Investigation of microstructure on phase transition kinetics of iron

Jidong Yu Hui Peng Songlin Yao Xiaoyang Pei

Institute of Fluid Physics,

China Academy of Engineering Physics

XIV ZABABAKHIN SCIENTIFIC TALKS
March 2019

Outline

- Background
- Experimental study of phase transition kinetics of annealed and cold-rolled polycrystalline iron
- Numerical study of microstructure evolution of martenstic phase transition
- Conclusion

Background

Laser Surface Modification

Strain rate

10^3/s

10^6/s

10^9/s

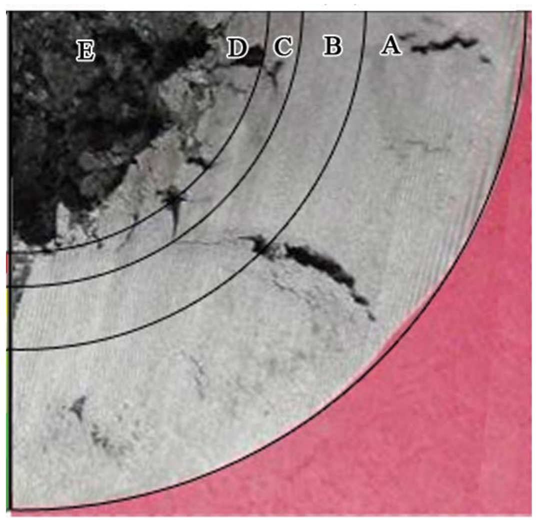
SHPB

Gas gun

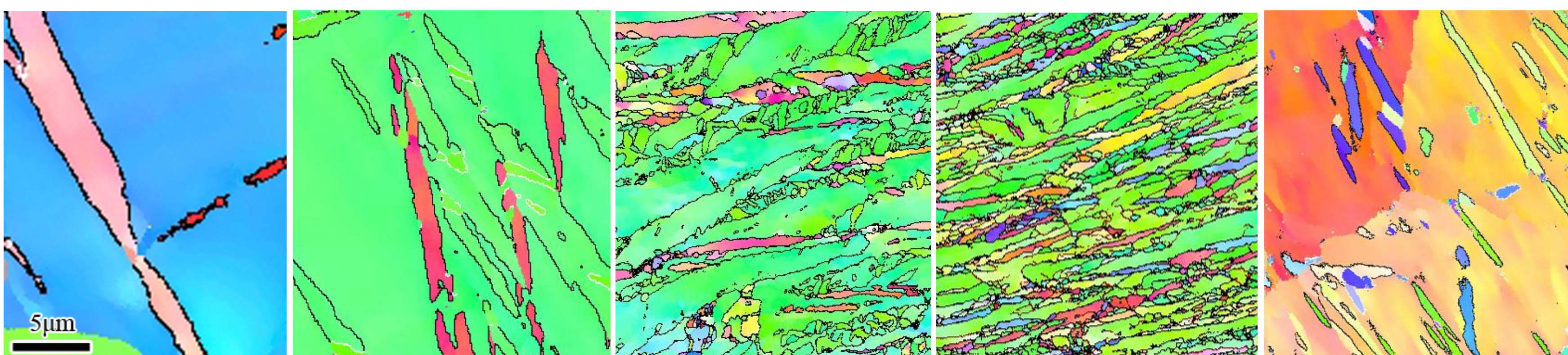
Laser

Background

Loading condition → **PT kinetic**



A: Deformation zone
B: Partial phase transition zone
C: Complete phase transition zone
D: Melting/Gasify zone
E: Hollow zone



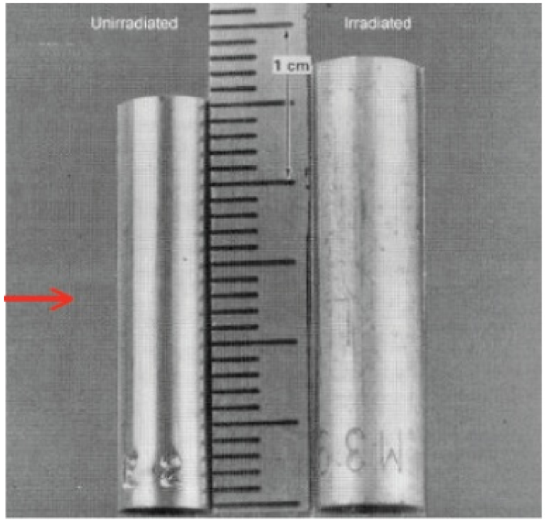
A1 **A2** B **C** **D**

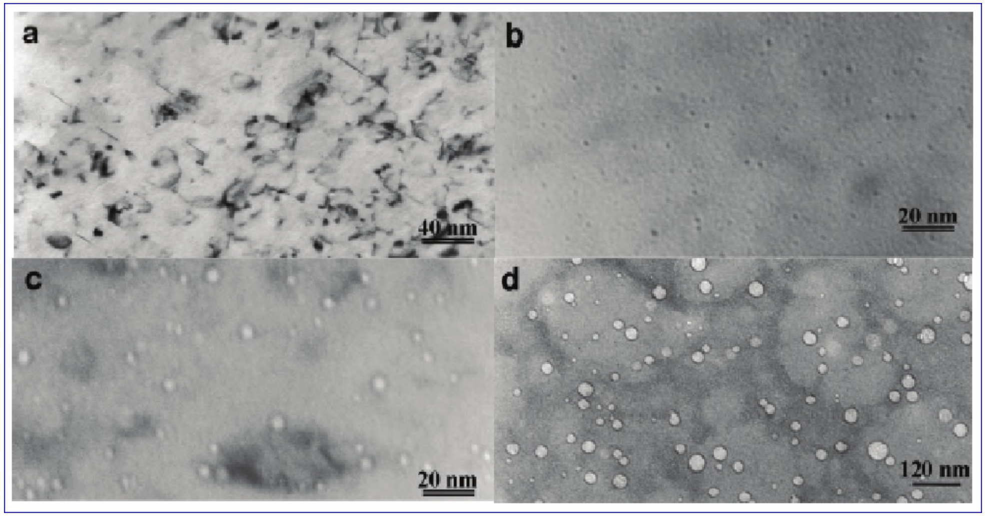
Wang SJ, Sui ML, *Scientific Report*, 2013

Background

Material character ⇒ PT kinetic

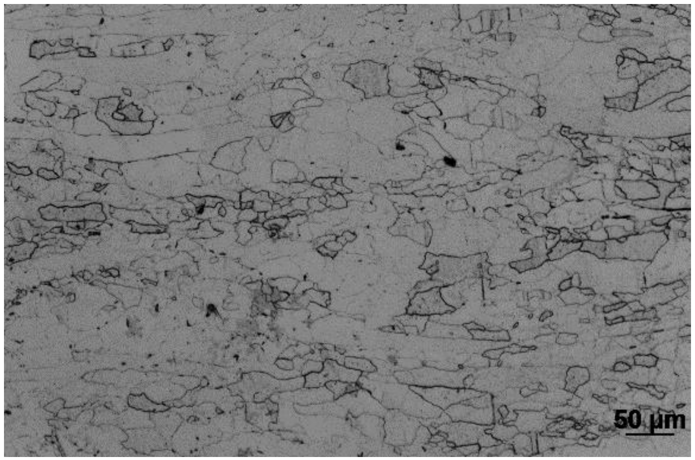
- Heat treatment
- Radiation
- Impurity
- …



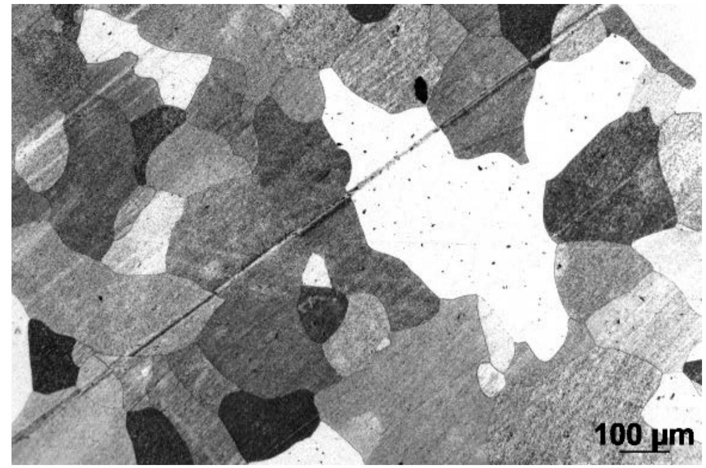


Experimental study of PT kinetics of annealed and cold-rolled polycrystalline iron

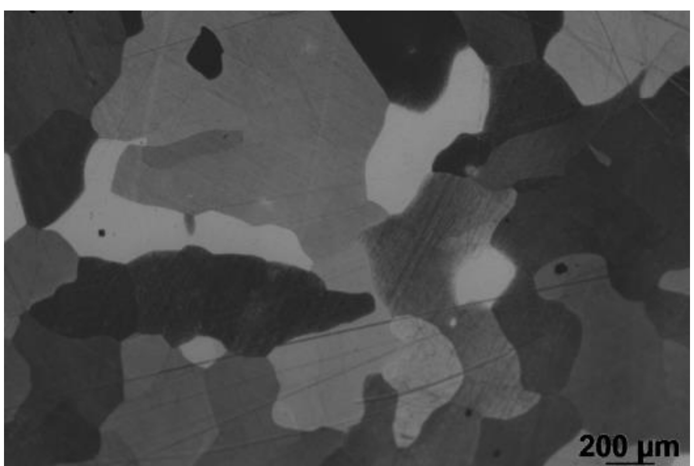
- **Grain size samples**



Grain size~10 μm
（cold rolling 80%; 800℃, 8hour, furnace colding）



Grain size~200 μm
（1150℃, 1.0Hour, furnace colding ）

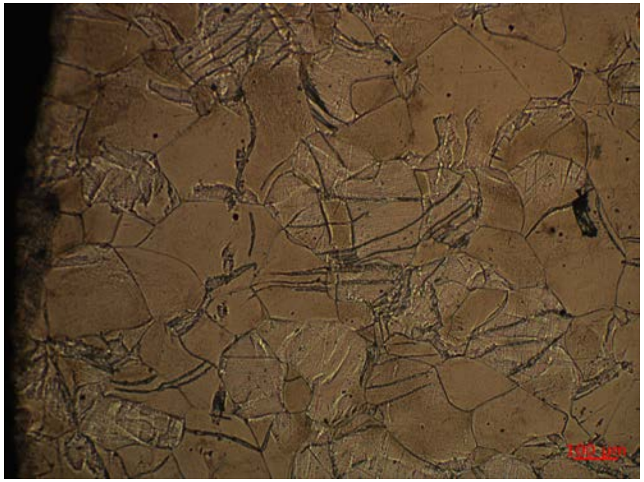


Grain size~500 μm
（1150℃, 4.0Hour, furnace colding ）

Experimental study of PT kinetics of annealed and cold-rolled polycrystalline iron

- **Cold rolling samples**

（cold rolling 50%）

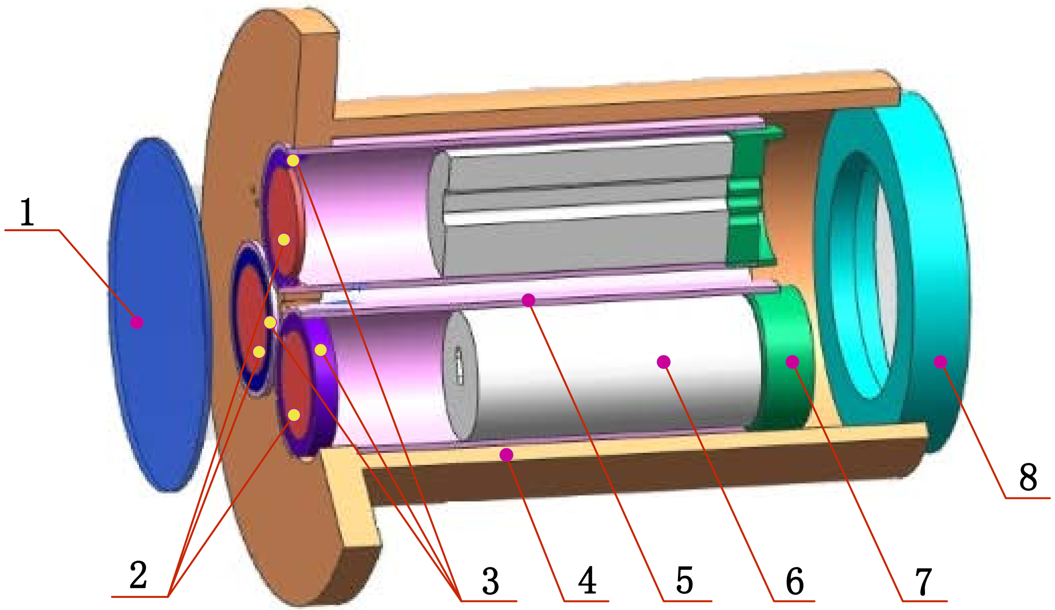


（cold rolling 70% ）

（cold rolling 90% ）

Experimental study of PT kinetics of annealed and cold-rolled polycrystalline iron

- **Experiment sketch**

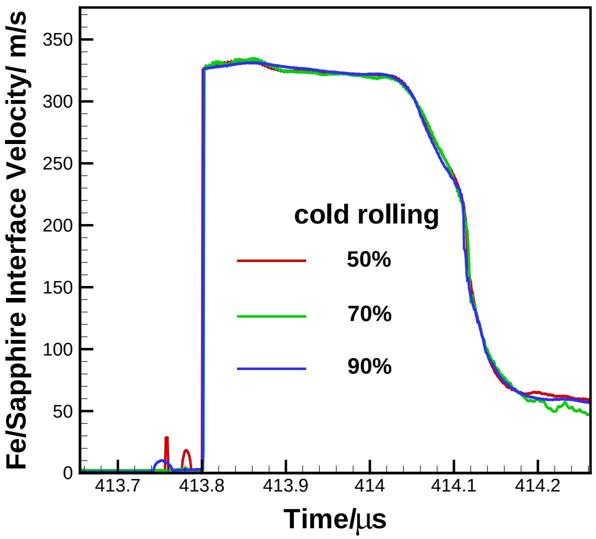


[1-flyer, 2-sample, 3-sample ring, 4-recycling bin, 5-sub-recycling bin, 6-buffer rubber, 7-lid 1，8-lid 2]

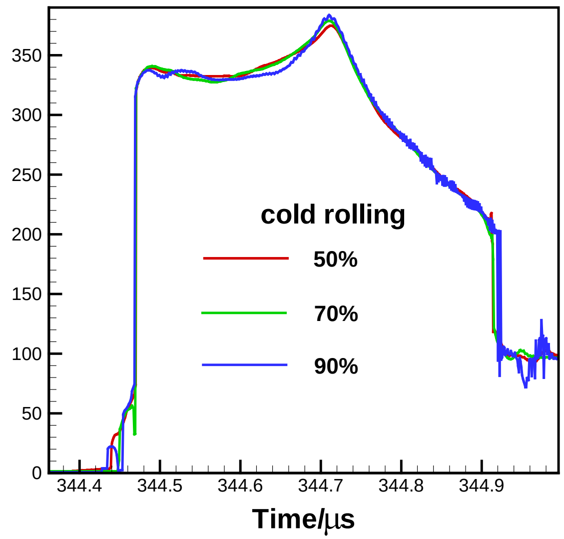
- Electric probes: tilt angle of flyer
- PDV: iron/sapphire interface velocity measurement;
- Recovery of samples

Experimental study of PT kinetics of annealed and cold-rolled polycrystalline iron

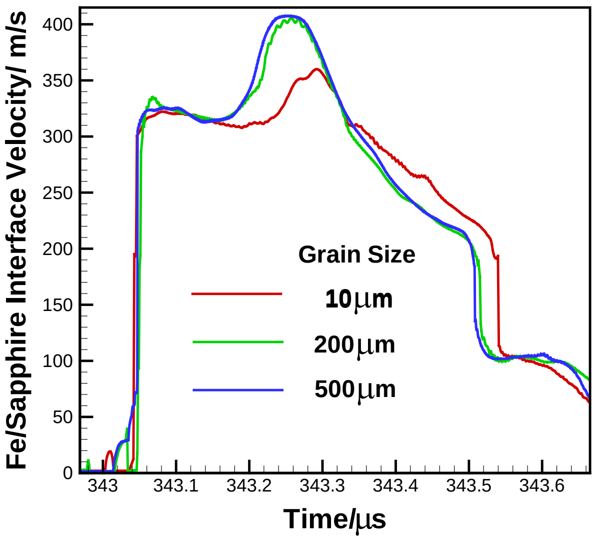
- **Loading consistency(interface velocity profile)**



Flyer velocity 666m/s



Flyer velocity 880m/s



Flyer velocity 886m/s

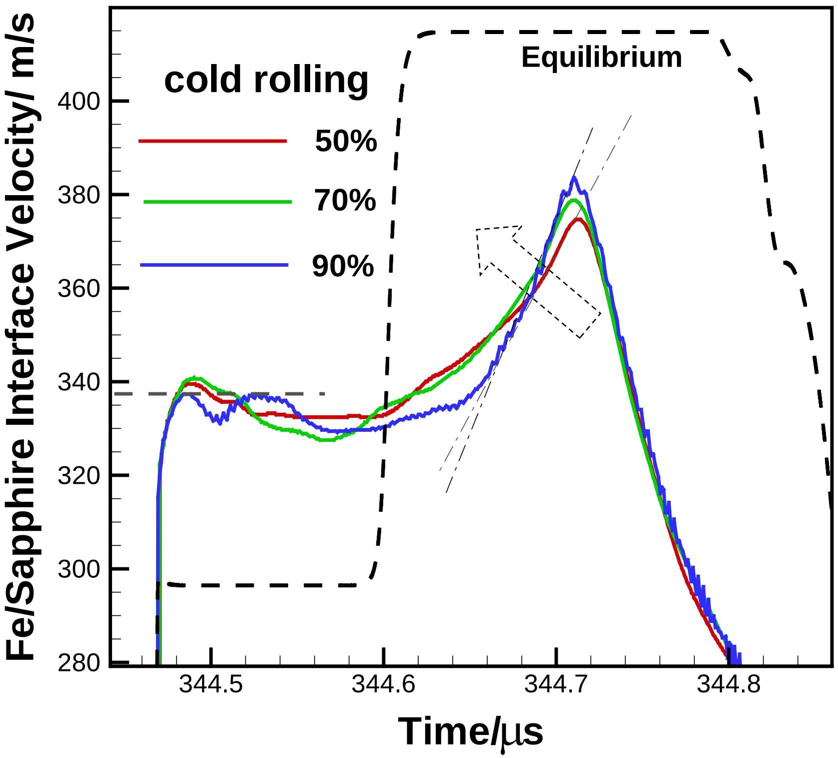
- Electric probes: tilt angle of flyer is less than 0.2°
- PDV: loading consistency is good

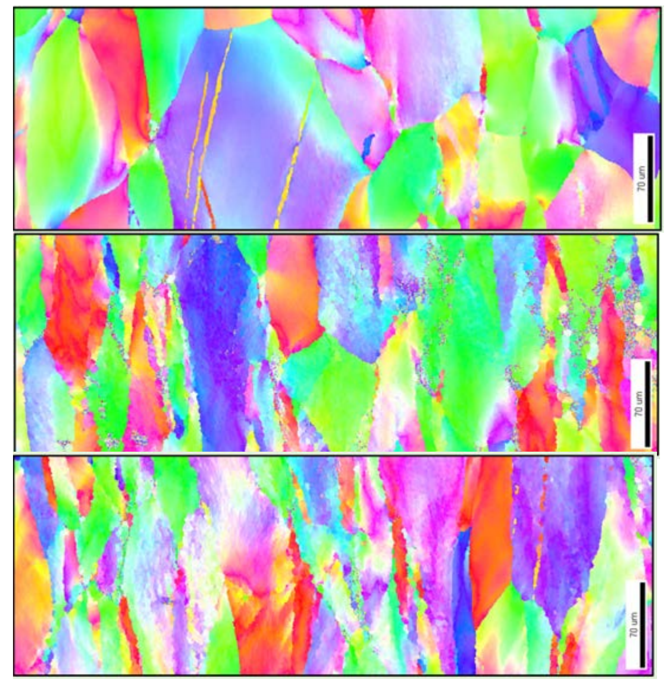
Experimental study of PT kinetics of annealed and cold-rolled polycrystalline iron

- **Complete recovery of samples**

Experimental study of PT kinetics of annealed and cold-rolled polycrystalline iron

- **Cold rolling samples**





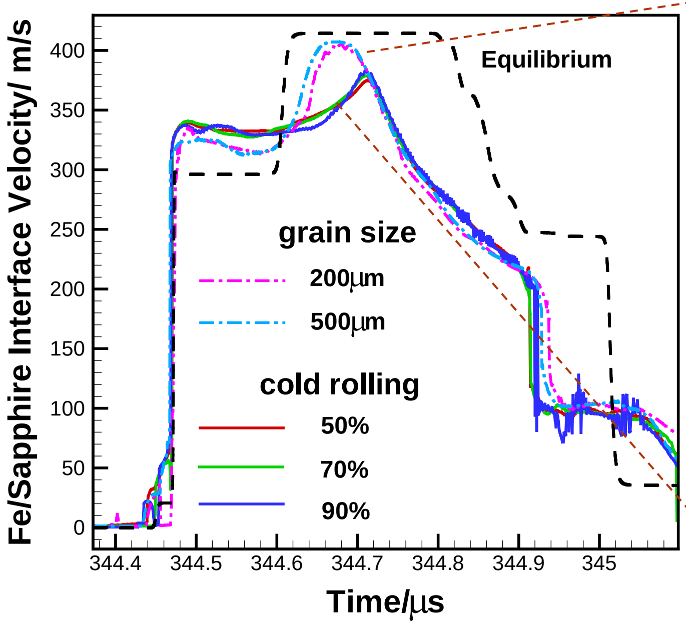
EBSD figs of initial samples

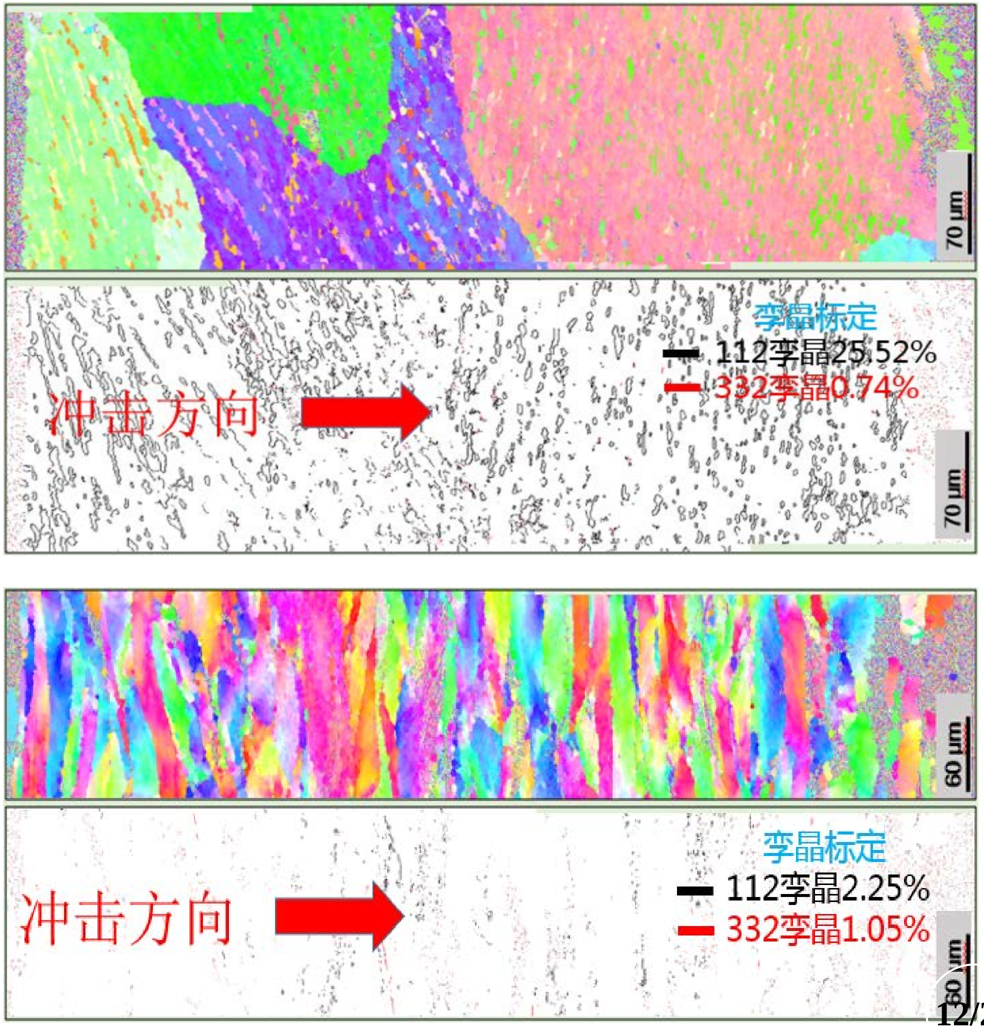
The PT rates are slightly increasing with the deformation of cold rolling

Initial defect ⟺ Nucleation density

Experimental study of PT kinetics of annealed and cold-rolled polycrystalline iron

- **Cold rolling and grain size samples(same loading condition)**



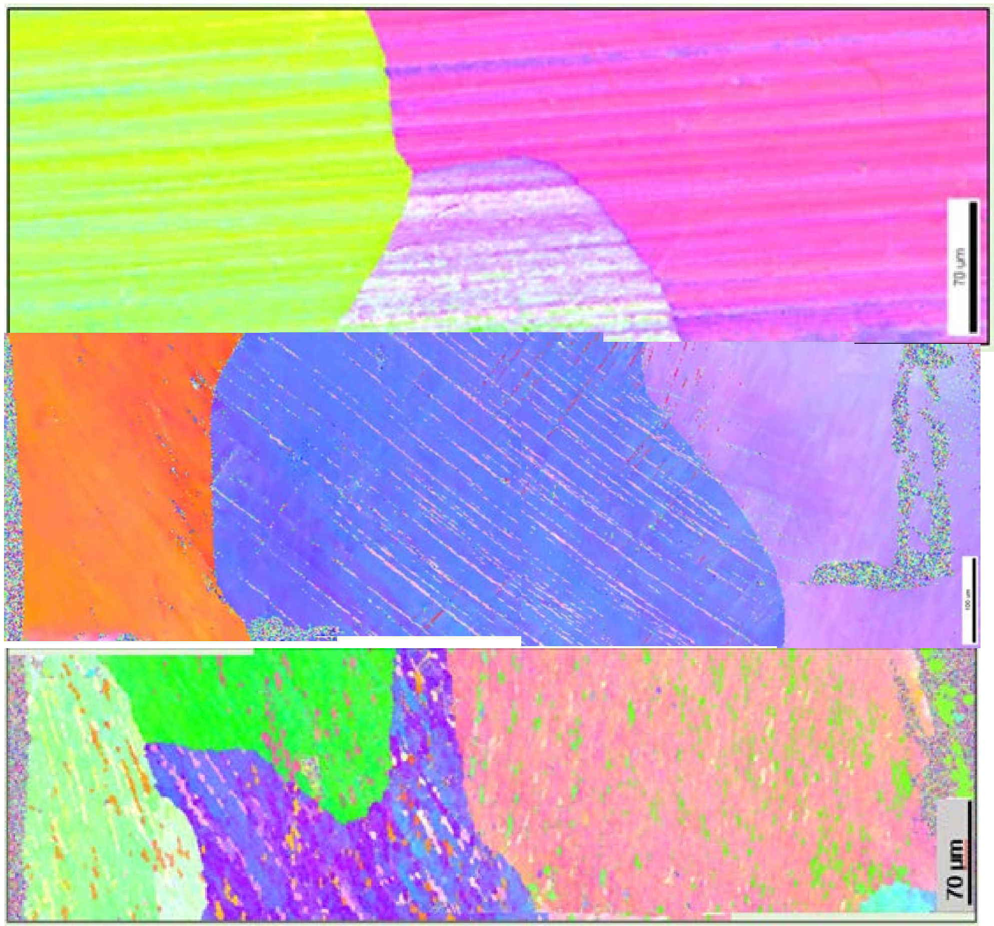


The PT rates of cold rolling samples are obviously slow than grain size samples

The grain boundary inhibit the growth of new phase

Experimental study of PT kinetics of annealed and cold-rolled polycrystalline iron

- **EBSD data of recovery samples at different loading velocity (grain size~200μm)**

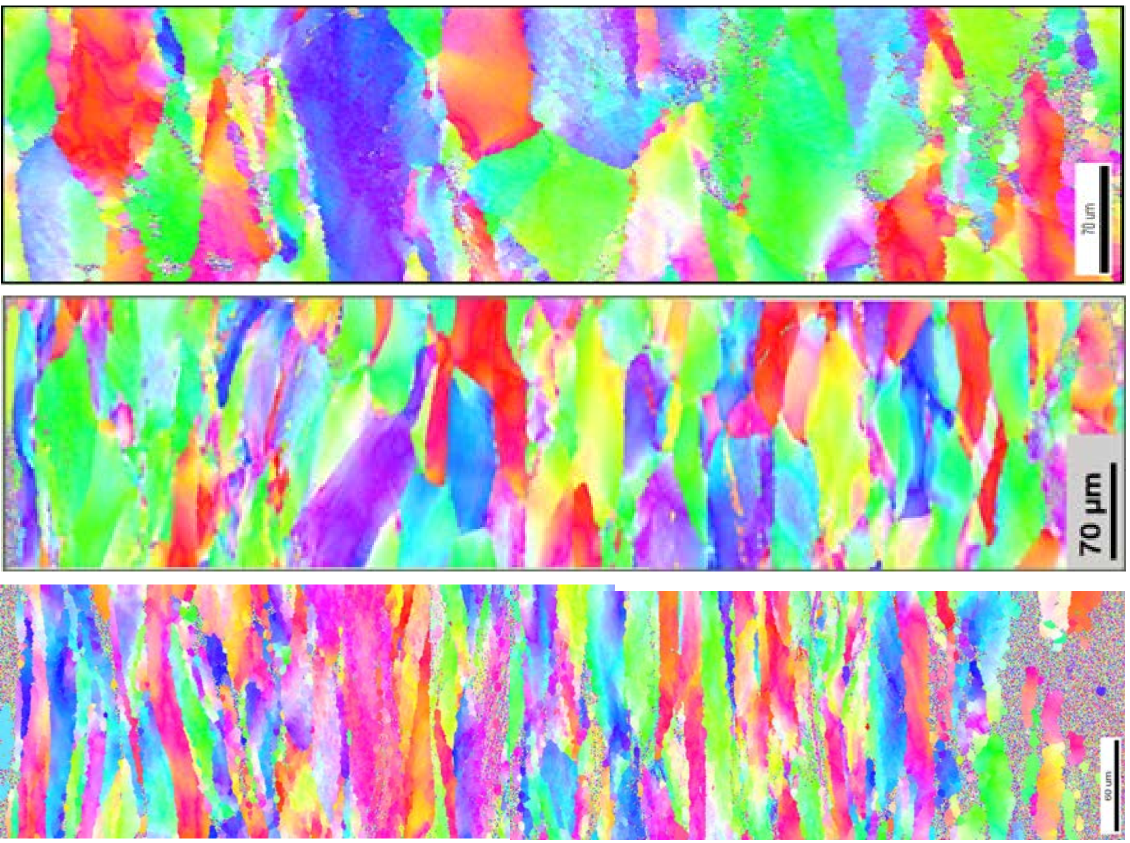


Loading velocity m/s	Peak pressure GPa	Fraction of PT	Average hardness HV
0	0	0	81.3
666	13.1	10%	155
886	16.4	85%	220

Shock loading direction

Experimental study of PT kinetics of annealed and cold-rolled polycrystalline iron

- **EBSD data of recovery samples at different loading velocity (cold rolling 70%)**

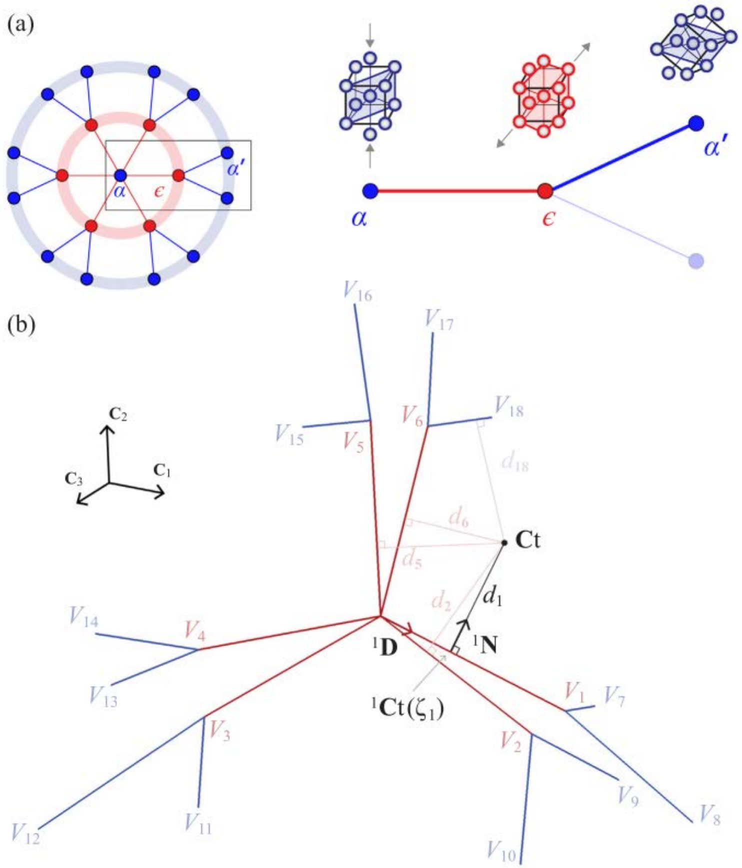


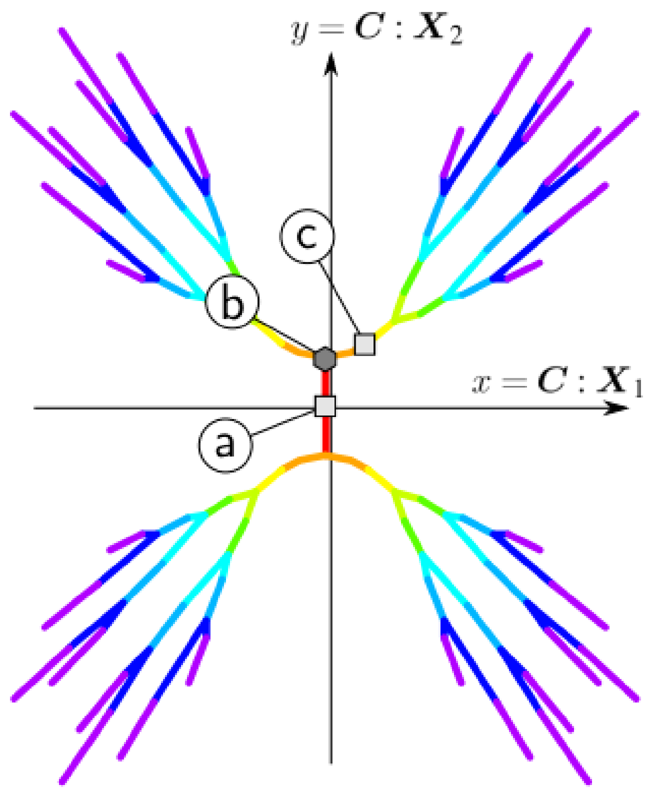
Loading velocity m/s	Peak pressure GPa	Fraction of PT	Average hardness HV
0	0	0	215.3
714	13.6	34%	220
880	16.4	85%	210

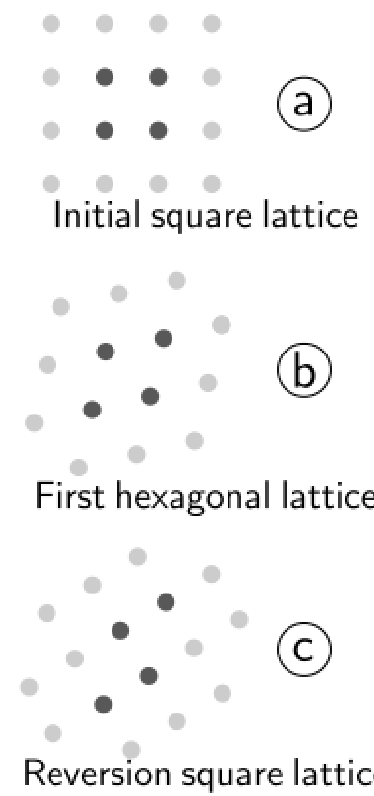
Shock loading direction

Numerical study of microstructure evolution of martenstic PT

- **Phase transition pathway theory**





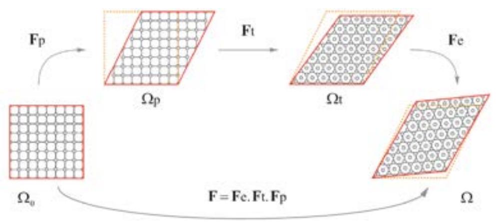


Hundred Variants

Denoual, *PRL*, 2010
Denoual, *JMPS*, 2016

Numerical study of microstructure evolution of martenstic PT

Deformation fradient decomposition:



$$\dot{\mathbf{F}} = \dot{\mathbf{F}}_e \cdot \mathbf{F}_t \cdot \mathbf{F}_p + \mathbf{F}_e \cdot \dot{\mathbf{F}}_t \cdot \mathbf{F}_p + \mathbf{F}_e \cdot \mathbf{F}_t \cdot \dot{\mathbf{F}}_p$$

Helmholtz free energy:

$$\psi \doteq \psi(\mathbf{Fe}, \mathbf{Ft}, \nabla\mathbf{Ft}) = \psi_e(\mathbf{Fe}, \mathbf{Ft}) + \psi_t(\mathbf{Ft}) + \psi_\nabla(\nabla\mathbf{Ft})$$

$$\dot{\psi} = \left.\frac{\partial \psi_e}{\partial \mathbf{Fe}}\right|_{\mathbf{Ft}} : \dot{\mathbf{Fe}} + \left.\frac{\partial \psi_e}{\partial \mathbf{Ft}}\right|_{\mathbf{Fe}} : \dot{\mathbf{Ft}} + \frac{\partial \psi_t}{\partial \mathbf{Ft}} : \dot{\mathbf{Ft}} + \frac{\partial \psi_\nabla}{\partial \nabla\mathbf{Ft}} \therefore \nabla\dot{\mathbf{Ft}}$$

Clausius-Duhem inequality

$$\int_{\Omega_0} \left(\mathbf{P} : \dot{\mathbf{F}} - \rho_0 \dot{\psi}\right) d\Omega_0 \geq 0$$

$$\int_{\Omega_0} \left\{ \left(\mathbf{P} \cdot \mathbf{Fp}^t \cdot \mathbf{Ft}^t - \rho_0 \left.\frac{\partial \psi_e}{\partial \mathbf{Fe}}\right|_{\mathbf{Ft}} \right) : \dot{\mathbf{Fe}} + \left(\mathbf{Fe}^t \cdot \mathbf{P} \cdot \mathbf{Fp}^t - \rho_0 \left.\frac{\partial \psi_e}{\partial \mathbf{Ft}}\right|_{\mathbf{Fe}} - \rho_0 \frac{\partial \psi_t}{\partial \mathbf{Ft}} \right) : \dot{\mathbf{Ft}} + \left(\mathbf{Ft}^t \cdot \mathbf{Fe}^t \cdot \mathbf{P} \right) : \dot{\mathbf{Fp}} - \rho_0 \frac{\partial \psi_\nabla}{\partial \nabla\mathbf{Ft}} \therefore \nabla\dot{\mathbf{Ft}} \right\} d\Omega_0 \geq 0$$

Phase transition driving force

$$\mathbf{Xt} = \mathbf{Fe}^t \cdot \mathbf{P} \cdot \mathbf{Fp}^t - \rho_0 \left.\frac{\partial \psi_e}{\partial \mathbf{Ft}}\right|_{\mathbf{Fe}} - \rho_0 \frac{\partial \psi_t}{\partial \mathbf{Ft}} + \rho_0 \nabla \cdot \frac{\partial \psi_\nabla}{\partial \nabla\mathbf{Ft}}$$

Vattre, Denoual, *JMPS*, 2016

Numerical study of microstructure evolution of martenstic PT

Small strain hypothesis: $\dot{\varepsilon} = \dot{\varepsilon}_V + \dot{\varepsilon}_d + \dot{\varepsilon}_p + \dot{\varepsilon}_t$

Volume strain rate	Deviatoric strain rate	Plastic strain rate	Phase transition strain rate
EOS	Anisotropic elastic constitution	Plasticitic constitution	$\dot{\varepsilon}_t = \frac{1}{2}\left(\dot{\mathbf{Ft}}\bullet\mathbf{Ft}^{-1} + \mathbf{Ft}^{-\mathrm{T}}\dot{\mathbf{Ft}}^{\mathrm{T}}\right)$

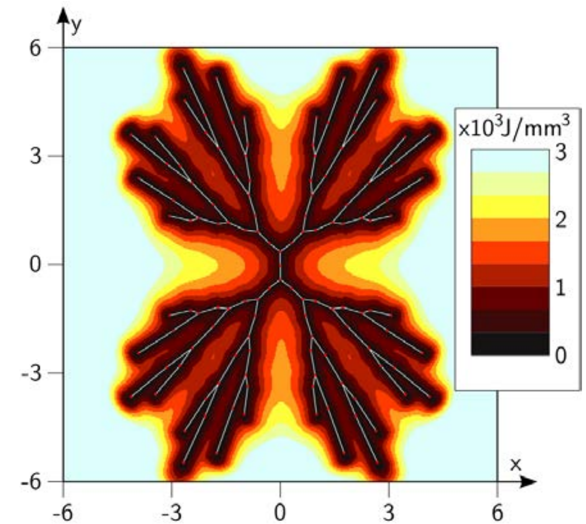
Phase transition deformation gradient evolution:

$$\eta\dot{\mathbf{Ft}} = \mathbf{Xt} = j\mathbf{Fe}^{\mathrm{T}}\bullet\boldsymbol{\sigma}\bullet\mathbf{Fe}^{-\mathrm{T}}\bullet\mathbf{Ft}^{-\mathrm{T}} + \lambda\nabla^2\mathbf{Ft} -$$
$$\sum_{i=1}^{18}\left[2\left(\rho_0\psi_{tk}(\zeta_k) + \sigma_h d_k(\mathbf{Ct})\right)\mathbf{Ft}\bullet\frac{\partial\omega_k(\mathbf{Ct})}{\partial\mathbf{Ct}} + 2\left(\rho_0\psi'_{tk}(\zeta_k)\mathbf{Ft}\bullet{}^k\mathbf{D} + 2\sigma_h\mathbf{Ft}\bullet{}^k\mathbf{N}(\mathbf{Ct})\right)\right]$$

Phase transition energy:

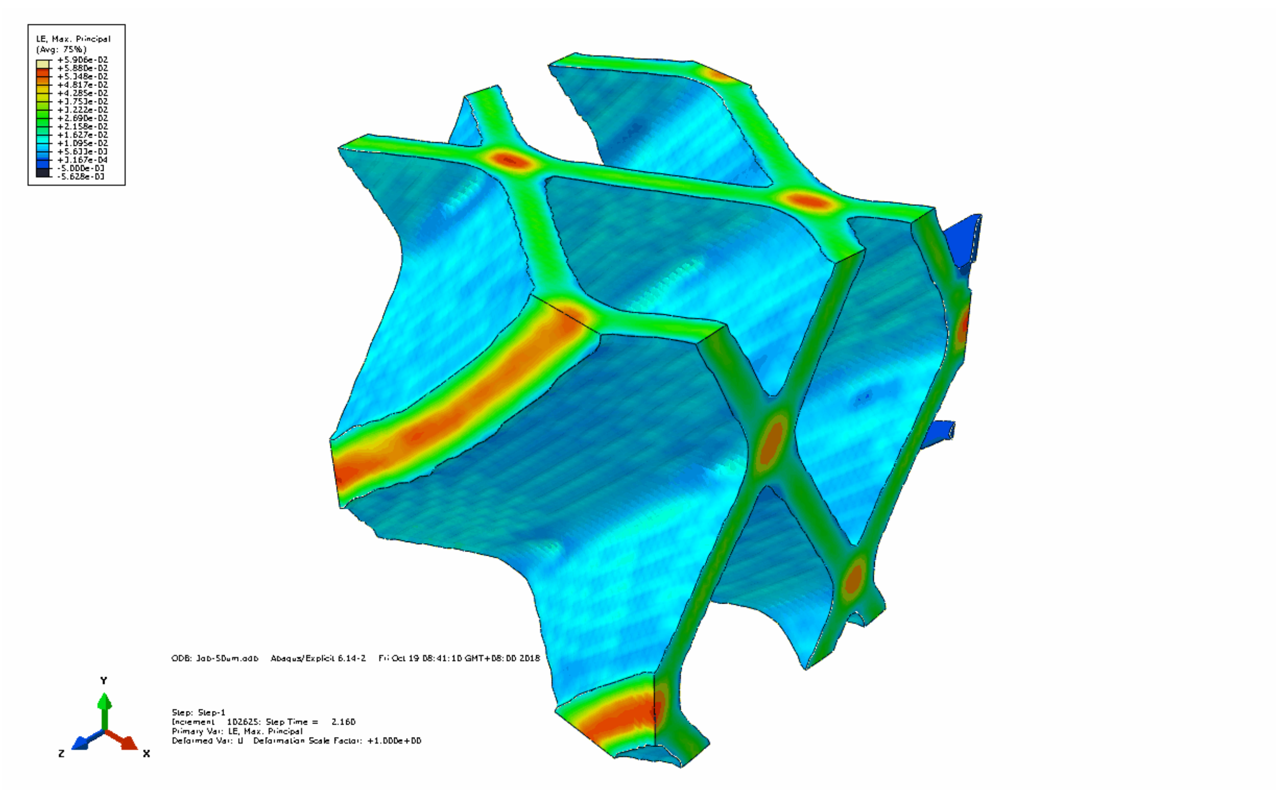
$$\psi_t(\mathbf{Ct}) = \sum_{k=1}^{18}\omega_k(\mathbf{Ct})\Psi_{tk}(\mathbf{Ct})$$

$$\Psi_{tk} = \rho_0\psi_{tk}(\zeta_k) + \sigma_h d_k(\mathbf{Ct}) \qquad \omega_k(\mathbf{Ct}) = \frac{d_k^{-h}(\mathbf{Ct})}{\sum_{i=1}^{18} d_i^{-h}(\mathbf{Ct})}$$



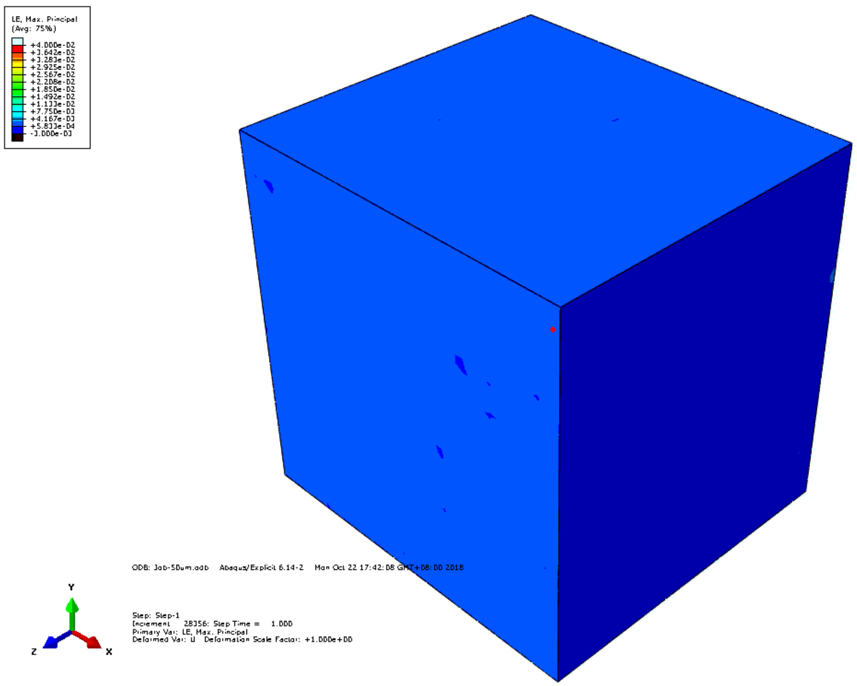
Numerical study of microstructure evolution of martenstic PT

- **Simulation results (1D strain)**

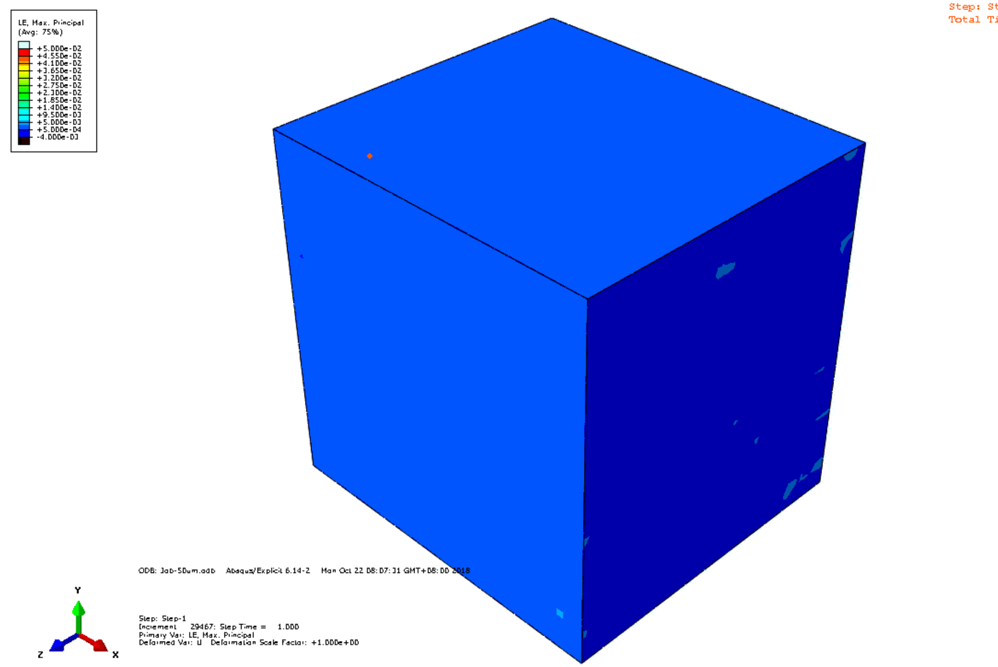


Z axis strain 0.09

Numerical study of microstructure evolution of martenstic PT



Z axis strain 0.092



Z axis strain 0.096

Conclusion and prospect

Conclusion

- The consistency of loading condition is important to decouple the effects of heat treatment of the sample on the phase transition kinetics;
- The phase transition rates of grain size samples is obviously fast than the cold rolling samples, and under the same heat treatment process the grain size and deformation of cold rolling will slightly affect the PT rates;
- Pathway theory will be very useful to investigate the microstructure evolution of reconstructive martenstic phase transition.

Prospect

- Crystal plasticity constitutive will be coupled in the pathway theory;
- The multi-variants evolution simulation results will be further validated by the microstructure analysis of the recovery samples.

Thanks for your attention!