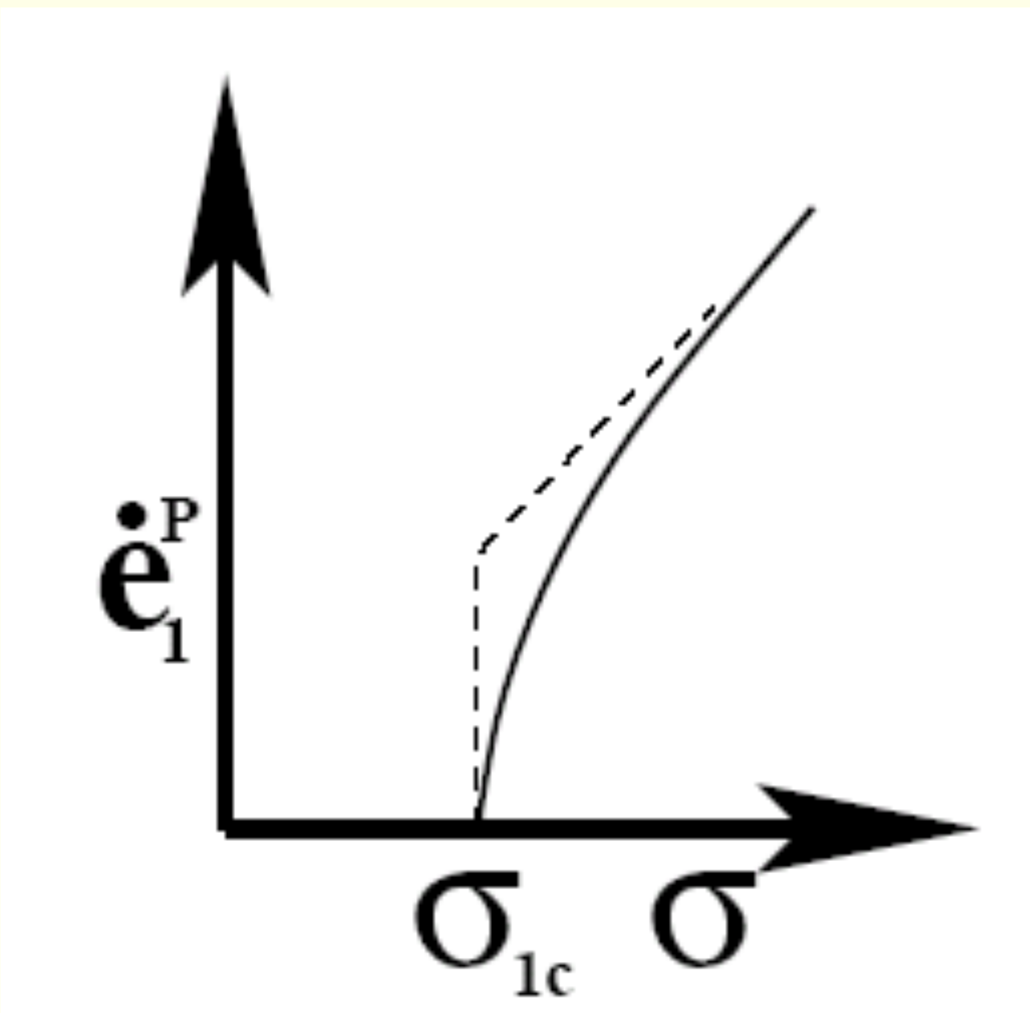


Elasto-plastic theory

$$
\begin{aligned}
\rho\ddot{e}_1 &= \nabla^2[a_1(e_1+e_1^P)-c_1\nabla^2 e_1+\gamma_1\dot{e}_1]+2\frac{\partial^2}{\partial x\partial y}\left(a_3e_3+\frac{\partial V}{\partial e_3}-c_3\nabla^2 e_3+\gamma_3\dot{e}_3\right)\\
&+ \left(\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}\right)\left(a_2e_2-c_2\nabla^2 e_2+\gamma_2\dot{e}_2\right),\\
\rho\ddot{e}_2 &= \nabla^2\left(a_2e_2-c_2\nabla^2 e_2+\gamma_2\dot{e}_2\right)+\left(\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}\right)[a_1(e_1+e_1^P)-c_1\nabla^2 e_1+\gamma_1\dot{e}_1],\\
\rho\ddot{e}_3 &= \nabla^2\left(a_3e_3^2+\frac{\partial V}{\partial e_3}-c_3\nabla^2 e_3+\gamma_3\dot{e}_3\right)+2\frac{\partial^2}{\partial x\partial y}[a_1(e_1+e_1^P)-c_1\nabla^2 e_1+\gamma_1\dot{e}_1].
\end{aligned}
$$

Elasto-plastic theory

$$
\begin{aligned}
\dot{e}_1^P &= -\frac{1}{\nu}\int_{-\infty}^{t} \sigma_1(t')e^{-\frac{(t-t')}{\tau}}dt' + c_p\nabla^2 e_1^P \qquad \text{if } |\sigma_1| > \sigma_{1c} \\
&= c_p\nabla^2 e_1^P \qquad \text{otherwise}
\end{aligned}
$$

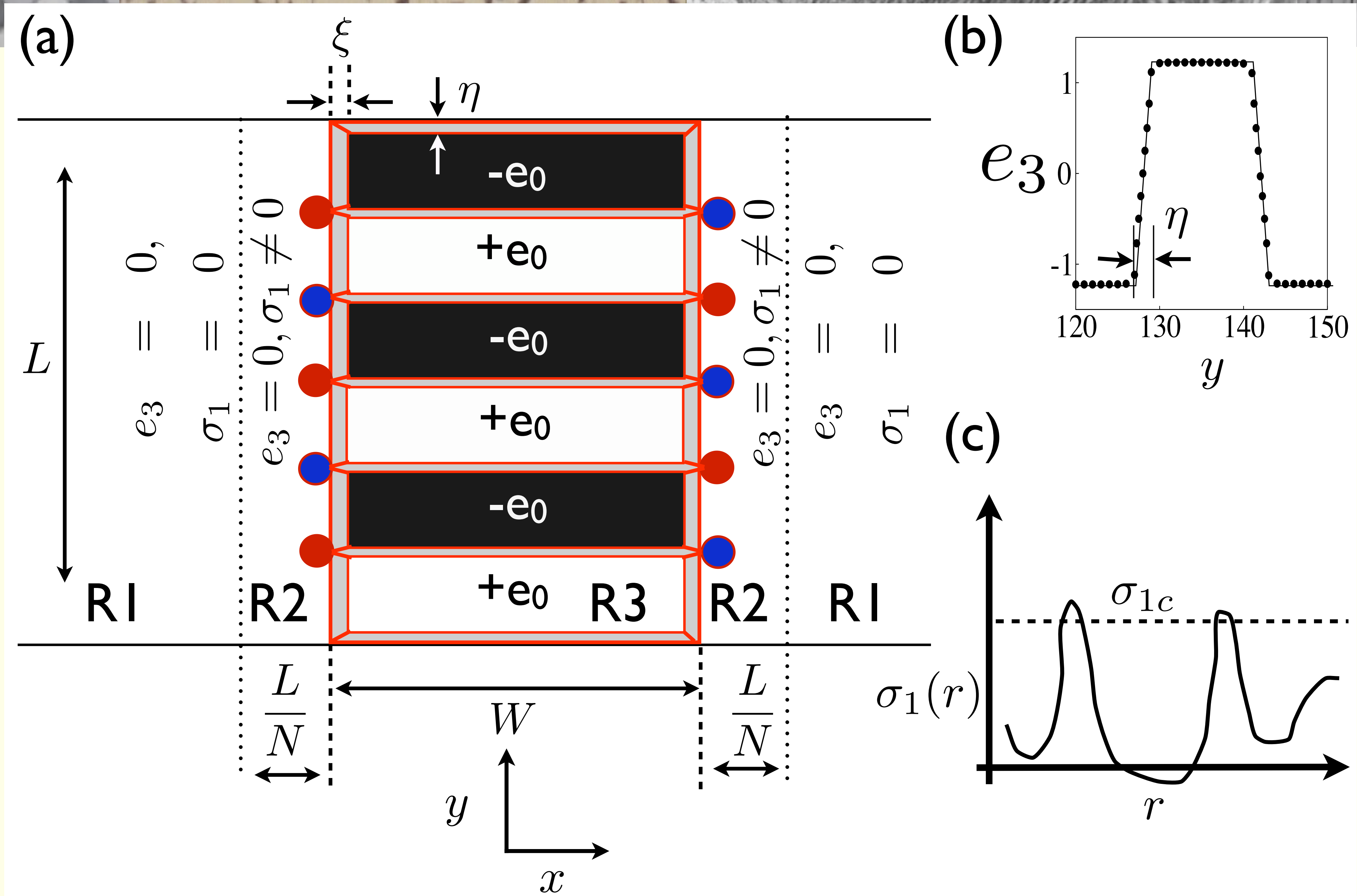


$$\nabla \times (\nabla \times \epsilon)^T \neq 0 = \nabla^2 e_1^P$$

$$
\begin{aligned}
\frac{1}{2}\left(-\frac{\partial e_1^P}{\partial y}, \frac{\partial e_1^P}{\partial x}\right) &= \nabla \times \epsilon^P \\
&= \text{Burger's vector density}
\end{aligned}
$$

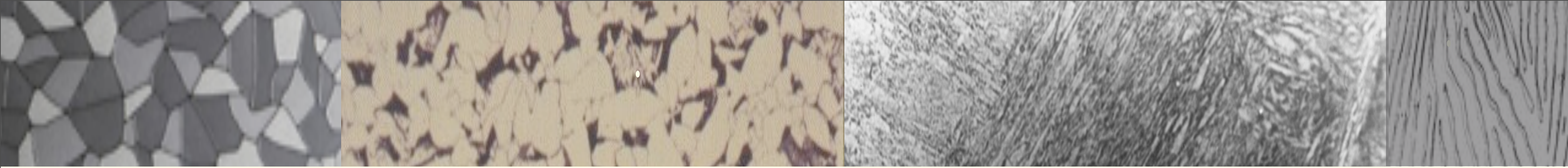
E. Kröner, *Z. Physik* **139**, 175–188 (1954).

Droplet model



Assume e_1 and interfacial widths ξ, η are *fast* variables slaved to e_3 and e_1^P is small

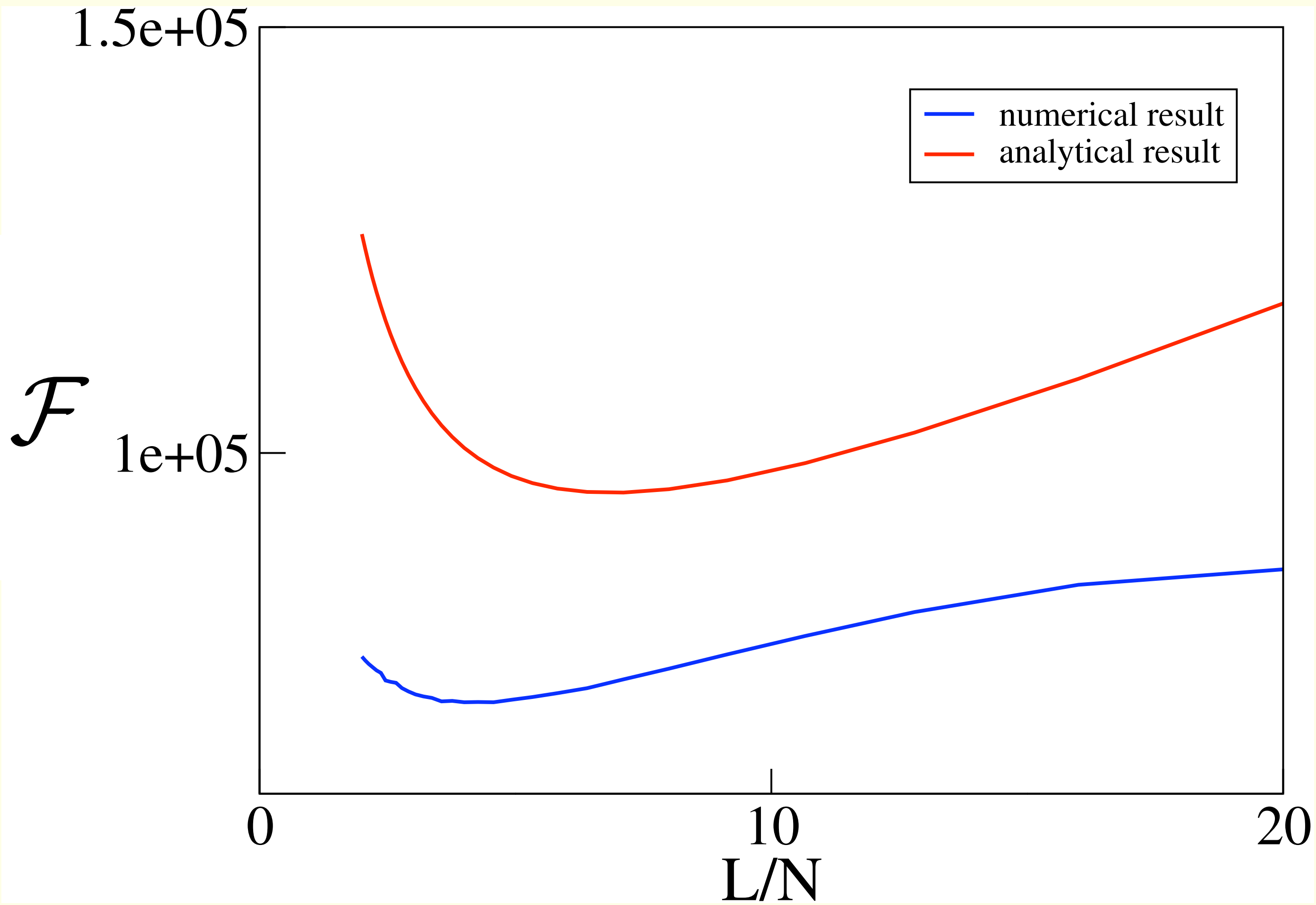
$$\nabla^2 e_1 = 2\left(\frac{a_2 - a_3}{a_1 + a_2}\right)\frac{\partial^2 e_3}{\partial x \partial y} - \nabla^2 e_1^p,$$

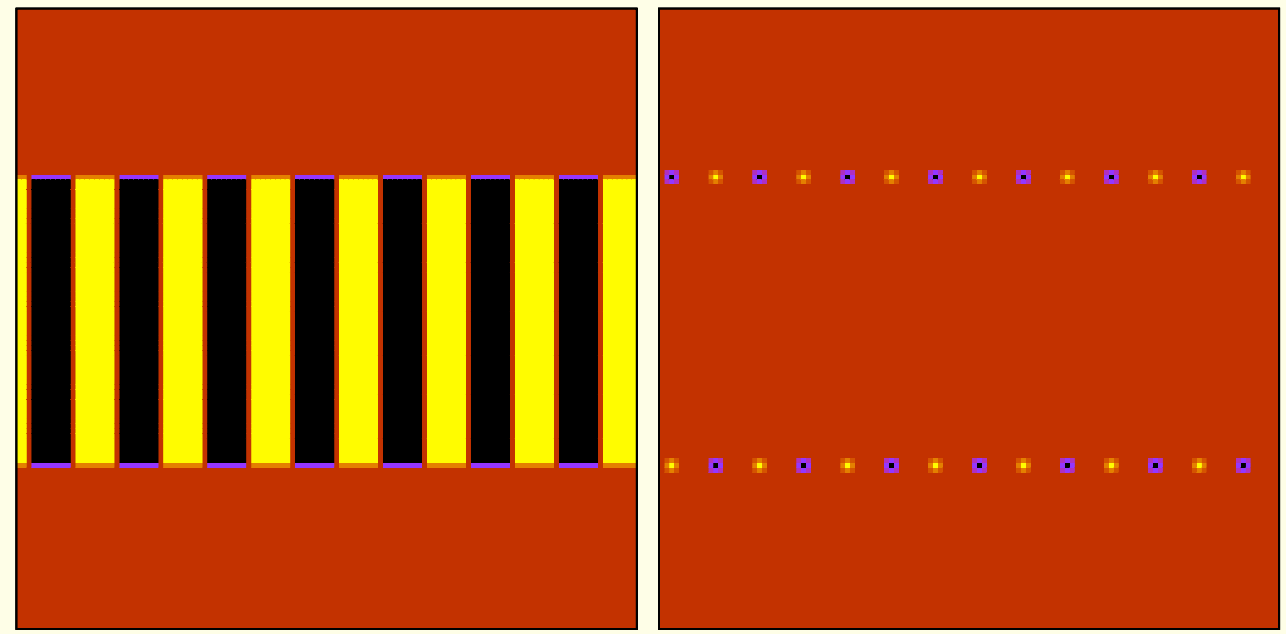


$$\mathcal{F} = \mathcal{F}_b LW + 2N\mathcal{F}_s\left(\frac{L\xi}{N} + \eta W\right) + 2Nc_3 e_0^2\left(\frac{L/N}{\xi} + \frac{W}{\eta}\right) + \frac{a_1\lambda^2 N}{4\pi^2}\left(\frac{L}{N}\right)^2$$

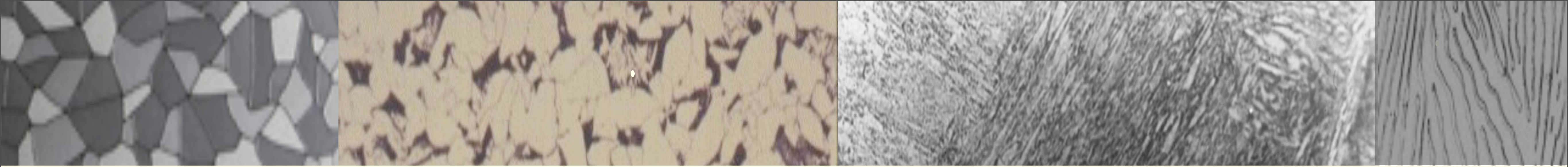
$$+\frac{Na_1 e_0^p(t)^2}{4}\left(\frac{L}{N}\right)\beta + \frac{a_1\lambda e_0^p(t)N}{\pi\sqrt{2\pi}}\left(\frac{L}{N}\right)^2$$

e_1^P **slow**





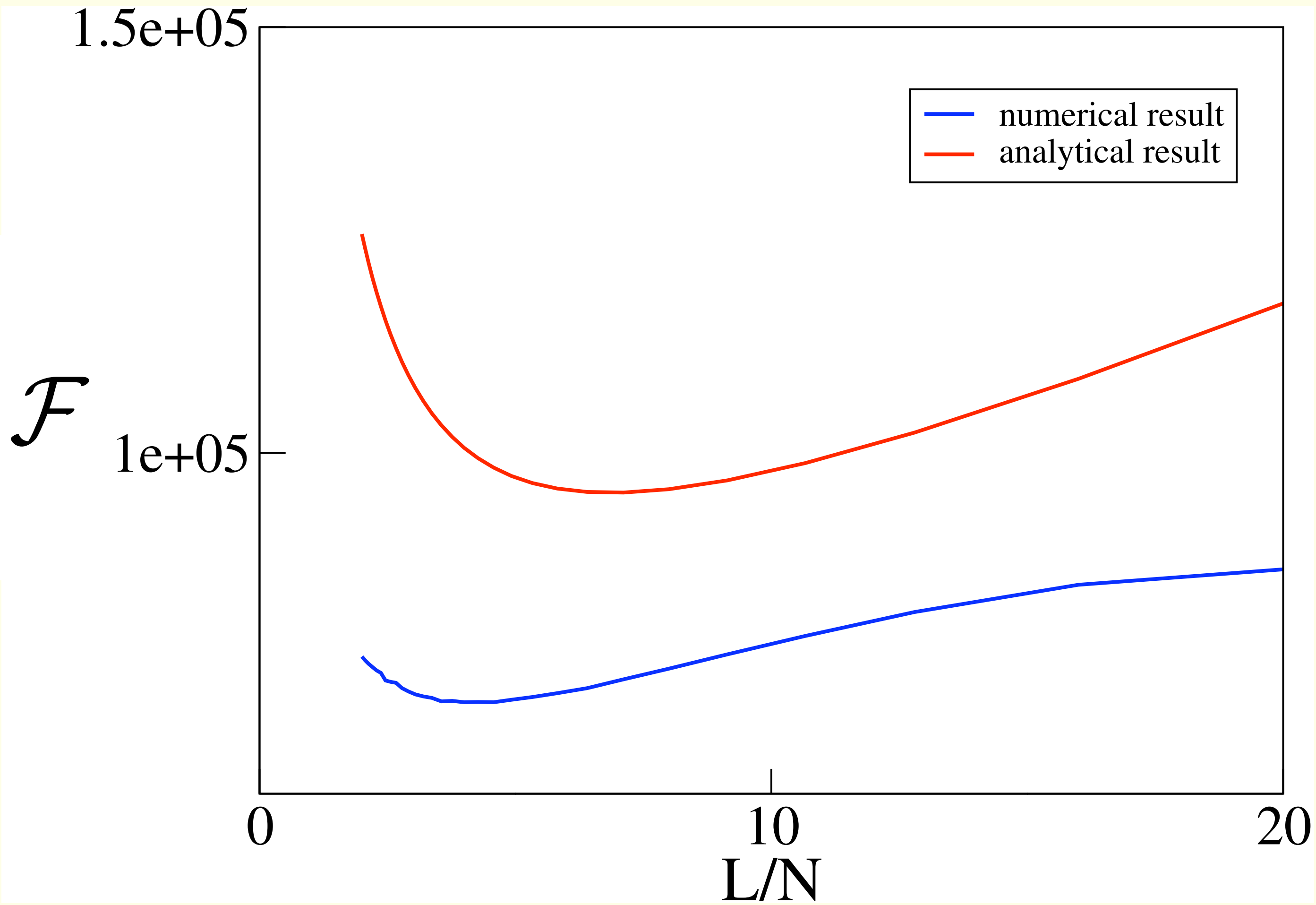
$e_3(x,y)$ $e_1(x,y)$

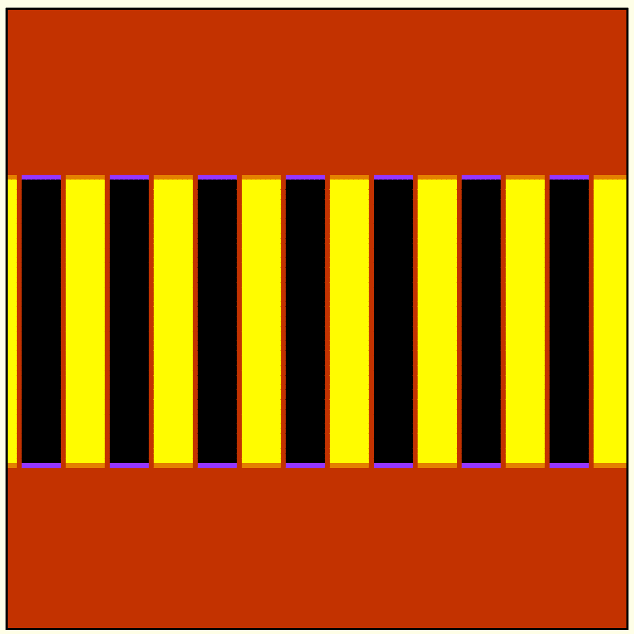


$$\mathcal{F} = \boxed{\mathcal{F}_b LW} + 2N\mathcal{F}_s\left(\frac{L\xi}{N} + \eta W\right) + 2Nc_3e_0^2\left(\frac{L/N}{\xi} + \frac{W}{\eta}\right) + \frac{a_1\lambda^2 N}{4\pi^2}\left(\frac{L}{N}\right)^2$$

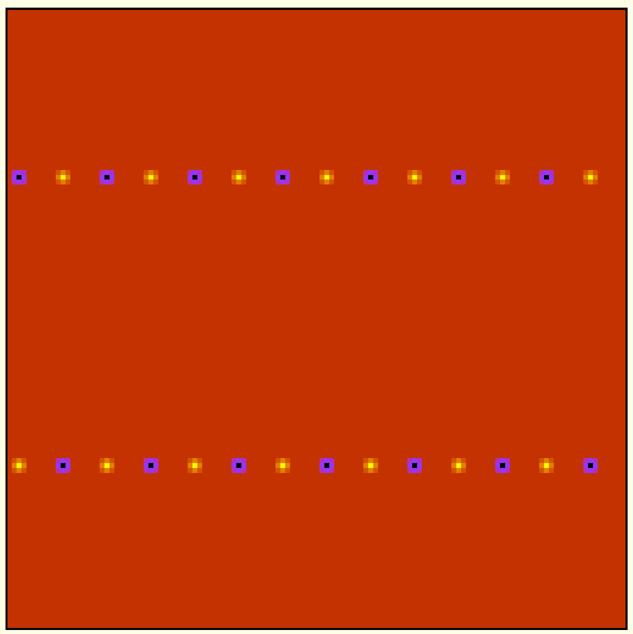
$$+\frac{Na_1e_0^p(t)^2}{4}\left(\frac{L}{N}\right)\beta + \frac{a_1\lambda e_0^p(t)N}{\pi\sqrt{2\pi}}\left(\frac{L}{N}\right)^2$$

e_1^P **slow**

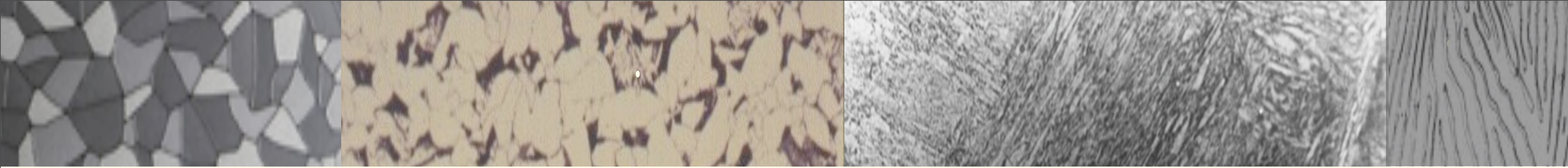




$e_3(x,y)$

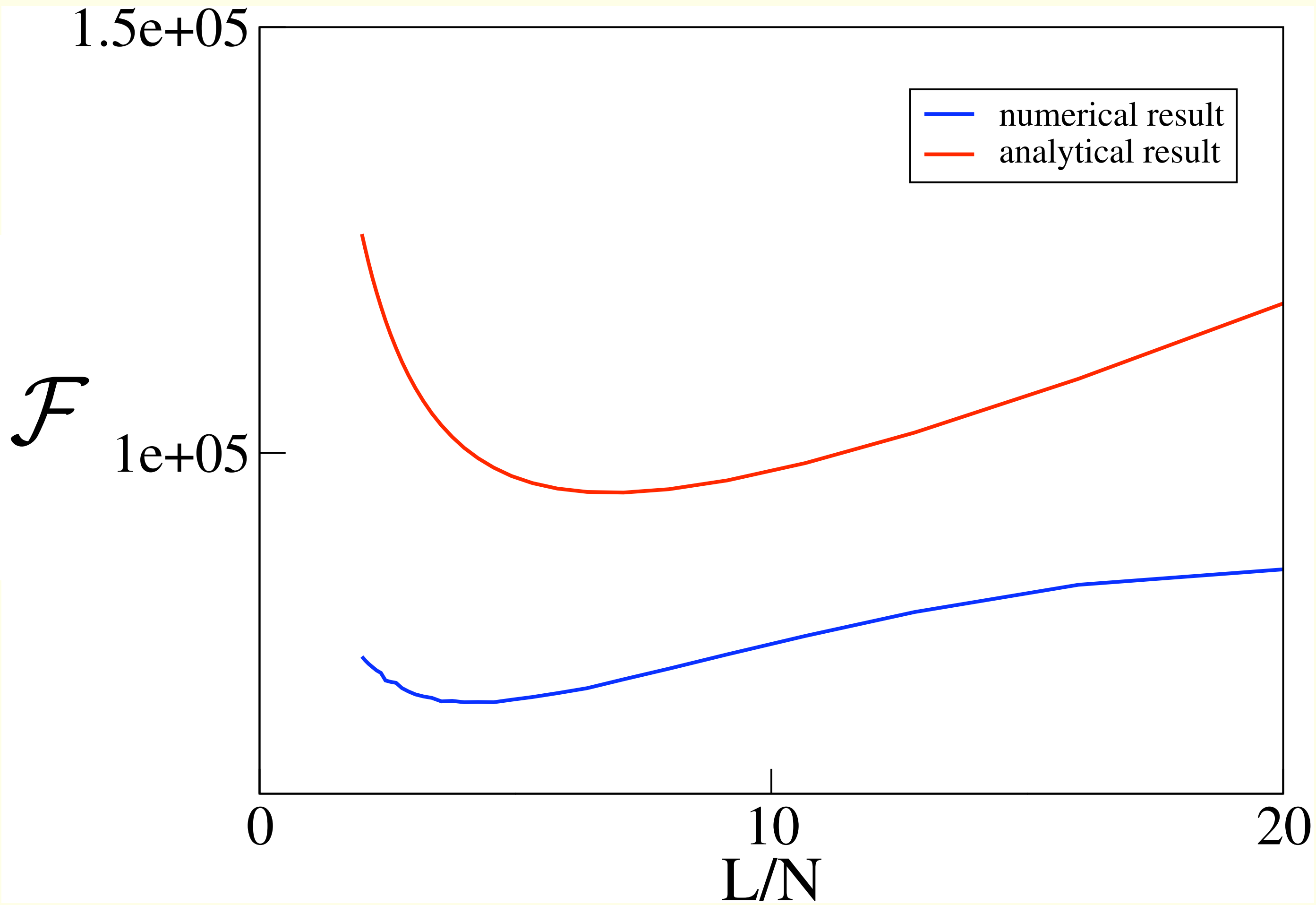


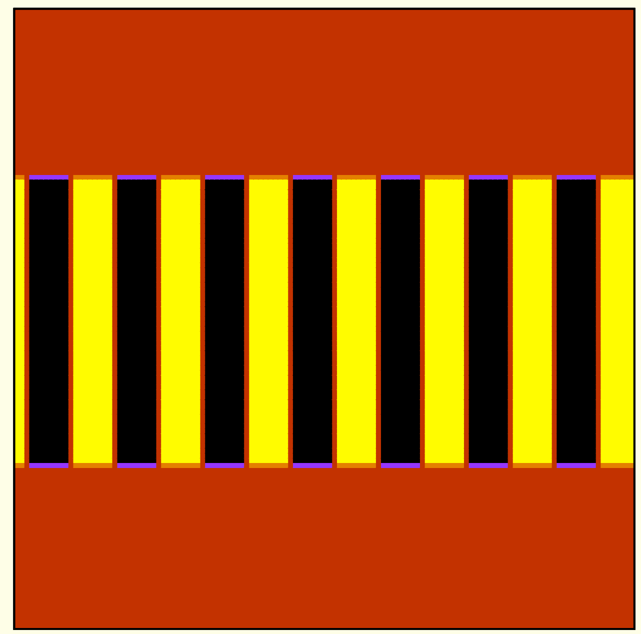
$e_1(x,y)$



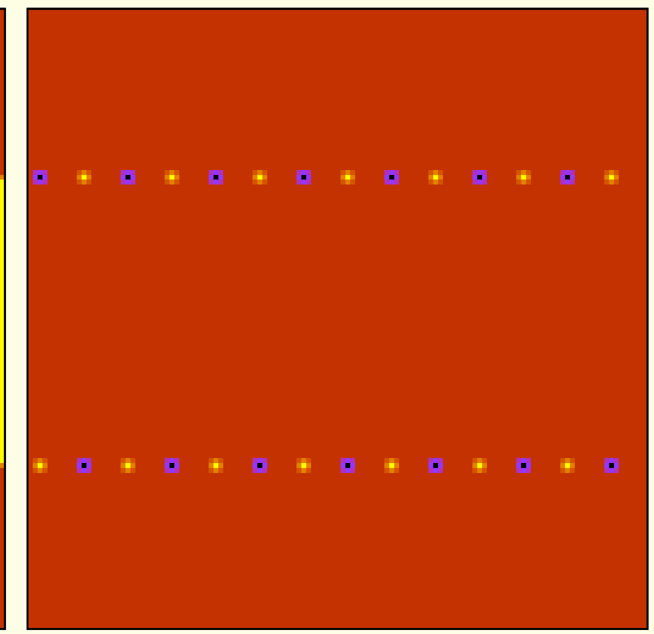
$$\mathcal{F} = \boxed{\mathcal{F}_b LW} + \boxed{2N\mathcal{F}_s\left(\frac{L\xi}{N} + \eta W\right)} + \boxed{2Nc_3e_0^2\left(\frac{L/N}{\xi} + \frac{W}{\eta}\right)} + \frac{a_1\lambda^2 N}{4\pi^2}\left(\frac{L}{N}\right)^2$$
$$+\frac{Na_1e_0^p(t)^2}{4}\left(\frac{L}{N}\right)\beta + \frac{a_1\lambda e_0^p(t)N}{\pi\sqrt{2\pi}}\left(\frac{L}{N}\right)^2$$

e_1^P **slow**

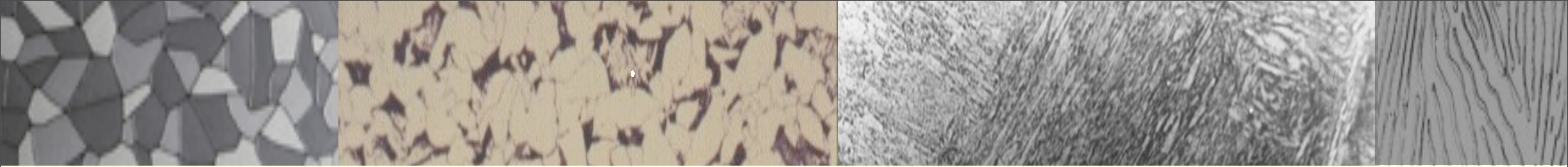




$e_3(x,y)$

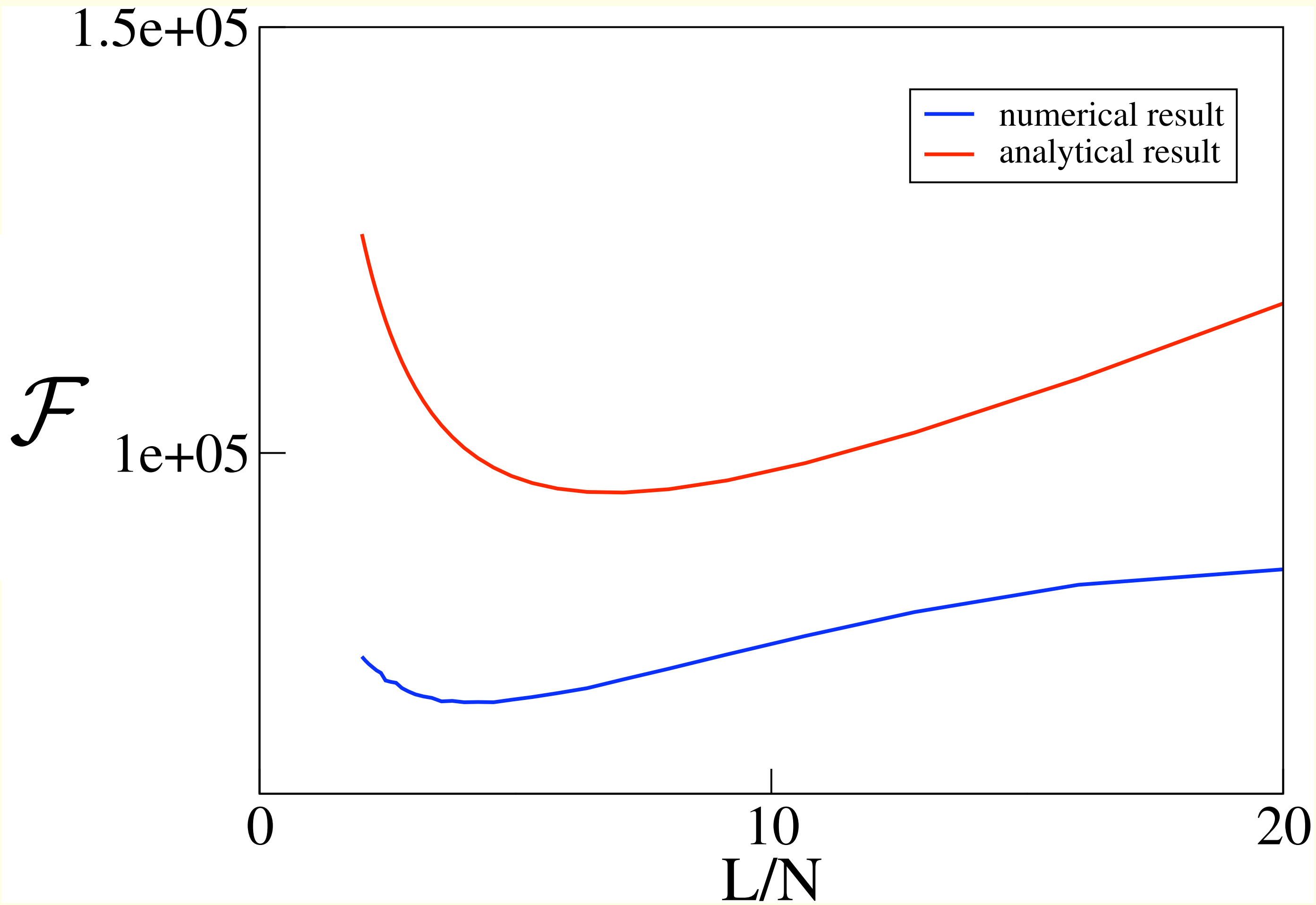


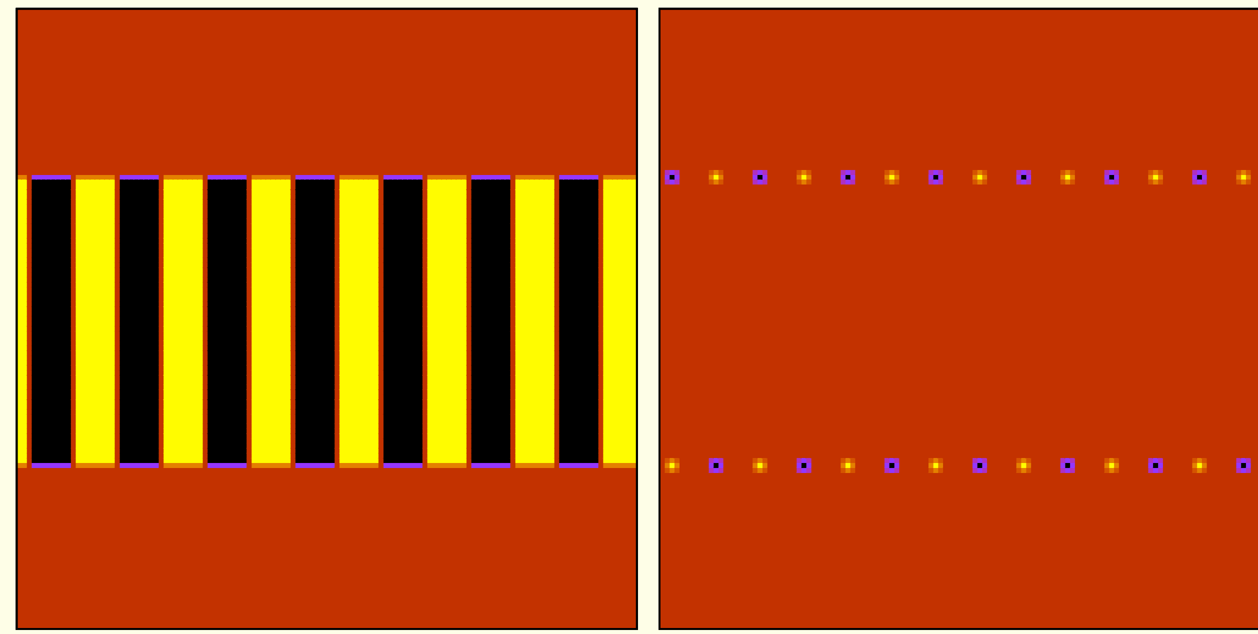
$e_1(x,y)$



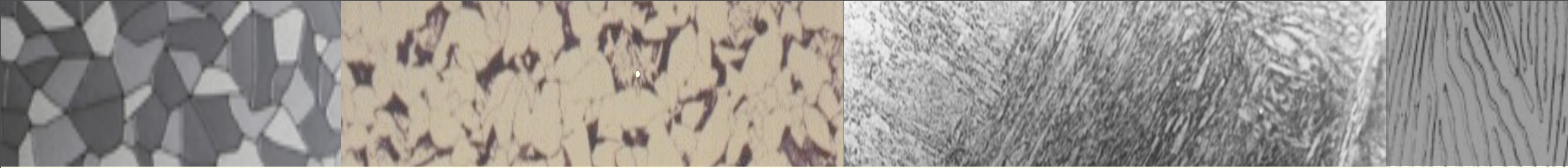
$$\mathcal{F} = \boxed{\mathcal{F}_b L W} + \boxed{2N\mathcal{F}_s\left(\frac{L\xi}{N} + \eta W\right)} + \boxed{2N c_3 e_0^2\left(\frac{L/N}{\xi} + \frac{W}{\eta}\right)} + \boxed{\frac{a_1\lambda^2 N}{4\pi^2}\left(\frac{L}{N}\right)^2}$$

$$+\frac{N a_1 e_0^p(t)^2}{4}\left(\frac{L}{N}\right)\beta + \frac{a_1\lambda e_0^p(t) N}{\pi\sqrt{2\pi}}\left(\frac{L}{N}\right)^2 \qquad e_1^P \ \textbf{slow}$$





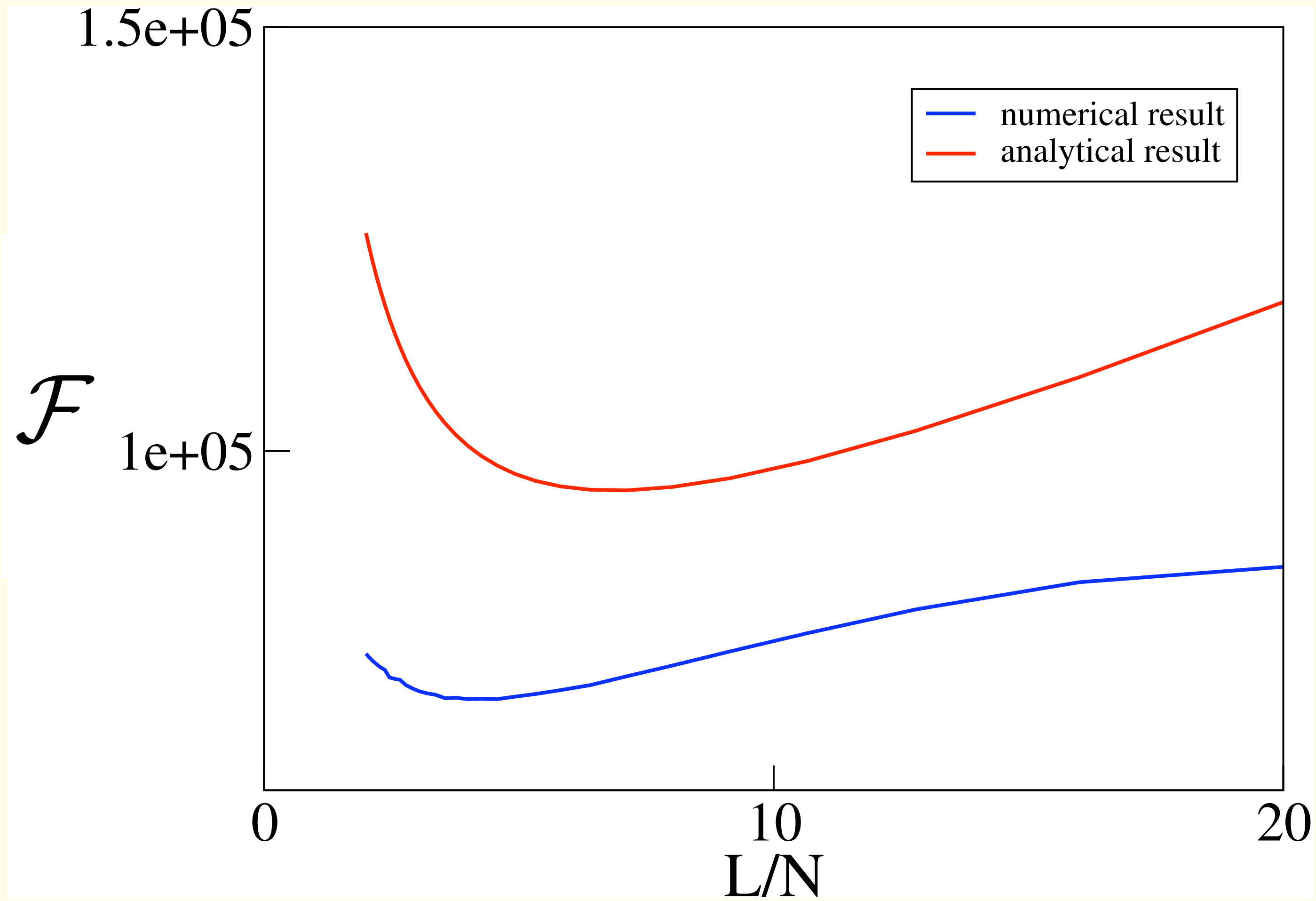
$e_3(x,y)$ $e_1(x,y)$

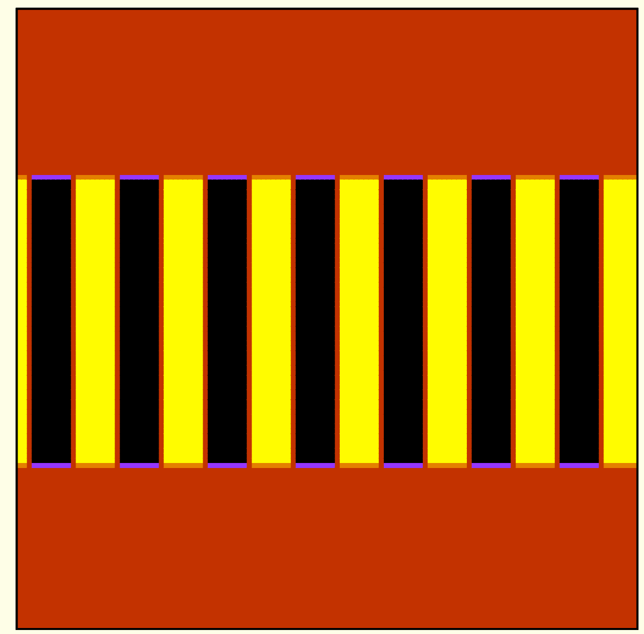


$$\mathcal{F} = \boxed{\mathcal{F}_b L W} + \boxed{2N\mathcal{F}_s\left(\frac{L\xi}{N} + \eta W\right)} + \boxed{2Nc_3 e_0^2\left(\frac{L/N}{\xi} + \frac{W}{\eta}\right)} + \boxed{\frac{a_1\lambda^2 N}{4\pi^2}\left(\frac{L}{N}\right)^2}$$

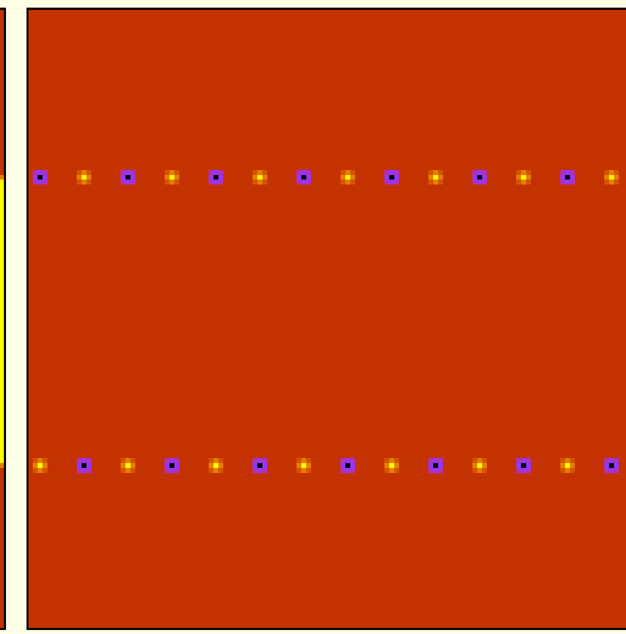
$$\boxed{+\frac{N a_1 e_0^p(t)^2}{4}\left(\frac{L}{N}\right)\beta + \frac{a_1\lambda e_0^p(t) N}{\pi\sqrt{2\pi}}\left(\frac{L}{N}\right)^2}$$

e_1^P **slow**

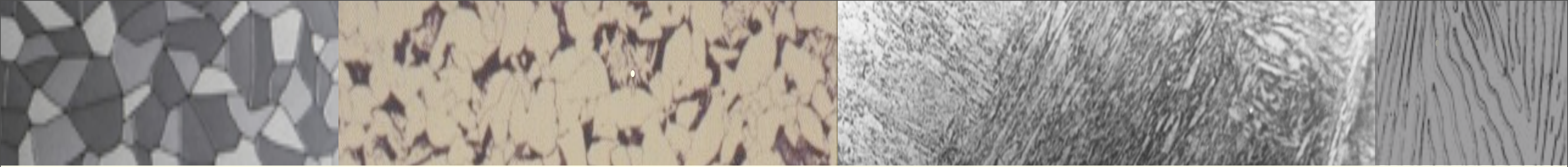




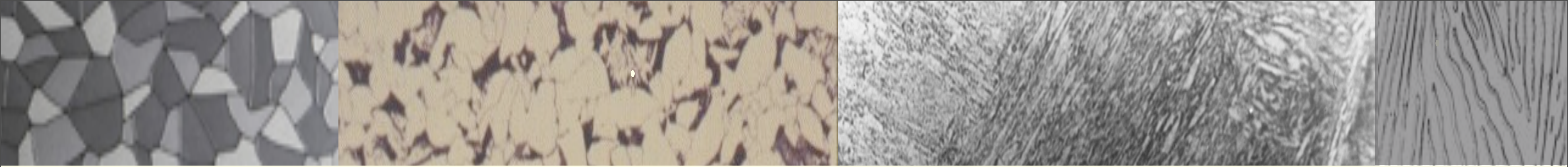
$e_3(x,y)$



$e_1(x,y)$

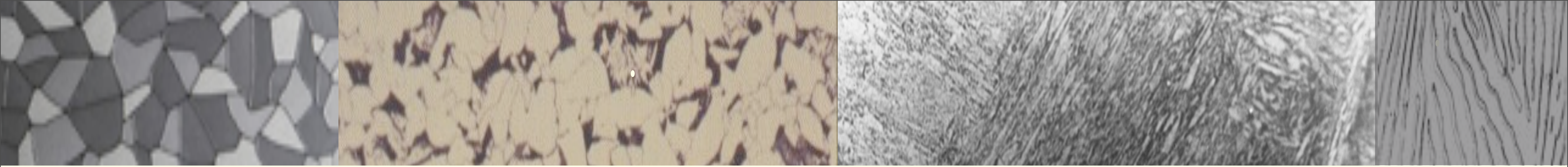


Elastic coupling makes energy of parent product interfaces go as $(L/N)^2$. This *favors* a twin structure.



Elastic coupling makes energy of parent product interfaces go as $(L/N)^2$. This *favors* a twin structure.

$$\left(\frac{L}{N}\right)^2 = \frac{16\pi^2 e_0 \sqrt{c_3 \mathcal{F}_s}}{a_1 \left(\lambda^2 + 4\sqrt{\frac{\pi}{2}}\lambda e_0^p(t)\right)} W$$

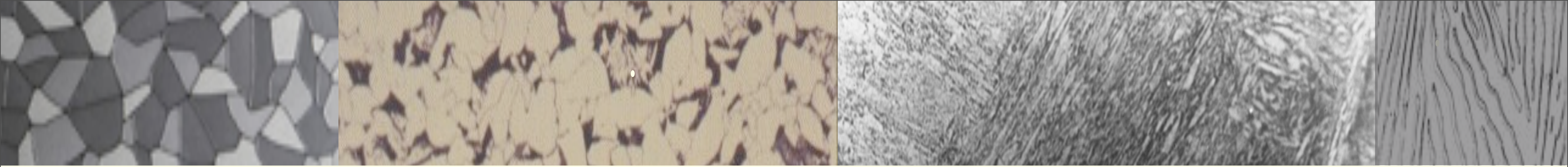


Elastic coupling makes energy of parent product interfaces go as $(L/N)^2$. This *favors* a twin structure.

$$\left(\frac{L}{N}\right)^2 = \frac{16\pi^2 e_0 \sqrt{c_3 \mathcal{F}_s}}{a_1\left(\lambda^2 + 4\sqrt{\frac{\pi}{2}}\lambda e_0^p(t)\right)} W$$

$$e_0^P(t) \rightarrow -\lambda\sqrt{\frac{1}{8\pi}}$$

$$\frac{L}{N} \rightarrow \infty$$



Elastic coupling makes energy of parent product interfaces go as $(L/N)^2$. This *favors* a twin structure.

$$\left(\frac{L}{N}\right)^2 = \frac{16\pi^2 e_0\sqrt{c_3\mathcal{F}_s}}{a_1\left(\lambda^2 + 4\sqrt{\frac{\pi}{2}}\lambda e_0^p(t)\right)} W$$

$$e_0^P(t) \rightarrow -\lambda\sqrt{\frac{1}{8\pi}}$$

$$\frac{L}{N} \rightarrow \infty$$

Too much of plasticity *destroys* twinned structure because it *screens* elastic interactions and makes them short ranged.

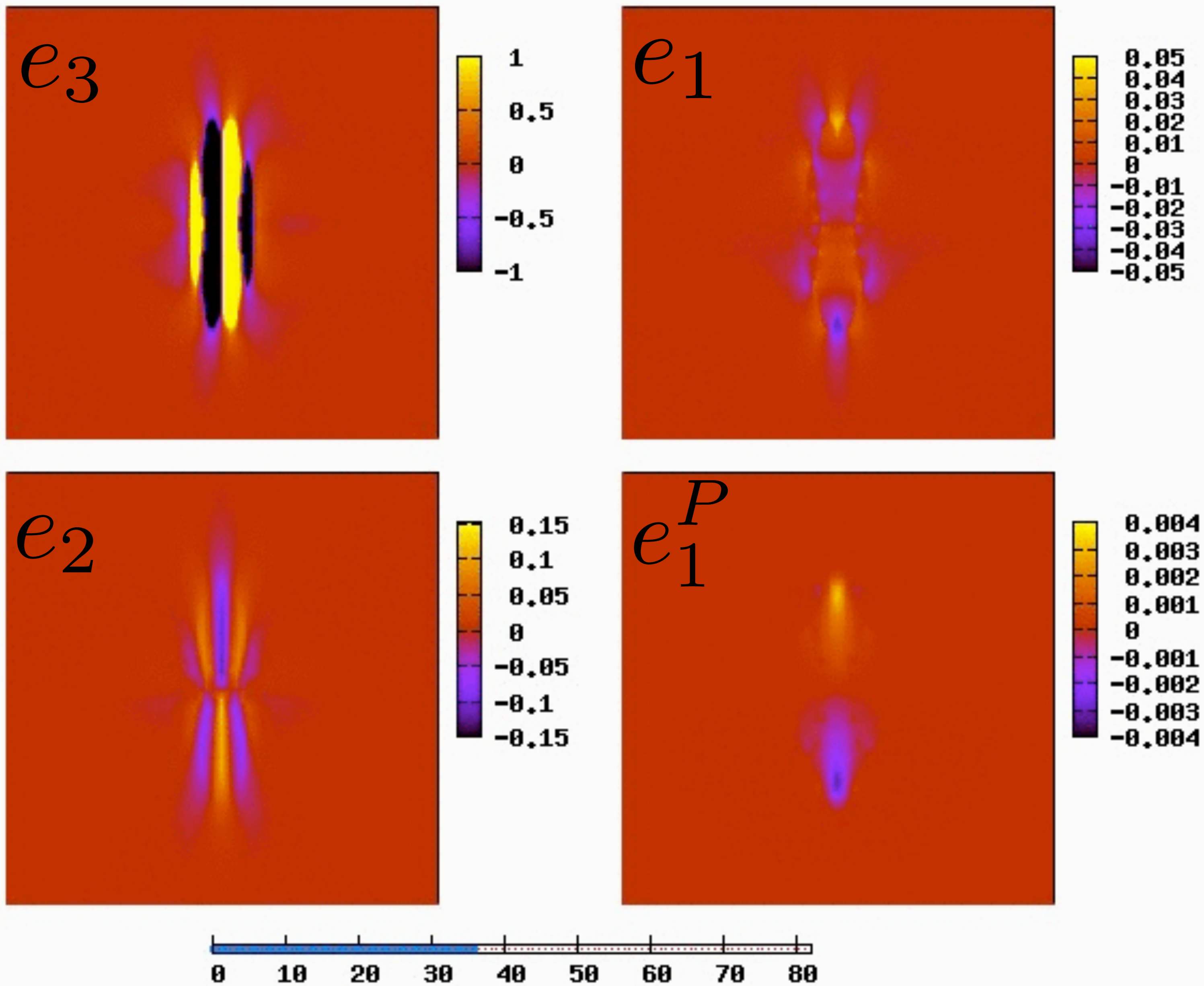
Dynamics

e_3 e_1

e_2 e_1^P

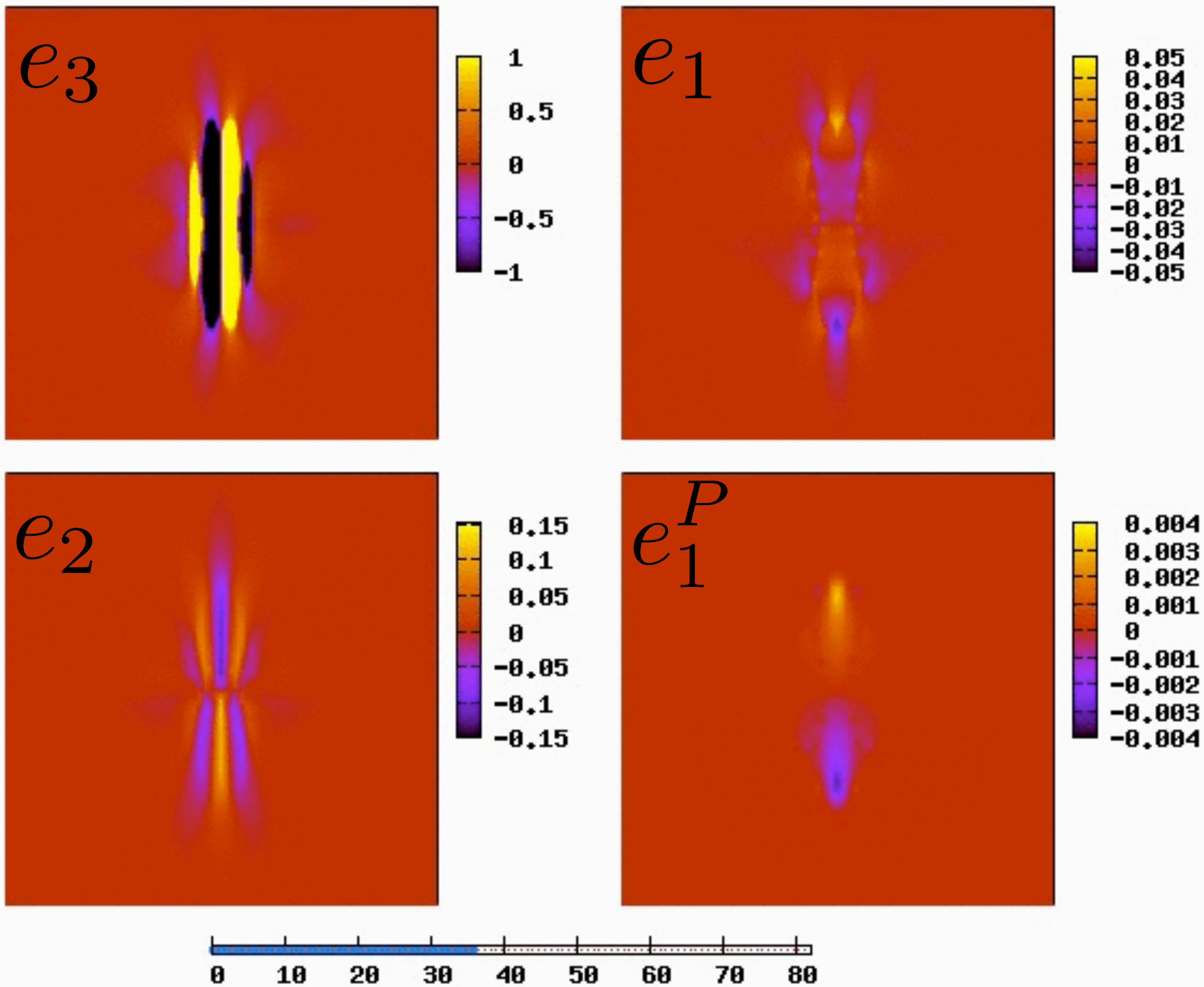
M-phase

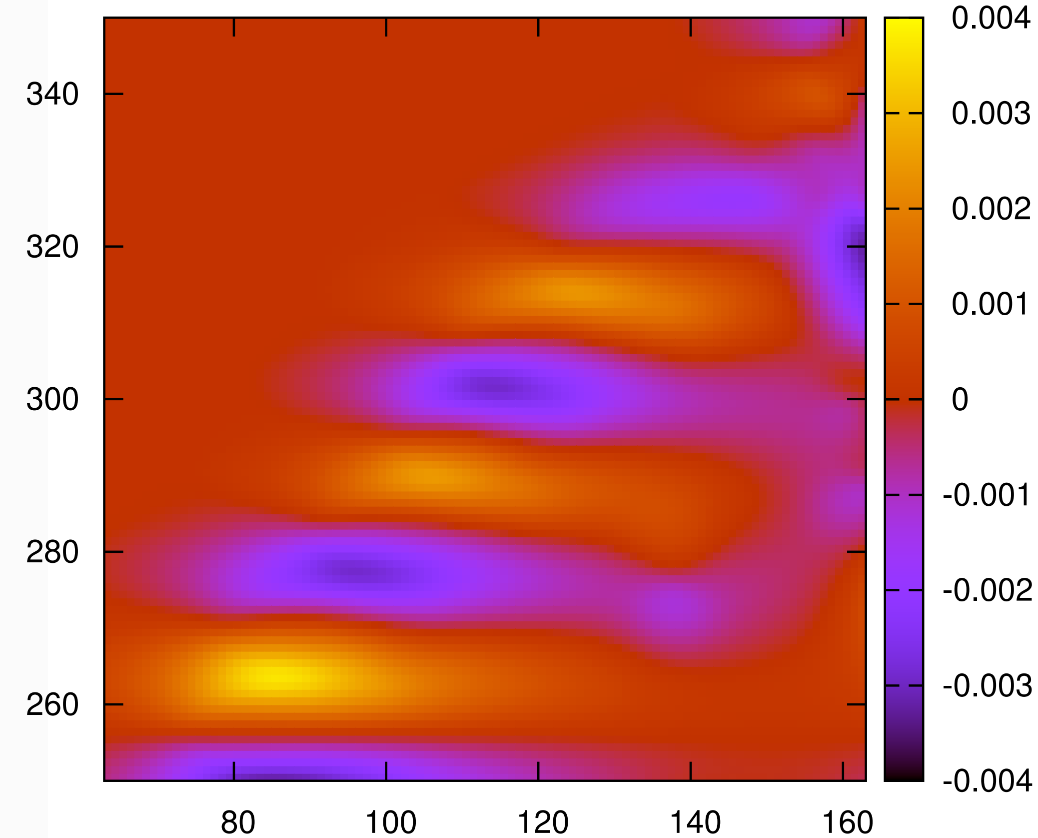
Dynamics



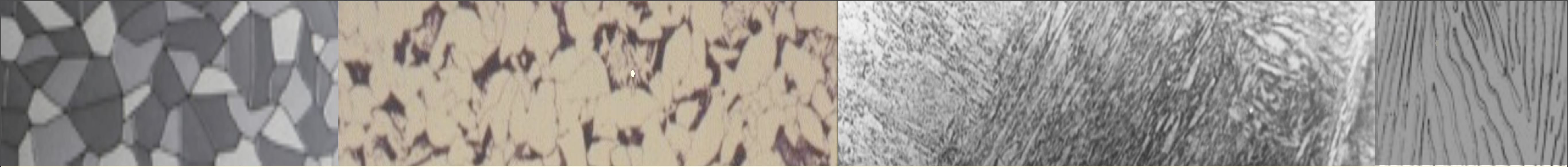
M-phase

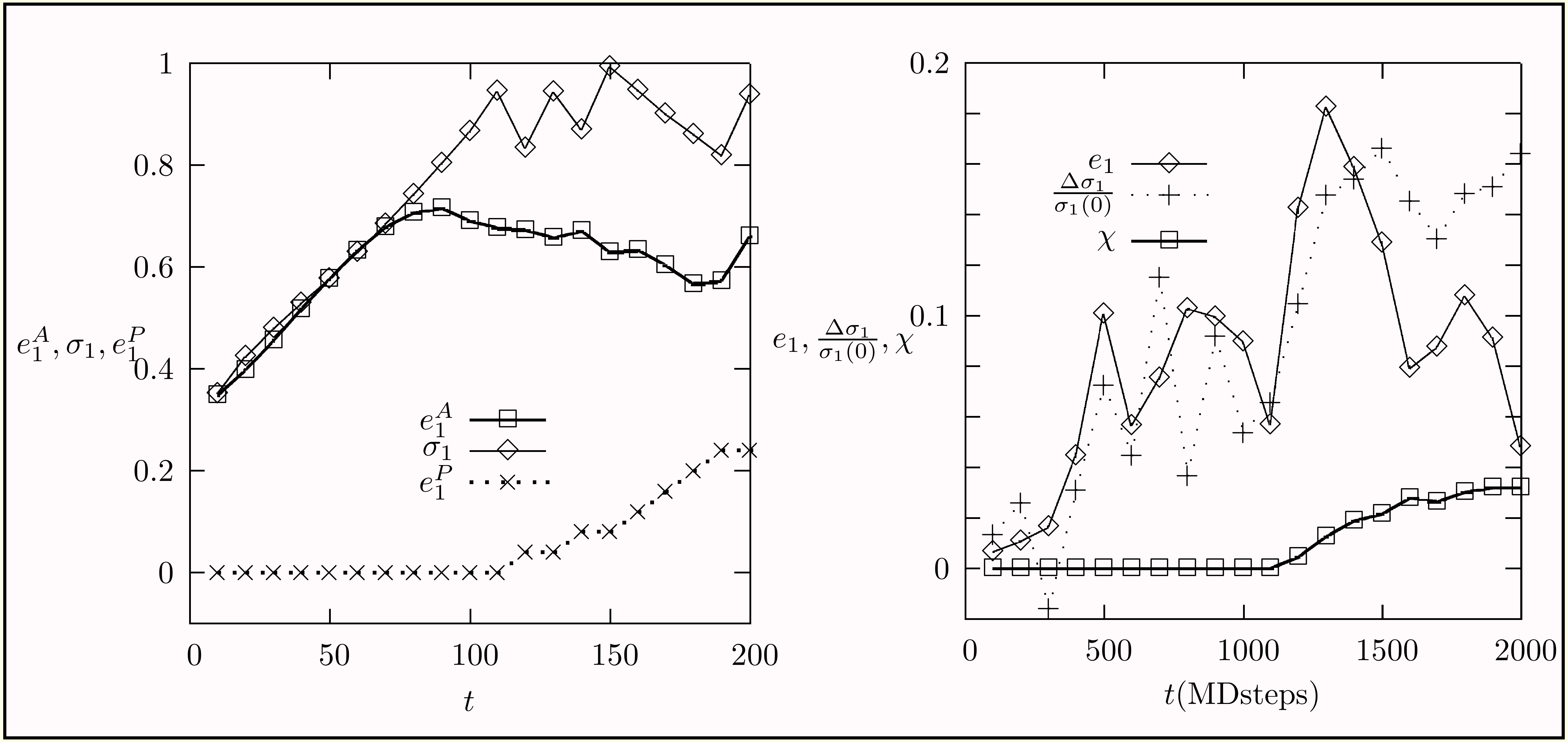
Dynamics

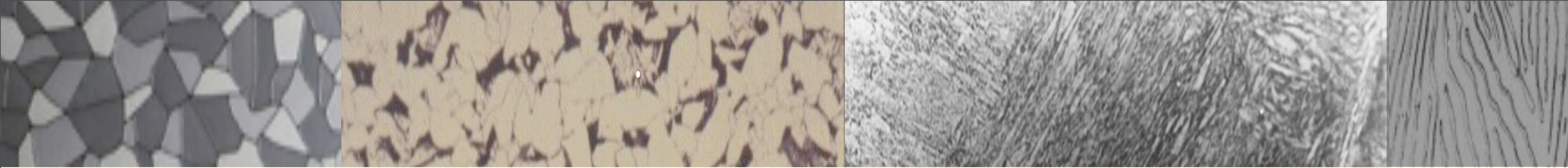




M-phase



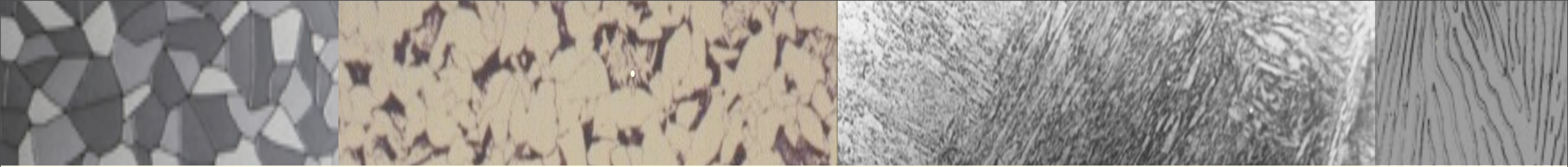

e_1^A, σ_1, e_1^P
t
0
50
100
150
200
0
0.2
0.4
0.6
0.8
1
e_1^A
σ_1
e_1^P
$e_1, \frac{\Delta\sigma_1}{\sigma_1(0)}, \chi$
t(MDsteps)
0
500
1000
1500
2000
0
0.1
0.2
e_1
$\frac{\Delta\sigma_1}{\sigma_1(0)}$
χ

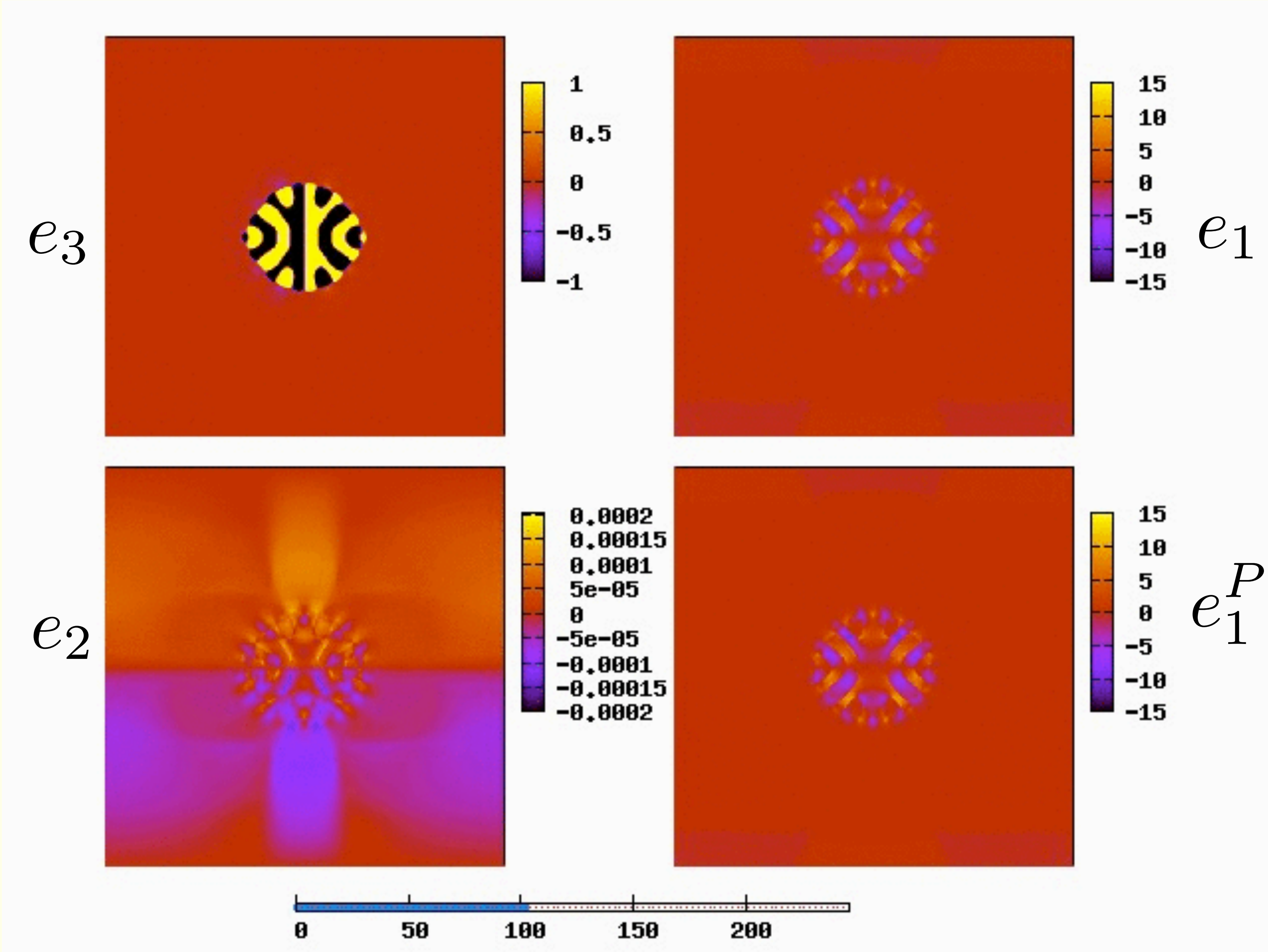


e_3 e_1

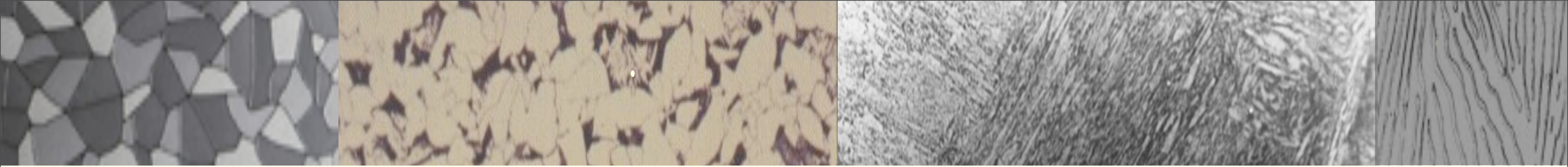
e_2 e_1^P

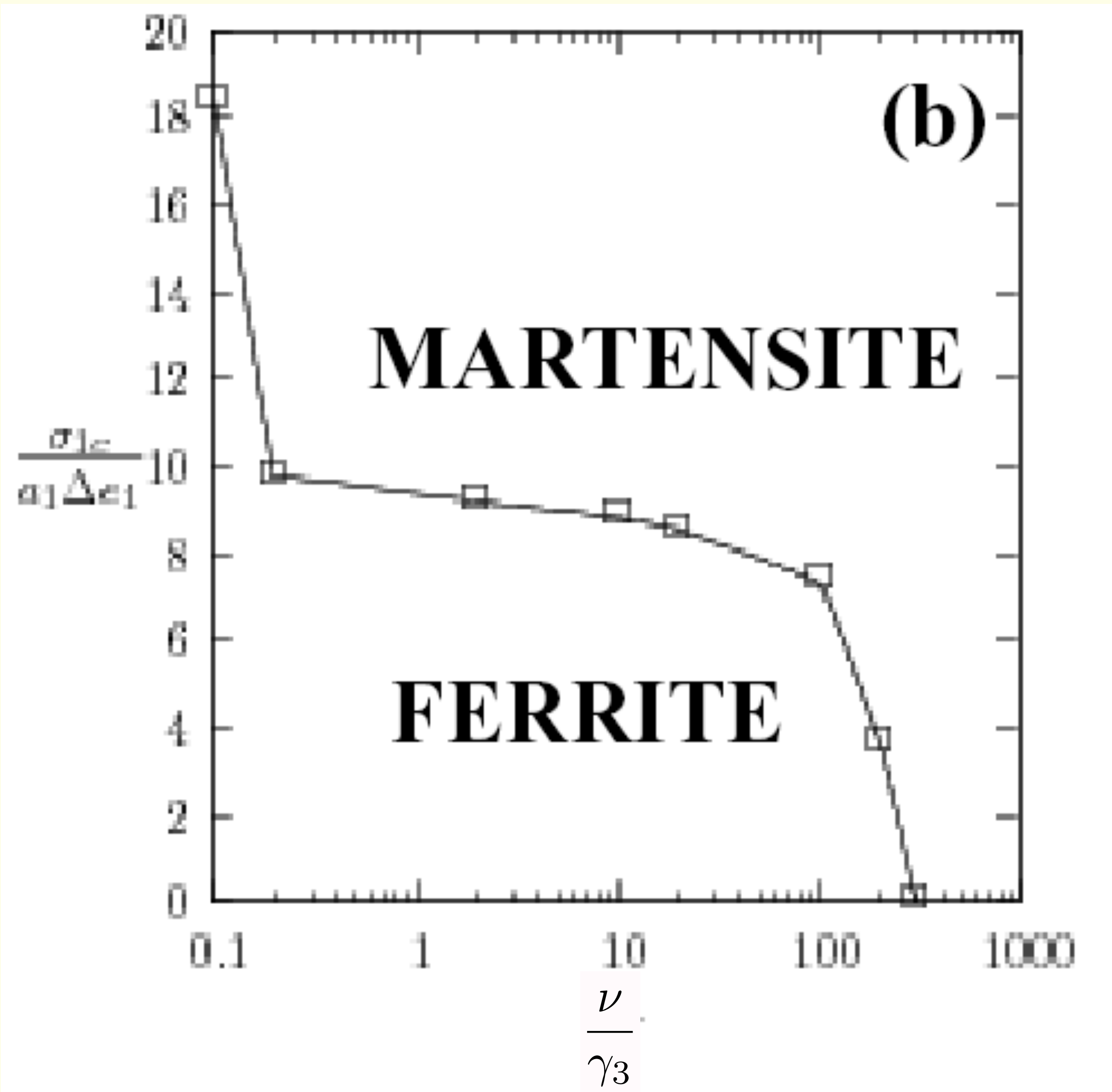
F-phase

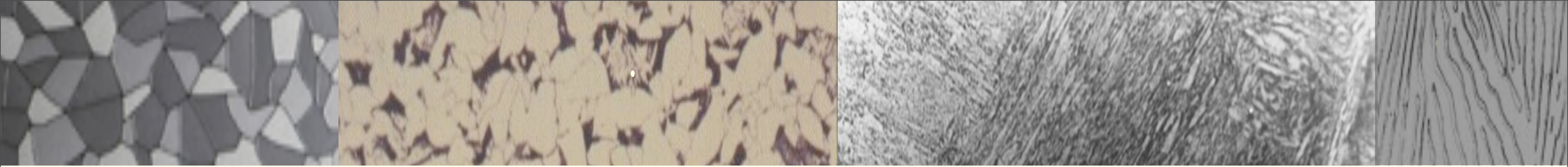


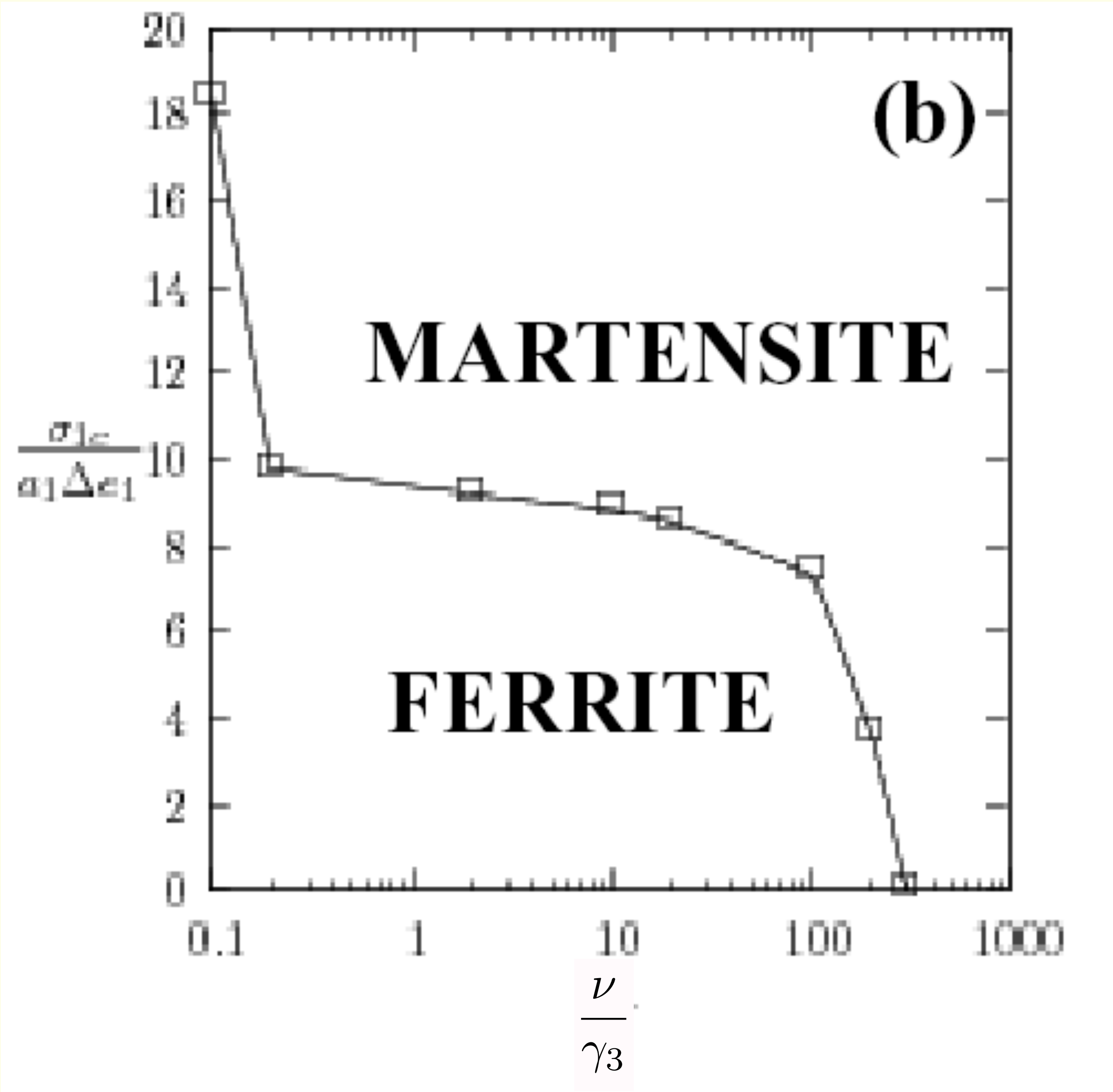

e_3
1
0.5
0
-0.5
-1
15
10
5
0
-5
-10
-15
e_1
e_2
0.0002
0.00015
0.0001
5e-05
0
-5e-05
-0.0001
-0.00015
-0.0002
15
10
5
0
-5
-10
-15
e_1^P
0
50
100
150
200

F-phase



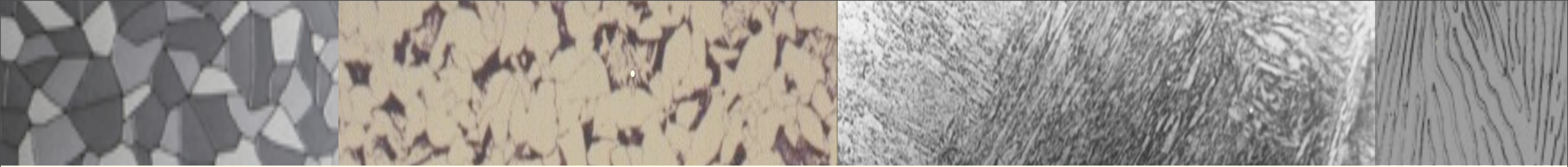

(b)
MARTENSITE
FERRITE
20
18
16
14
12
10
8
6
4
2
0
0.1
1
10
100
1000
$\frac{\sigma_{1c}}{a_1 \Delta e_1}$
$\frac{\nu}{\gamma_3}$

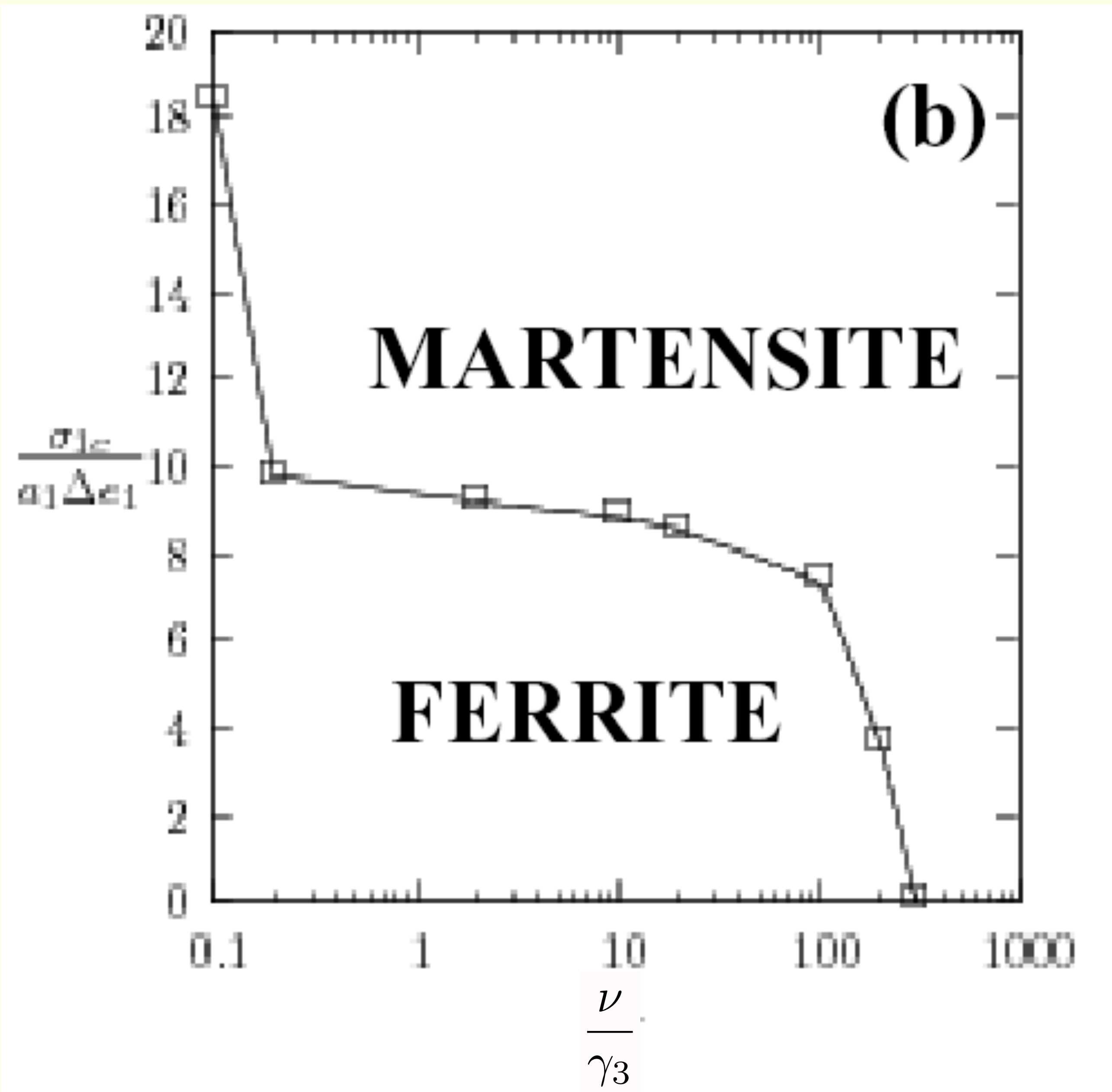




σ_{1c}

given by local elastic modulus times atomic strain threshold (<13%)



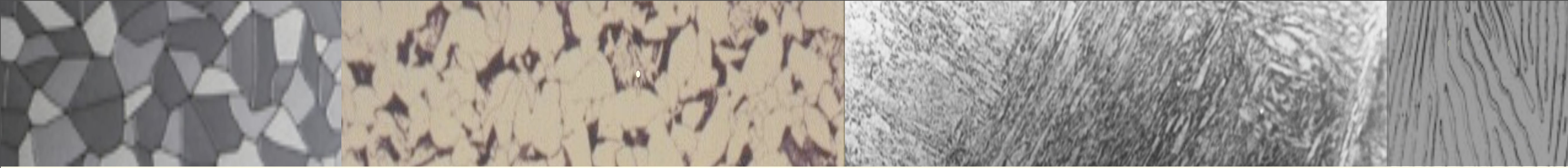


σ_{1c}
given by local elastic modulus times atomic strain threshold (<13%)

$\frac{\nu}{\gamma_3}$ is a *Deborah* number = $\frac{\text{Growth velocity}}{\text{plasticity production rate}}$

Future directions

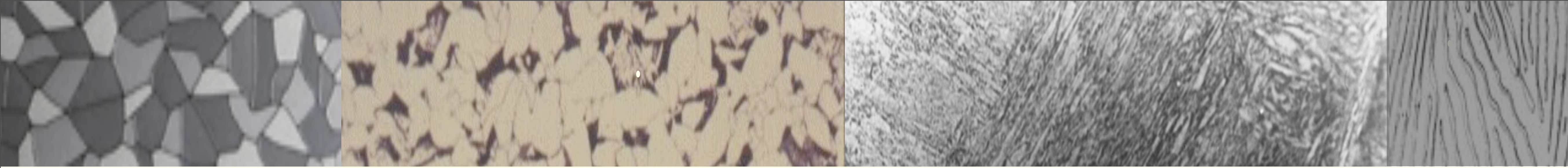
- Is this phenomenon generic? Other models in 2D and 3D showing structural transitions between incompatible solids.
- Other kinds of approaches: intermediate scale dynamics for NAZs - connections with STZ theory.
- Spin ($S=\pm 1,0$) models *with plasticity*.
- and ....



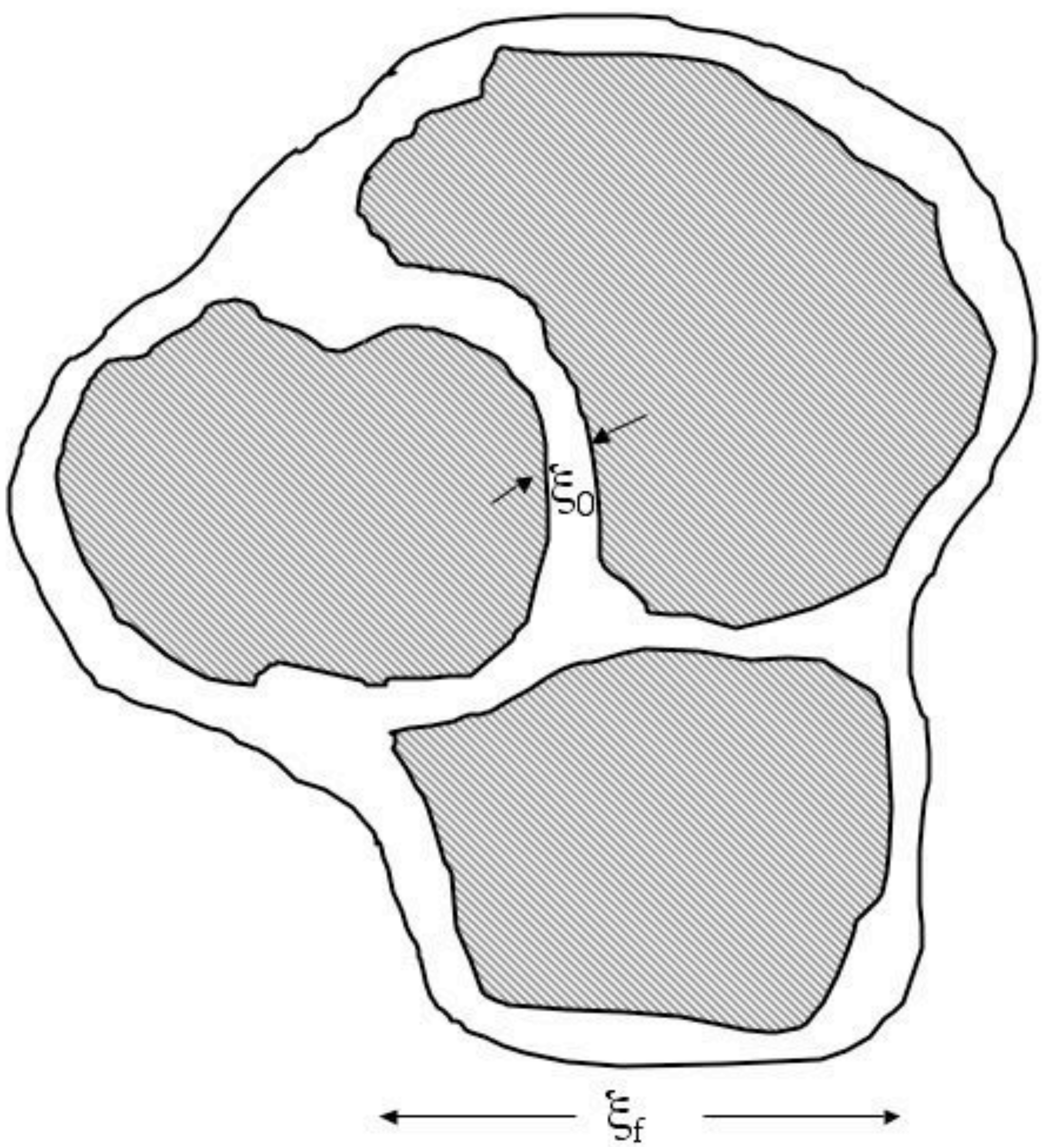
Is there a solid-solid route to microstructural glass?

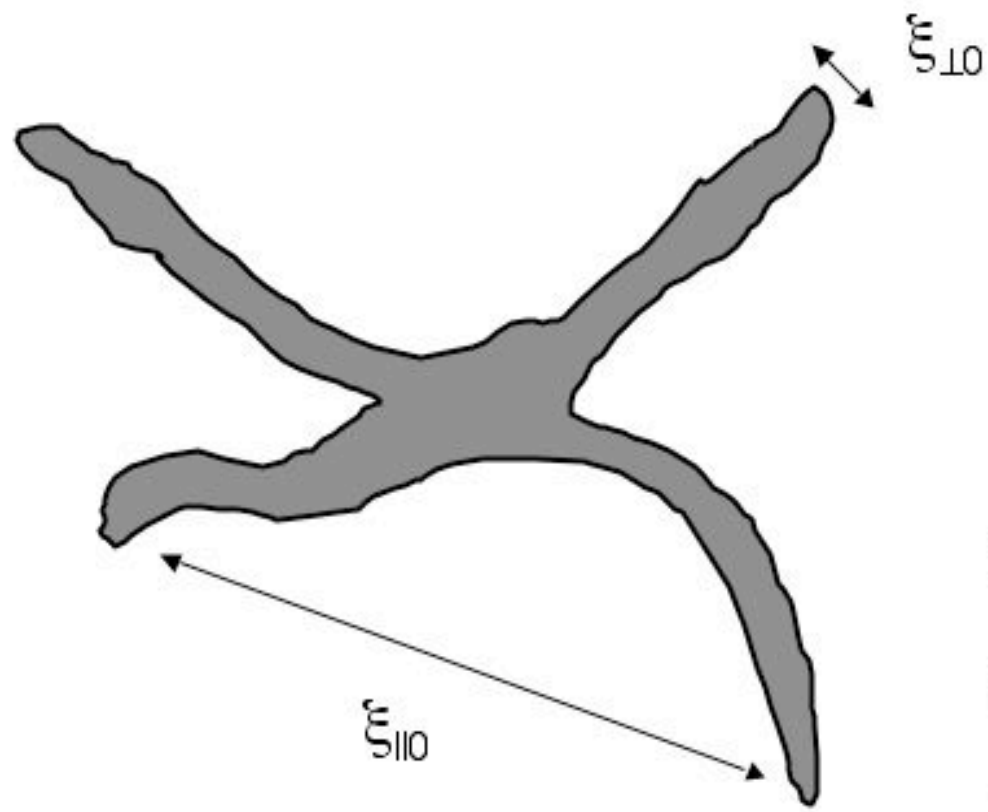
Glass = frozen-in liquid

Microstructural glass = a messed up solid



when size of NAZ comparable to grain size (ferrite)





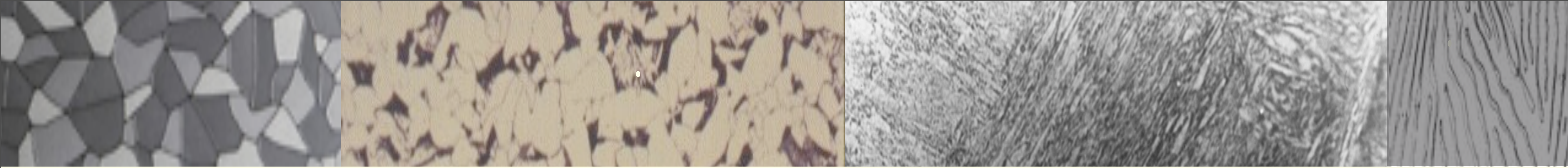
$$\xi_{\parallel 0} \sim (T-T_0)^{-\nu_{\parallel}}$$

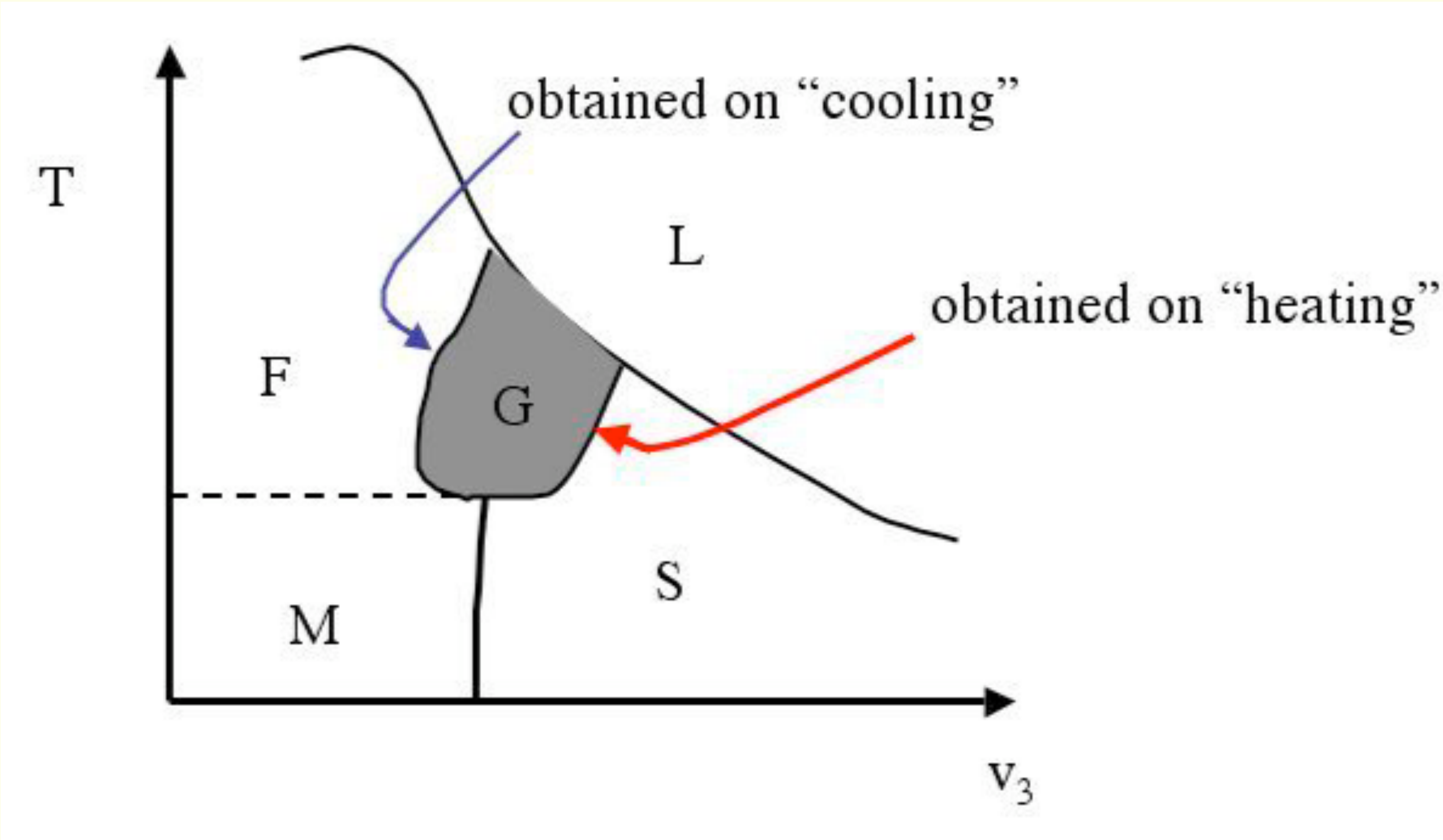
$$\xi_{\perp 0} \sim (T-T_0)^{-\nu_{\perp}}$$

$$\nu_{\parallel} = \nu_{\perp} \ (?)$$

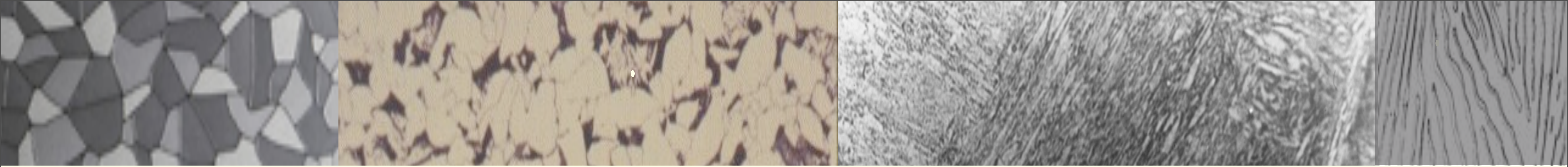
$$D = D_0 \exp(-\xi_{\parallel 0}/T_{eff})$$

Vogel-Fulcher!





"Microstructural glass"?
How different will this be from quenching from liquid?



The dynamical heterogeneities which will get larger as one gets into the microstructural glass phase, will also be characterized by such stress behaviour. The inherent structures that these configurations will fall into will be `proximal' or have some memory of the crystalline phase (and hence will be different from the conventional glass).