Introduction of Dislocation-mediated Plasticity and Discrete Dislocation Dynamics

Department: Mechanical Engineering
Presenter: Haijian Yang

Time: Oct. 24th 2024

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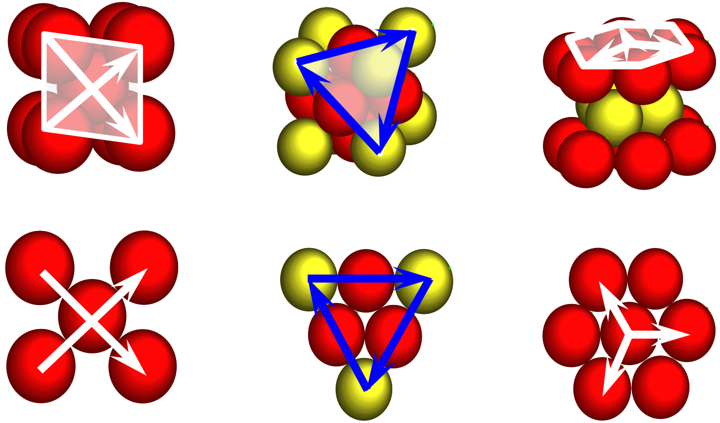
Part 1 Dislocation-mediated Plasticity

1. Plasticity Deformation

1.1 Single Crystal

- **Slip system**: A spatial orientation relationship consisting of a slip plane and slip direction.
- **Slip direction**: general happens at close stacking plane
- **Slip planes** are usually the most densely packed planes, and slip directions are usually the most densely packed directions.
- Under the same conditions, the more slip directions there are, the better the plasticity. And the more slip planes there are, the better the plasticity



	BCC	FCC	HCP
Slip Plane	**{110}**	**{111}**	**{0001}**
Slip Direction	**<111>**	**<110>**	**< $11\bar{2}0$ >**

1.2 Polycrystalline
- misorientation
- grain boundary

Grain boundary impede dislocation slip

Misorientation impede dislocation slip

↓

Impede dislocation tranverse grian boundary

↓

Dislocation pile up

↓

Pile stress

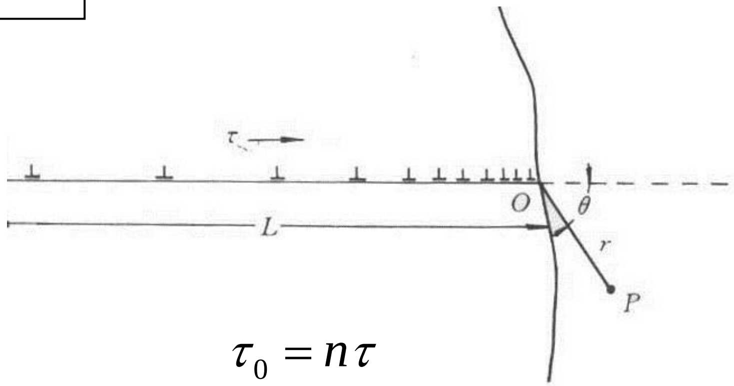
↓

Start slip system

Misorientation twisted → Dislocation through boundary

↓

Deformation delivered

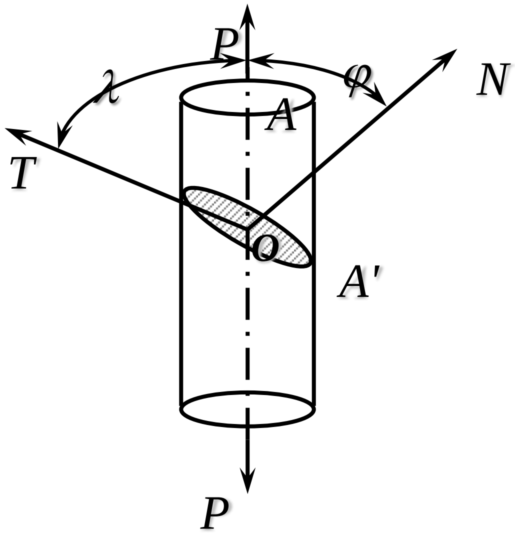


$$\tau_0 = n\tau$$

Dislocation Pile Up

1.3 Critical Shear Stress

minimum shear stress to start slip



φ —— load slip plane in normal direction

λ ——load slip direction

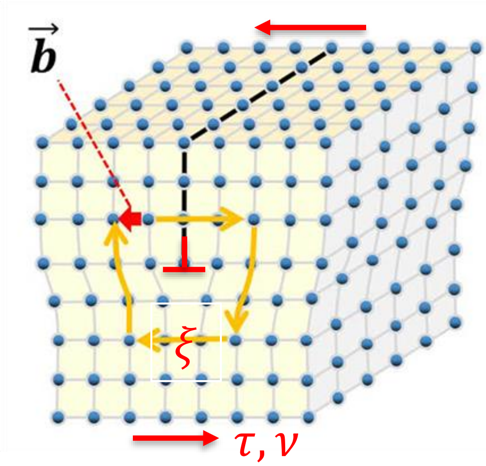
$$\tau = \sigma \cos\lambda \cos\varphi$$

- main mechanism → slip
- phenomenon → slip line/slip belt
- specific slip plan/direction → slip system
- load force → critical shear stress
- micro mechanism → Dislocation?

2. Dislocation

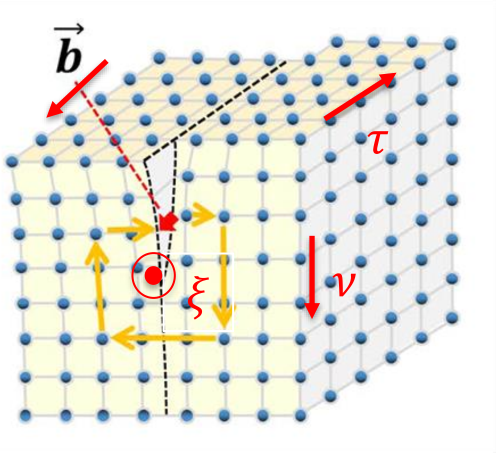
2.1 Definition: the boundary of slipped and un-slipped regions in the slip plane

Classification: edge, screw, mix



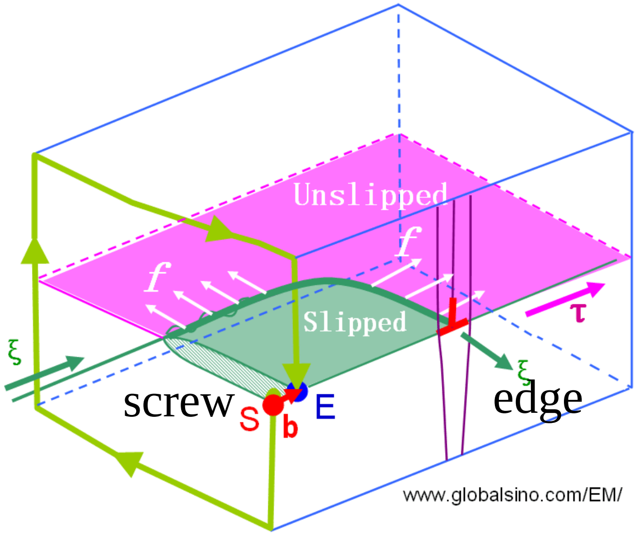
$\tau \parallel \nu \parallel \bar{b}\,;\, \bar{b} \perp \xi$

Edge $\bar{b} \perp \xi$



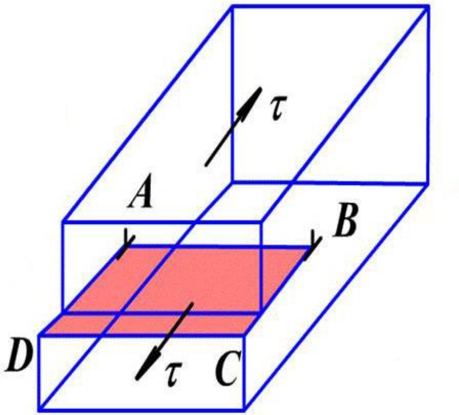
$\xi \parallel \tau \parallel \bar{b}\,;\, \bar{b} \perp \nu$

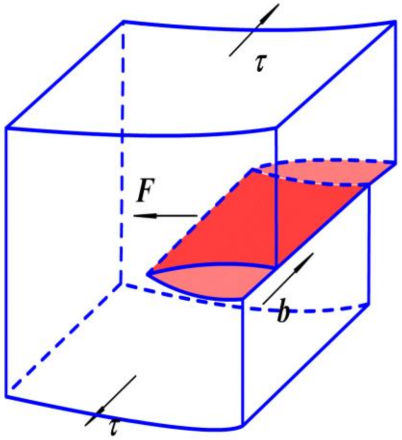
Screw $\bar{b} \parallel \xi$



Mix

2.2 Force on

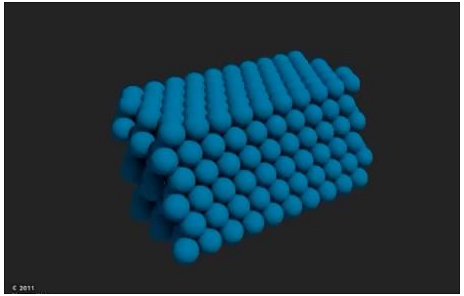


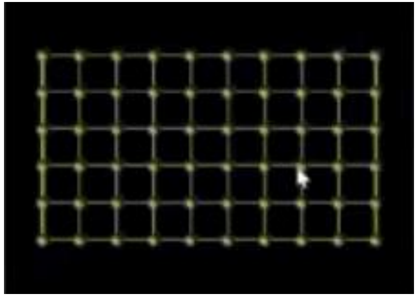


F= τ*b

τ is the shear stress on the Burgers vector

b is the Burgers vector





Dislocation density

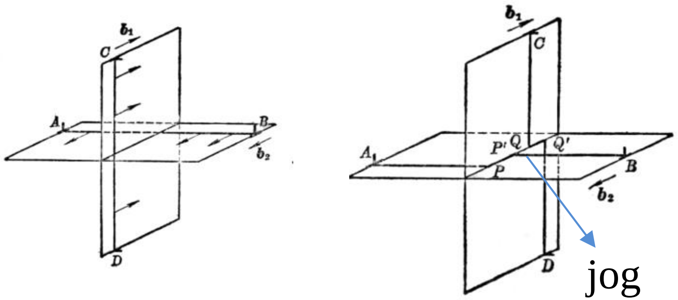
- Dislocation length in unit volume

$$\rho = \frac{S}{V} \quad m/m^3$$

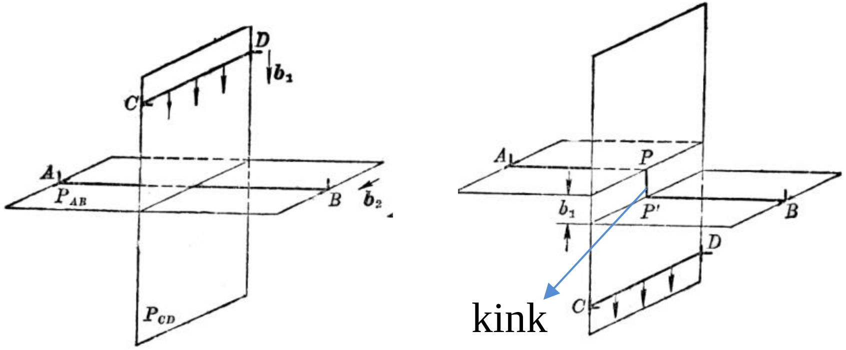
- Dislocation length per cross section area

$$\rho = \frac{n}{A} \quad 1/m^2$$

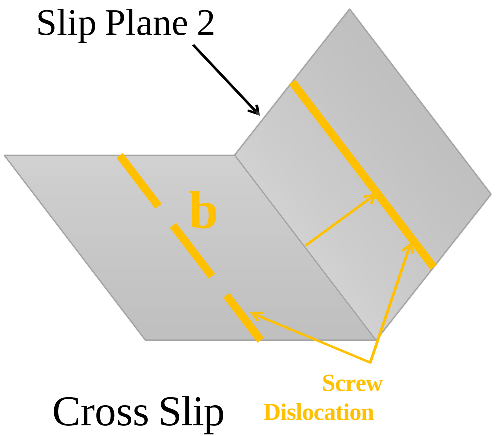
2.3 Dislocation Mobility and Interaction



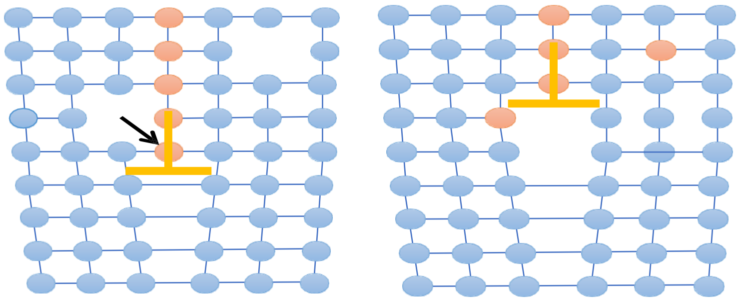
Parallel B interception of edge dislocation



Vertical B interception of edge dislocation

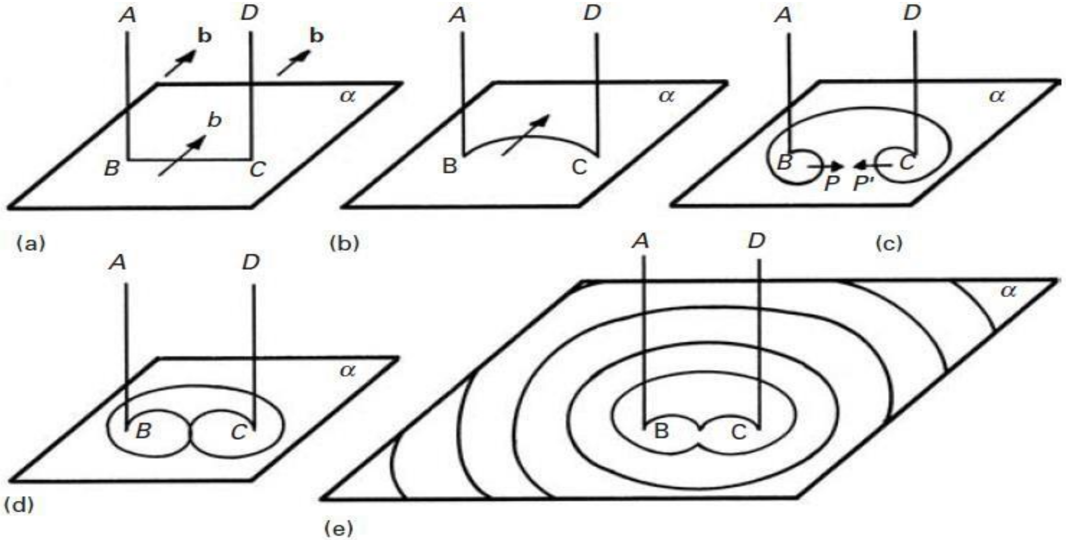


Cross Slip



Dislocation Climb

2.4 Dislocation Generation: Frank-Read



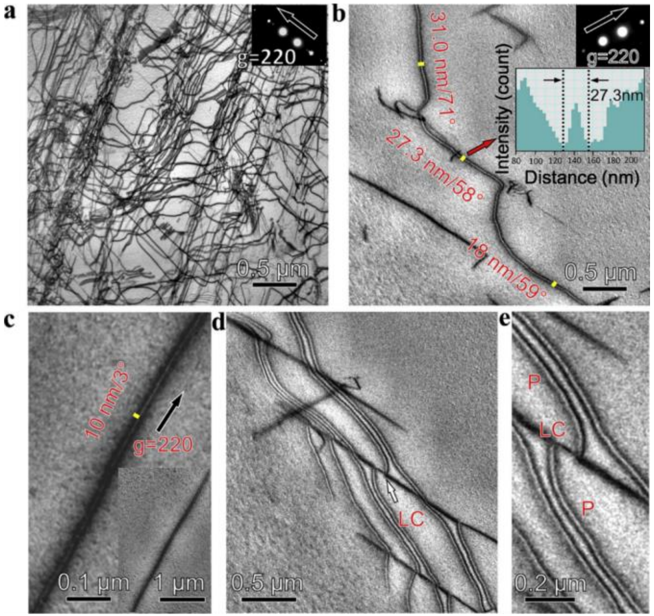
$$\tau = \frac{G * b}{l}$$

B:burgers vector

L: length of dislocation

Part 2 Dislocation Study Approaches

1. Experimental: TEM



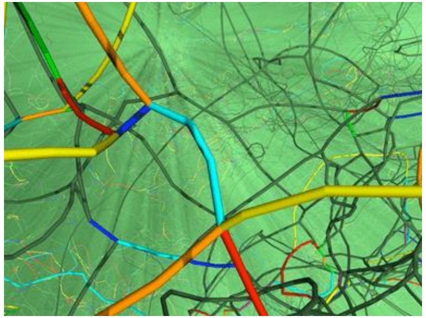
loop radius is $r_l = 5$ nm

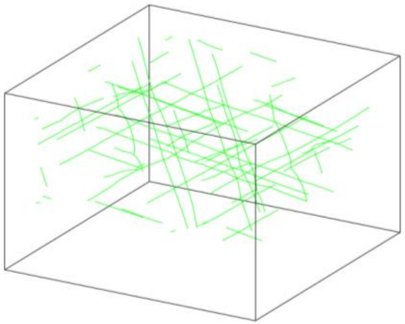
Precipitate size parameter is $R_p = 5$ nm

2. Simulation

- **Discrete Dislocation Dynamics (DDD)**
- Phase Field Method
- Finite Element Method (FEM)
- Molecular Dynamics (MD)
- Continuum Dislocation Dynamics (CDD)
- Crystal Plasticity Finite Element Method (CPFEM)

Reason: closer to the real situation by space discrete and time step



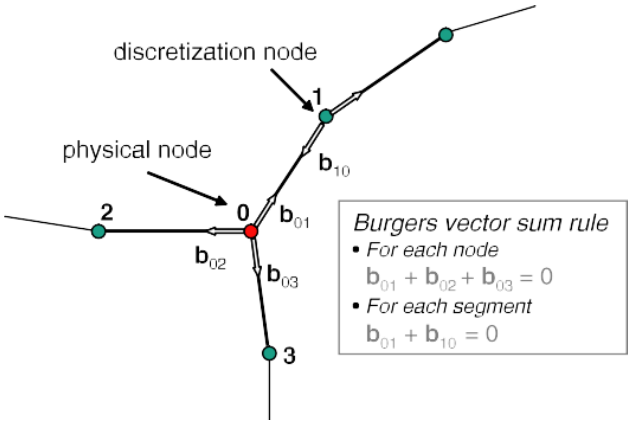


Xu X D, Liu P, Tang Z, et al. Transmission electron microscopy characterization of dislocation structure in a face-centered cubic high-entropy alloy Al0. 1CoCrFeNi[J]. Acta Materialia, 2018, 144: 107-115.

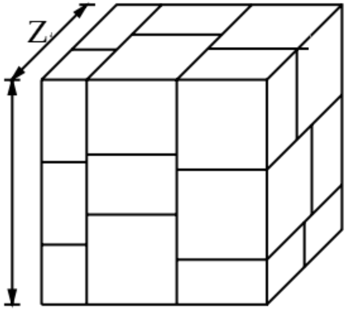
https://www.dierk-raabe.com/movies-and-animations/discrete-dislocation-dynamics-ddd/

Part 3 Discrete Dislocation Dynamics (Parallel Dislocation Simulator)

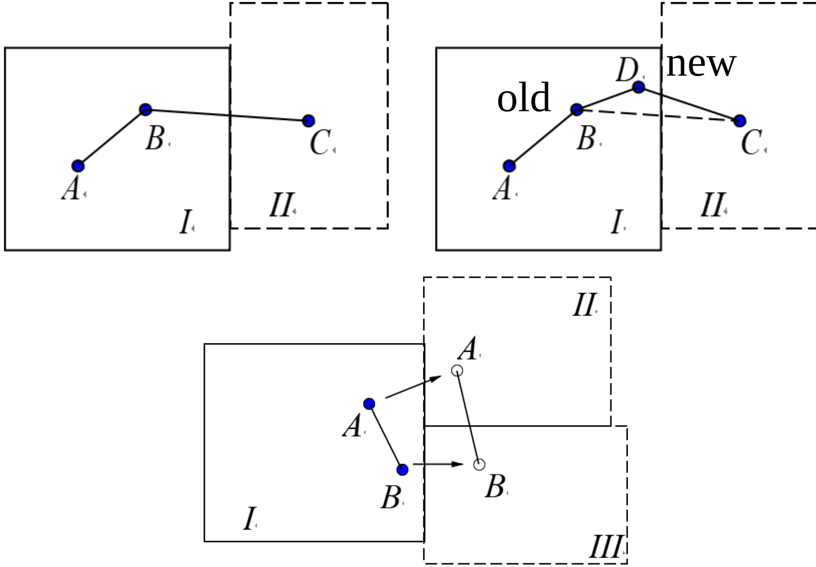
3.1 Discrete Dislocation Calculation Principle



Node (arms, segments)



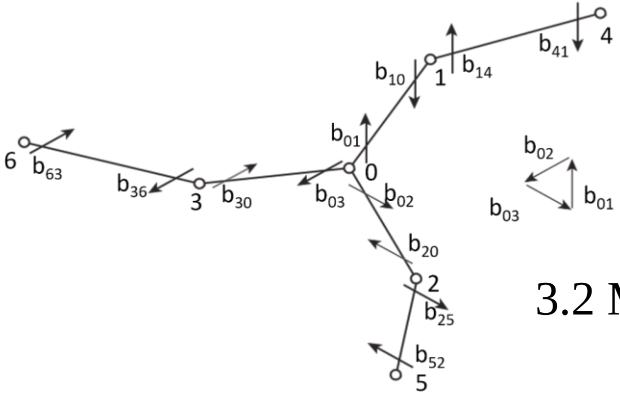
Domains
3*3*2



MPI: Massage Passing Interface(nodes)

ParaDiS User's Guide, Version 4. V. V. Bulatov, N. R. Bertin, S. Aubry, A. Arsenlis, W. Cai. August 23, 2023

3.2 Mobility



3.1 Force

$$\vec{f_i} = -\frac{\partial E(\{N_i\})}{\partial \vec{r_i}}$$

$N_i=[\vec{r_i};\overrightarrow{b_{ij}}, j = 1,2, \ldots . ni]$,where n_i is the connectivity of node i;

$E(\{N_i\})$,is the total elastic energy of dislocation network

$$\partial E(\{N_i\}) \sum_{<i,j>} W_s(ij) + \frac{1}{2} \sum_{<i,j>;<k,l>} W_I(ij, kl)$$

Where $W_s(ij)$ is the self energy of segments $< i, j >$
W_I (ij,kl) is the interaction energy between segments <i,j> and <k,l>

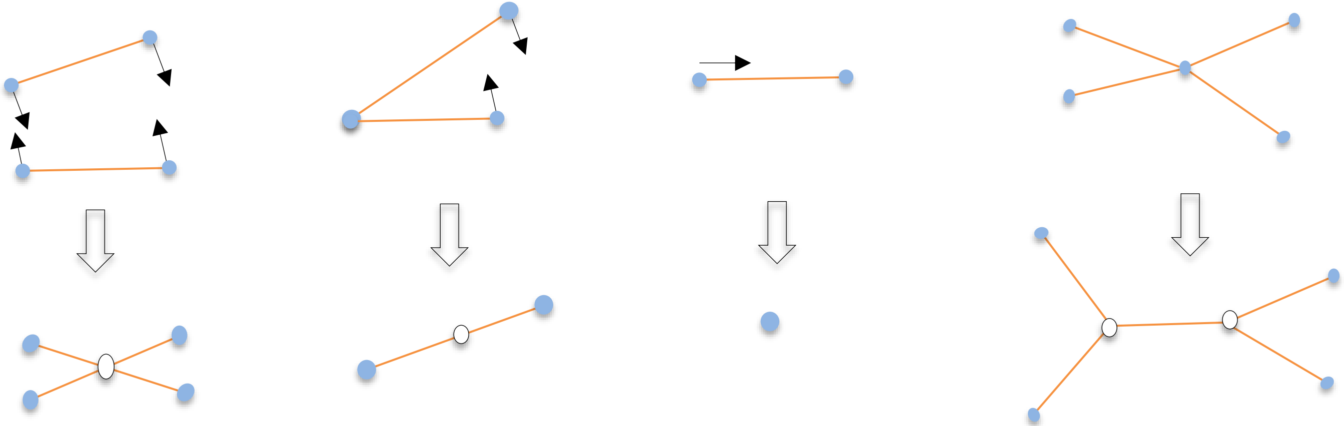
3.2 Mobility Laws

$$F = \tau * b \qquad M = \frac{v}{F} \qquad M = \frac{v}{\tau * b}$$

M: the mobility function of velocity v of dislocation in response to the driving force f, 1/(Pa*s)
v: dislocation velocity b/s;
b: Burgers length, 2.75e-10 m;(BCC)4
τ: shear stress on the Burgers vector, Pa
F: force on the dislocation, Pa*b

ParaDiS User's Guide, Version 4. V. V. Bulatov, N. R. Bertin, S. Aubry, A. Arsenlis, W. Cai. August 23, 2023

3.3 4 types dislocation event detection



collision zipping shrinking dissociation

Parallel Dislocation Dynamics DD3d User's Manual. M. Bartelt, V. Bulatov, W. Cai, M. Hiratani, T. Pierce, M. Rhee, M. Tang. June 4, 2003

Part 4 Preliminary Results

Initial dislocation cube and running parameters of mobility and stress set

Initial parameters set up	
Dislocation type	Screw
Cube length	3500 (b)
Maximum length	500 (b)
No. chains	100
Node count	1400
Dis density	1400 (mm^-2)

numXdoms	1	mobilityLaw	FCC_linear	Unit
numYdoms	1	shearModulus	2.70E+10	Pa
numZdoms	1	pois	0.347	
numXcells	4	YoungModulus	7.27E+10	Pa
numYcells	4	burgMag	2.86E-10	b
numZcells	4	MobEdge	-	$pa^{-1}*s^{-1}$
maxSeg	500 (b)	MobScrew	-	$pa^{-1}*s^{-1}$
minSeg	100 (b)	MobClimb	-	$pa^{-1}*s^{-1}$
BoundType	Periodic/free	appliedStress	-	Pa
enableCrossSlip	Enabled	loadType	constant strain rate/stress	
maxstep	5000	edotdir	[1,0,0]	

Part 4 Preliminary Results

4.1 Frank Reed Dislocation Resource

Initial dislocation condition set	
Dislocation type	Screw
Cube length	3500 (b)
Maximum length	500 (b)
No. chains	2
Node count	22
Dis density	3.1E12 (mm^-2)

Initial running parameters set				
numXdoms	1	mobilityLaw	FCC_linear	Unit
numYdoms	1	shearModulus	2.70E+10	Pa
numZdoms	1	pois	0.347	
numXcells	4	YoungModulus	7.27E+10	Pa
numYcells	4	burgMag	2.86E-10	b
numZcells	4	MobEdge	1.0E4	$pa^{-1}*s^{-1}$
maxSeg	500 (b)	MobScrew	1.0E4	$pa^{-1}*s^{-1}$
minSeg	100 (b)	MobClimb	-	$pa^{-1}*s^{-1}$
BoundType	Periodic/free	appliedStress	1.0E+08	Pa
enableCrossSlip	Enabled	loadType	constant strain rate/stress	
maxstep	5000	edotdir	[1,0,0]	

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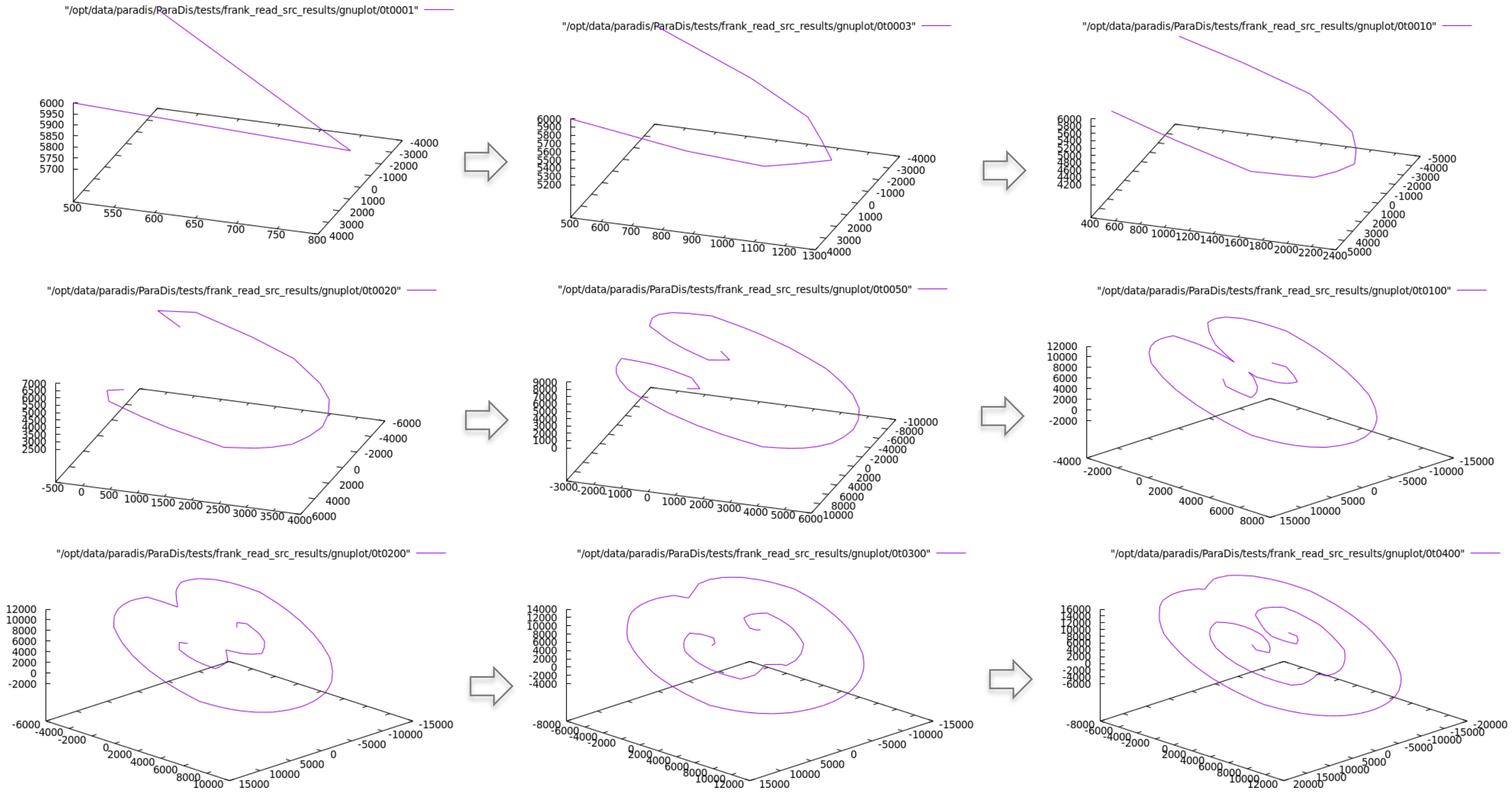
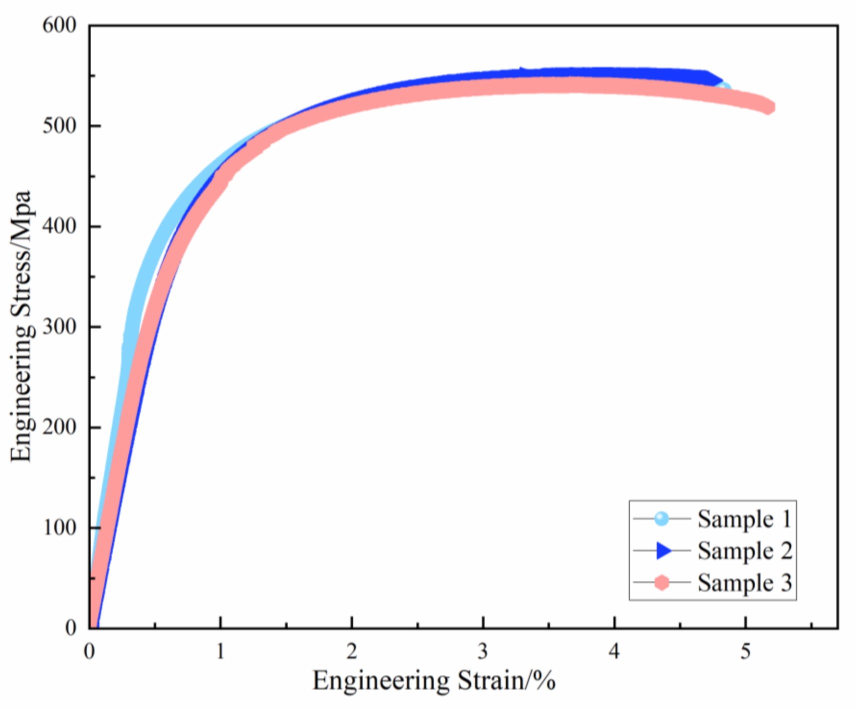
Frank-Reed dislocation case



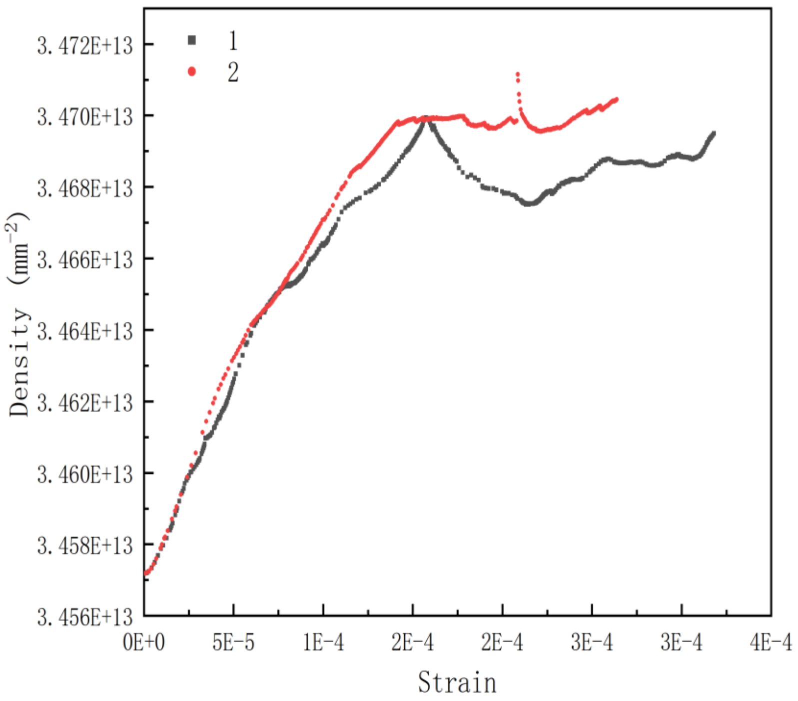
4.2 Aluminum uniaxial & creep simulation case

No.	Load type	Erate	Applied Stress	MobEdge	MobScrew	MobClimb	Steps set	Step stop by
Tensile 1	Uniaxial (constant strain rate)	1.0E+03	1.0E+08	1.0E+04	1.0E+04	100	50000	50000
Tensile 2	Uniaxial (constant strain rate)	1.0E+03	1.0E+07	1.0E+04	1.0E+04	100	50000	6276
Creep 1	Creep (constant stress)	1.0	1.0E+8	1.0E+04	1.0E+04	100	50000	3680
Creep 2	Creep (constant stress)	1.0	5.0E+07	1.0E+04	1.0E+04	100	50000	3996

Uniaxial (tensile)

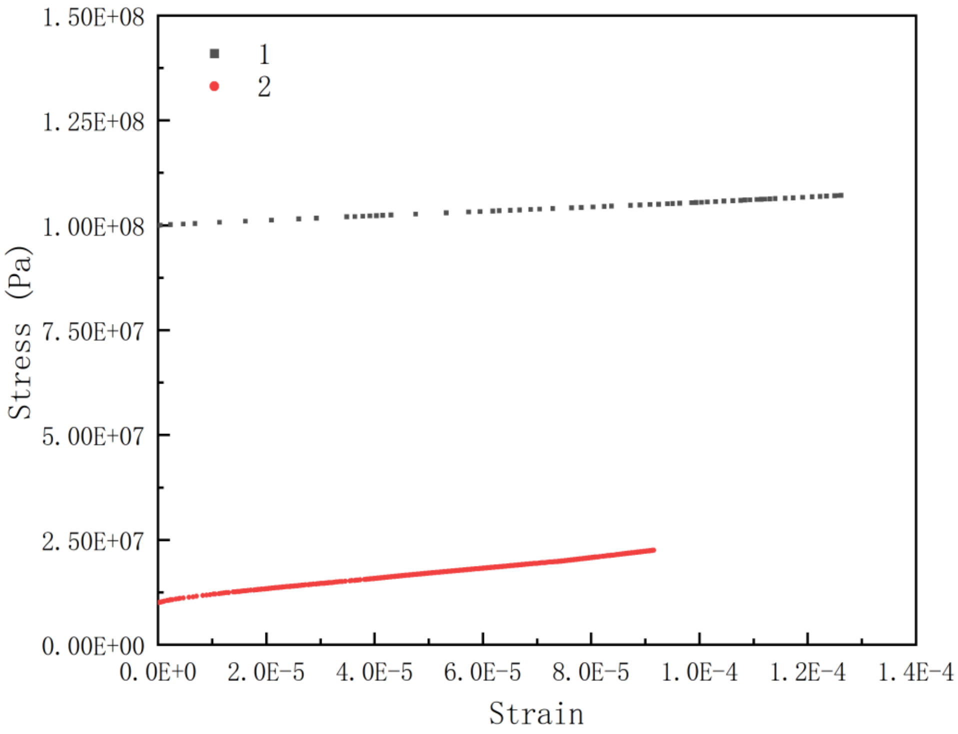


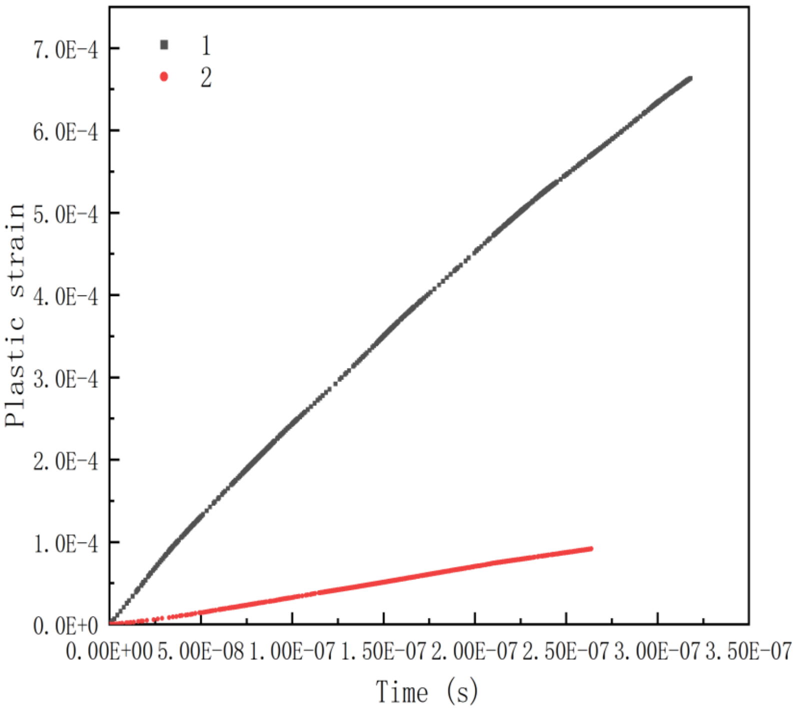
Al-Ce-Zr tensile test at room temperature



AppliedStress: 1) 1.0E+08; 2) 1.0E+07

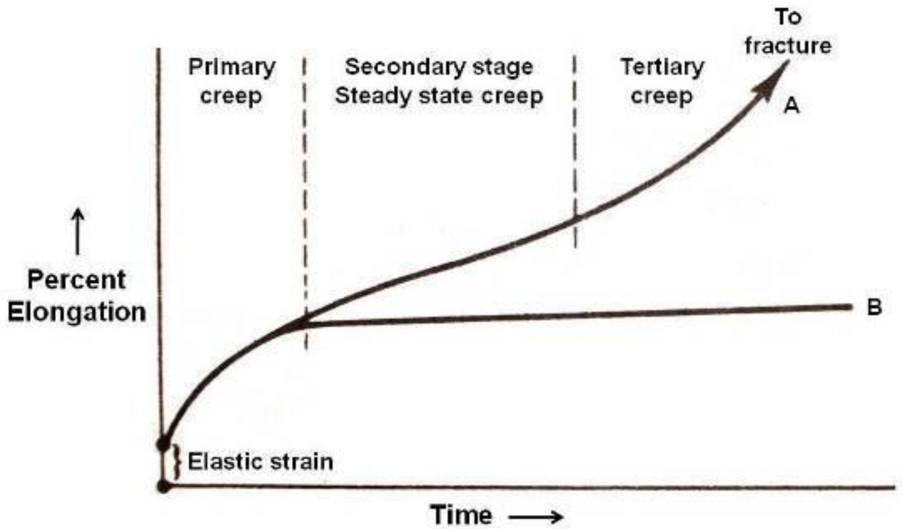
Uniaxial (tensile)



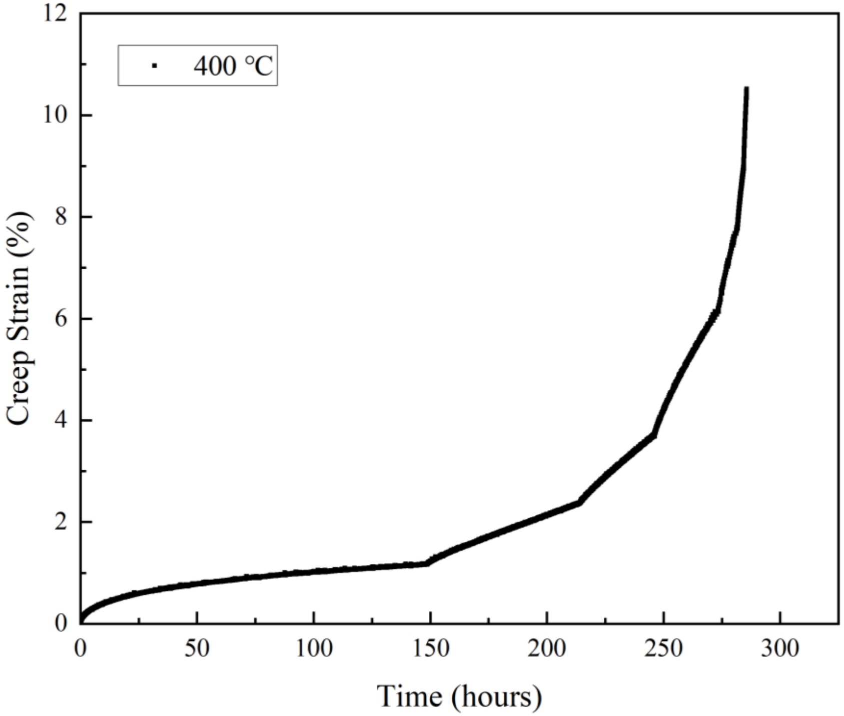


AppliedStress: (1) 1.0E+08; (2) 1.0E+07

Creep

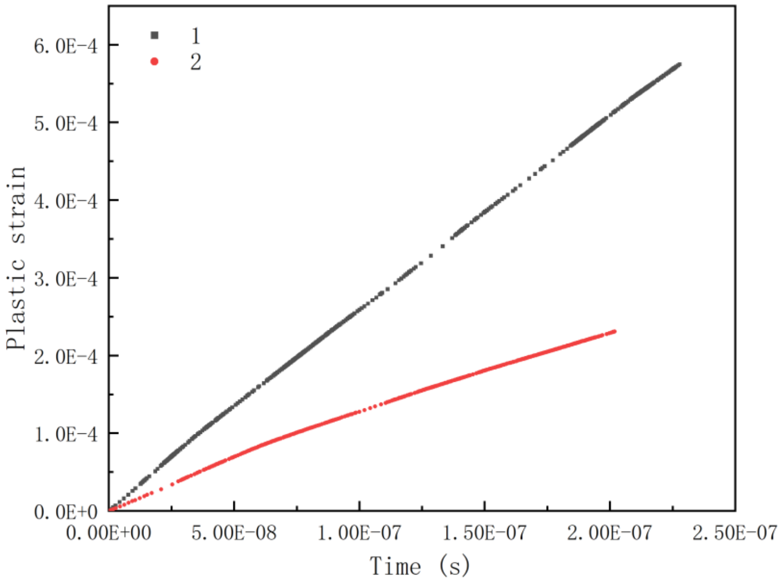


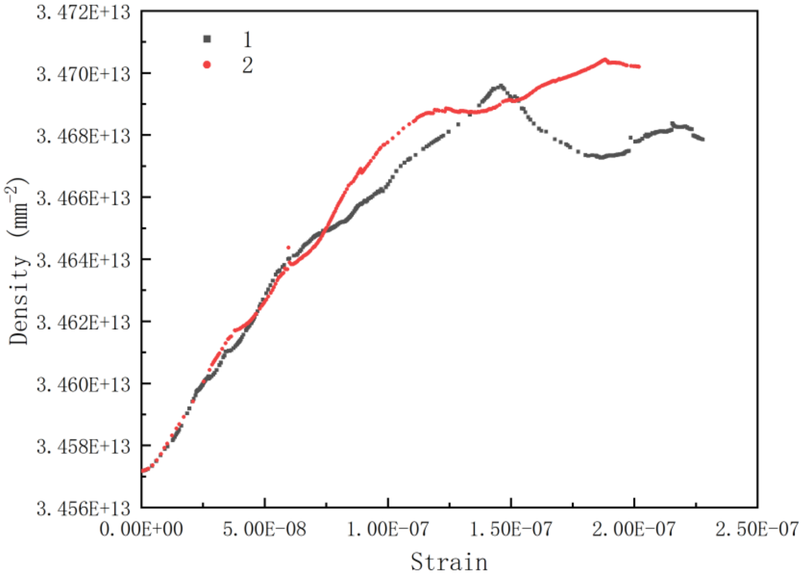
Typical Creep Curves



Al-Ce-Mg Creep test at 400 C

https://practicalmaintenance.net/?p=989





AppliedStress: (1) 1.0E+08; (2) 5.0E+07

Thank you