Molecular Dynamics Study on Drawing Process of Metallic Wire: Effect of Nano-sized Texture on Friction and Plasticity

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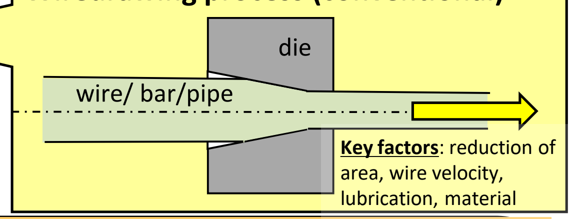
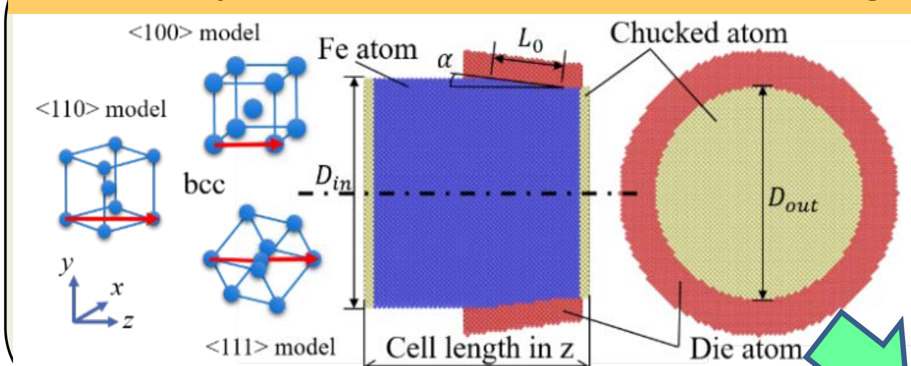
Background (open questions)

- ✓ Can wiredrawing process (plastic working) perform in nano-sized scale? (Possible)
- ✓ Will nano-sized texturing (new idea) reduce friction between die and wire?
- ✓ How microscopic plasticity (i.e. dislocation) in drawing is affected by nano-sized texturing? (in particular, from atomistic point of view)

Wiredrawing process (conventional)



Molecular dynamics model for Nano-sized wiredrawing



- Materials: iron and steel
- FS potential (many-body type)
- Velocities of entrance and exit are determined by conservation of volume law.
- Interaction between die and wire is weakened by ω<1 (artificial lubrication model).

Lubrication model (for FS potential)

Total energy

$$E = \sum_i \left\{ F_i(\rho) + \frac{1}{2}\sum_{j\neq i} \phi_{ij}(r_{ij}) \right\}$$

Many-body term $F(\rho) = \sqrt{\rho}$

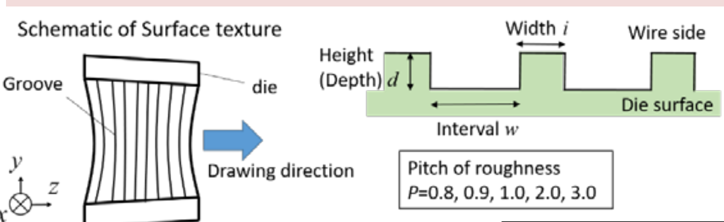
electron density $\rho_i = \sum_{j\neq i} \omega\, \rho(r_{ij})$

→ Lubrication factor ω

Table Computation condition for nano-sized **wiredrawing**

Drawing direction	<100>	<110>	<111>
The number of atoms [-]	211757	214285	209745
Cell size in x,y,z [nm]	9.88, 9.88, 13.8		
Velocity V_{in}, V_{out} [m/s]	21.9, 30.0		
Diameter D_{in}, D_{out} [nm]	13.8, 12.8		
Length of die L_0 [nm]	4.12		
Lubrication factor ω	0.01		

Nano-sized texturing (Ntxt) set-up for MD analysis



$$P = \frac{w+i}{d}$$

Pitch ratio (non-dimensional factor)

we are trying to apply **Ntxt** to wiredrawing model, so...

Simple Flat surface contact MD model with Ntxt

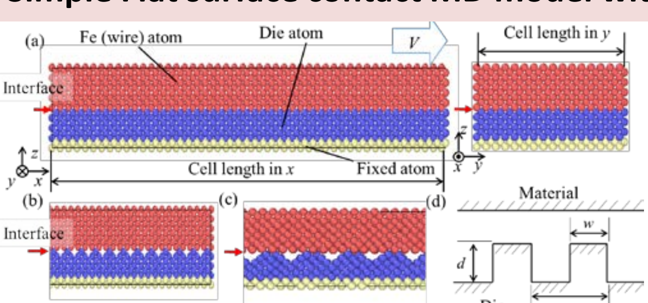


Fig. MD models with nano-sized texture (NTxt) (a)Pattern 1 (b)Pattern 2 (c)Pattern 3 (d)Geometric parameters of NTxts

Table Calculation condition **NTxt** model by MD

	Pattern 1	Pattern 2	Pattern 3
The number of atoms	13056	12672	12288
Cell size in x,y,z [nm]	13.728, 4.576, 2.288		
Velocity V [m/s]	100.0		
Depth d [nm]	-	0.143	0.286
Width w [nm]	-	0.286	0.572
Pitch p [nm]	-	0.572	1.144
Temperature T [K]	300.0		

Dislocation analysis in MD (wiredrawing model)

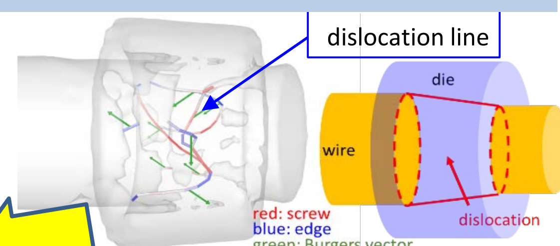


Fig. Example view obtained in dislocation analysis of nano-sized **wiredrawing** by using DXA method (drawing direction <110>, Die semi-angle α=5 deg, Velocity V_{out}=10 m/s, No texturing)

DXA (Dislocation Extraction Algorithm)

Flow of DXA (Ovito)

1. Detecting lattice defects by CNA
2. Patching surface around dislocation
3. Identifying Burger's circuit
4. Determining and indicating dislocation line

Stukowski, A., et al., Model.Simul.Mater.Sci. Eng.,**18**, 025016 (2010).

Results (examples)

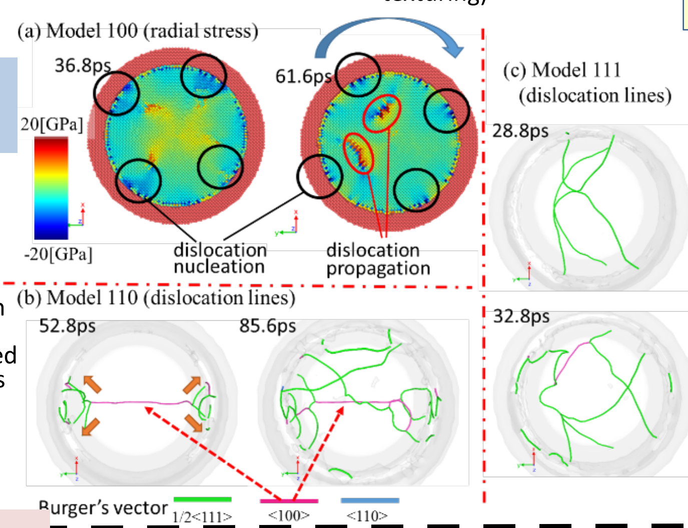
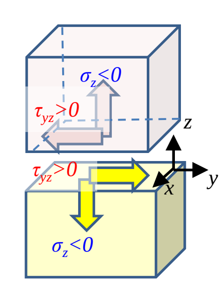


Fig. Distribution of radial stress (σ_r) and detected dislocation lines in α-Fe wire model, viewing from drawing direction



stress components in sliding motion

Results (Ntxt)

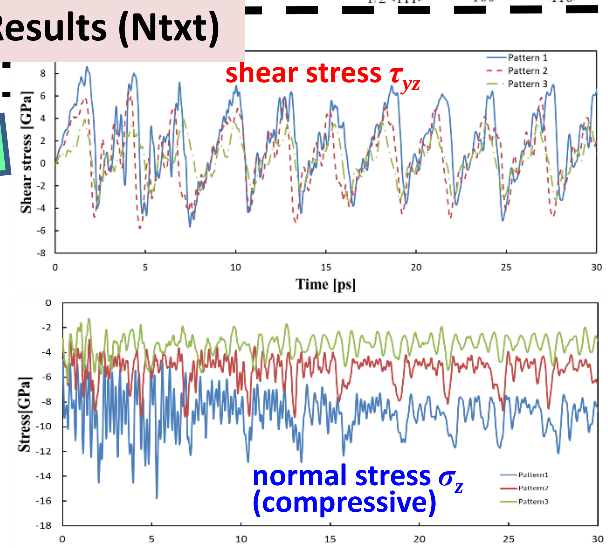


Fig. Time transition of stresses

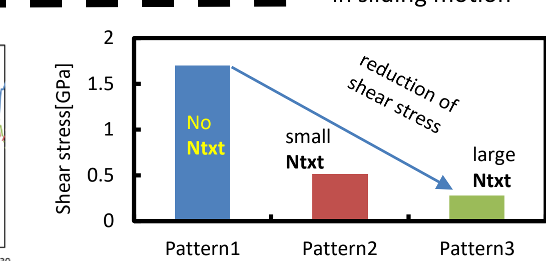


Fig. Averaged stress τ_{yz}

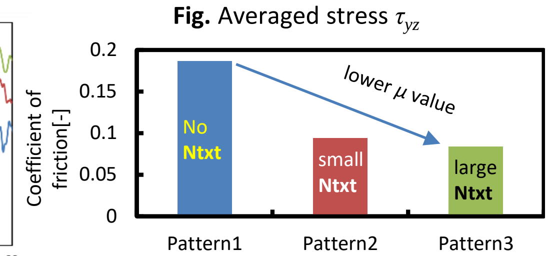
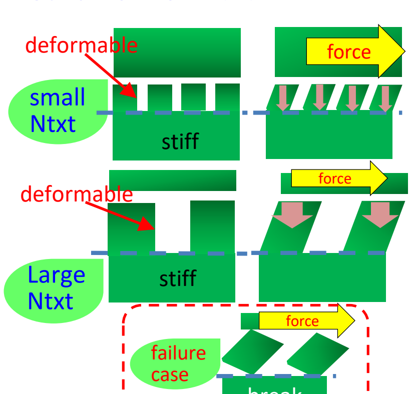


Fig. coefficient of friction $\mu = \tau_{yz}/\sigma_z$

Discussion (Ntxt)

Mechanism of Ntxt



- Stiffness of **Ntxt** depends on texture size.
- Large **Ntxt** can be deformed by smaller force.
  - Large **Ntxt** is subjected to larger normal force per one.
  - Too large **Ntxt** does not endure the force (plasticity, buckling).
- Optimized size and structure of **Ntxt** should be designed.

Summary: In this study, possibility of nano-sized **wiredrawing** was studied by using molecular dynamics (MD) simulations. In particular, effect of **nano-sized texturing** (**Ntxt**: here, single type of periodic grooves perpendicular to sliding direction) on die surface was investigated. Friction behavior is continuous stick-and-slip. Larger-sized **Ntxt** results in smaller shear stress on the materials, and accordingly smaller coefficient of friction in sliding. However it seems it largely depends on stability of **Ntxt** structure. In designing, the structure of **Ntxt** should be optimized as for size, shape as well as arrangement.