Amikor a véletlen felszínre tör

Mikrooszlopok deformációja

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ELTE, Anyagfizikai Tanszék

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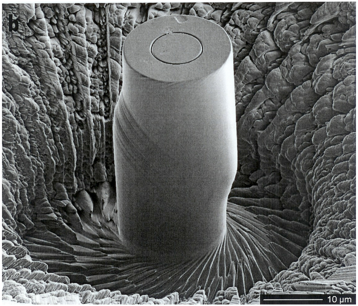
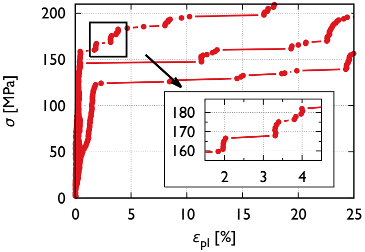
Összefoglaló

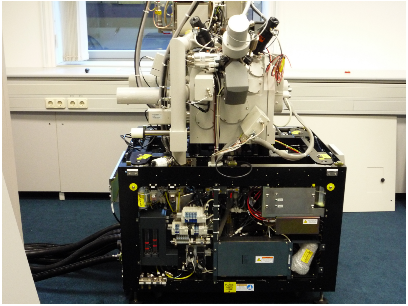
- Motiváció
- Molekula dinamika
- Depinnin modell
- Diszlokáció dinamika
- Lavinák tulajdonságai
- Összefoglaló

Mikrooszlop

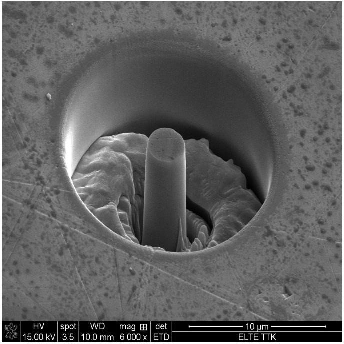




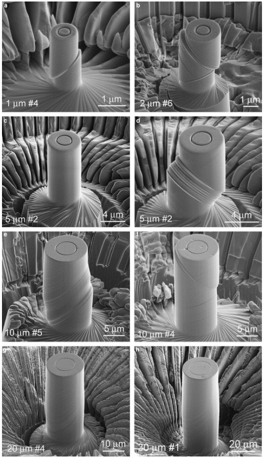
Feszültség-deformáció görbe

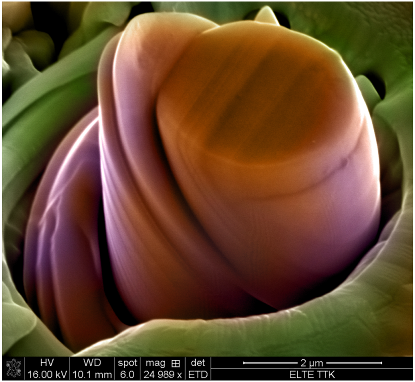


Focuses Ion Beam mikroszkóp

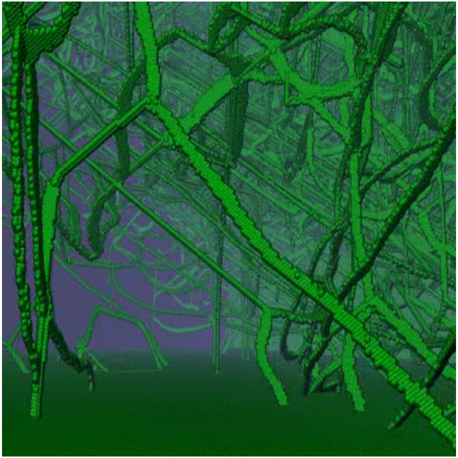


Méretfüggés





Molekula dinamika



Molekula dinamika módszerei

- Empírikus párpotenciál

$$V = \frac{1}{2}\sum_{i,j} V_d(\vec{r}_i - \vec{r}_j, A, B, C, ...)$$

  Egyszerű példa (Lennard-Jones potenciál)

$$V_d(\vec{r}) = \frac{A}{r^{12}} - \frac{B}{r^6}$$

- Sokrészecske potenciál, (megosztás)

$$V = \frac{1}{2}\sum_{i,j} V_d(\vec{r}_i - \vec{r}_j, A, B, C, ...) + F(\sum_{i,j} \Phi(\vec{r}_i - \vec{r}_j, E, F, G, ...))$$

- Első elvekből történő számolás (local density approximation)

Hőtartály hozzáadása

Ekvipartíció tétel

$$\left\langle \sum_i \frac{1}{2} m v_i^2 \right\rangle = \frac{3}{2} NkT$$

Sebesség átskálázás
Automatizálás (Nosé Hoover termosztát)

$$t' = st$$

Legyen $s(t')$ egy dinamikus változó

Módosított Lagrange függvény

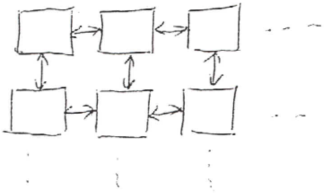
$$L'(\vec{r}_i, \vec{v}_i', s, \dot{s}) = \sum_i \frac{1}{2} m_i s^2 v_i'^2 + \frac{1}{2} \sum_{i,j} V_d(\vec{r}_i - \vec{r}_j) + \frac{1}{2} A\dot{s}^2 - NfkT \ln s$$

Variálás után

$$s^2 m_i \vec{a}_i' = -\frac{\partial V}{\partial \vec{r}_i} - 2\dot{s} s m_i \vec{v}_i'$$

$$As \frac{d^2 s}{dt'^2} = NfkT - \sum_i \frac{s^2}{2} m v_i'^2$$

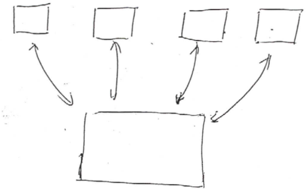
Array processzor



- $SX = X$
- $SX = Shift(SX)$
- $DO \quad I = 1 \quad TO \quad N$
- $F = F + f(X - SX)$
- $SX = Shift(SX)$
- $END \quad DO$

Master Slave

Slaves



Master

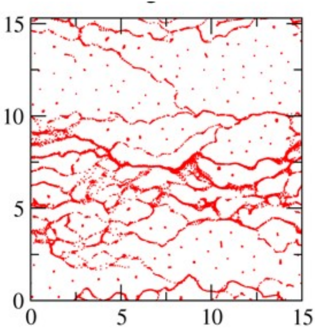
Master

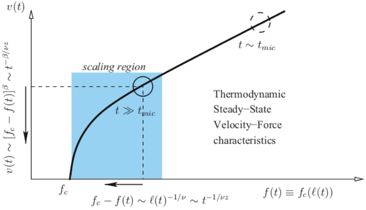
- $SlaveBoot$
- $Send(X)$
- $Receive_Force$
- Sum_Force
- $Update_X$

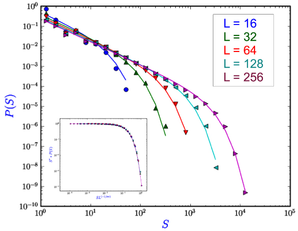
Slave

- $Receive_X$
- $Force_calc$
- $Send_Force$

Deppining átmenet







Deppining modellezése

Mozgásegyenlet

$$\eta \frac{\partial u(\vec{r},t)}{\partial t} = F + \int J(\vec{r}-\vec{r}')[u(\vec{r}',t) - u(\vec{r},t)]d\vec{r}' - f_p[\vec{r}, u(\vec{r},t)]$$

általában

$$J \propto A \triangle^2 \delta(\vec{r}) + \frac{K(\phi)}{r^\alpha}$$

Diszklét verzió

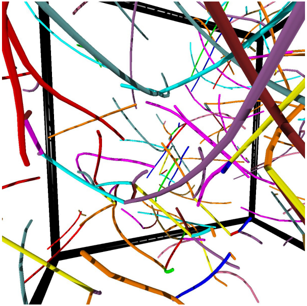
$$\eta \frac{\partial u_i(t)}{\partial t} = F + \sum_j J_{i,j}(u_j(t) - u_i(t)) + \zeta(u(t))$$

Végtelen hatótávolság+átlagtér közelítés $J_{ij} = J/N$

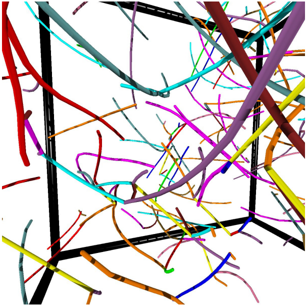
$$\eta \frac{\partial u_i(t)}{\partial t} = F + J(< u(t) > -u_i(t)) + \zeta(u(t))$$

ahol $< u >= \frac{1}{N} \sum_i u_i$

Diszlokáció dinamika



3D diszlokáció konfiguráció



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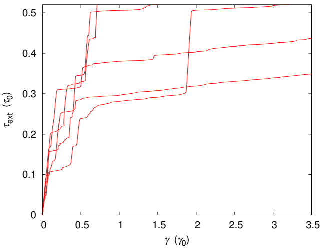
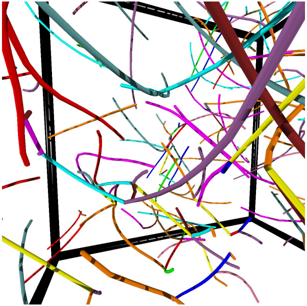
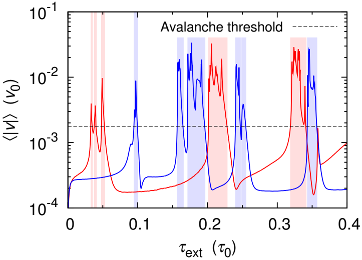


feszültség-deformáció györbe

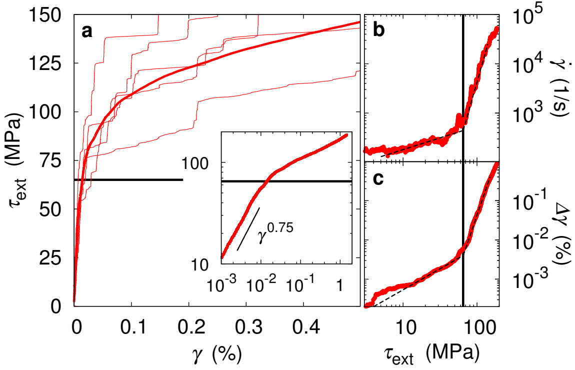


3D diszlokáció konfiguráció

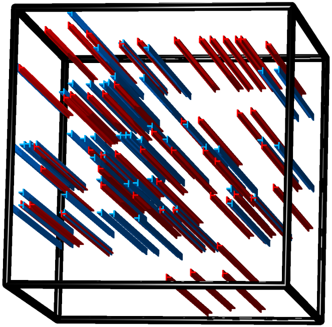


$<\dot{\gamma}>$ különböző futtatások

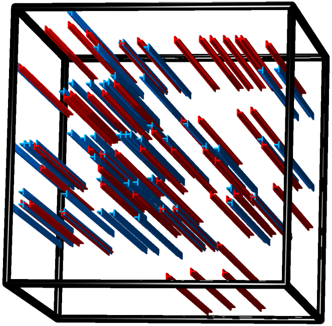
$<\gamma>$, $<\dot{\gamma}>$, $<\Delta\gamma>$



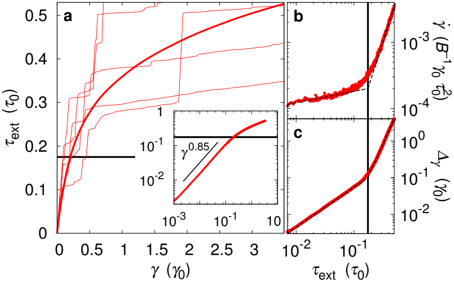
2D szimukáció



2D diszlokáció konfiguráció

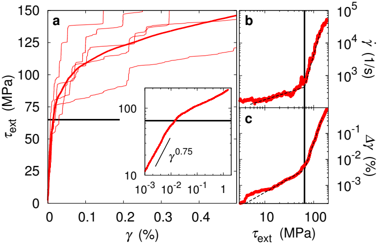


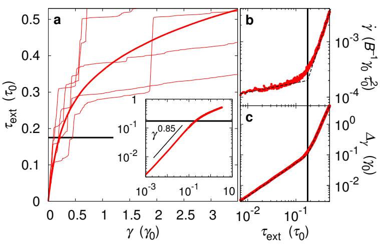
2D diszlokáció konfiguráció



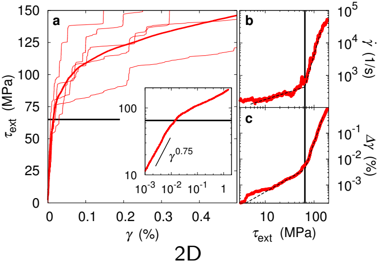
feszültség-deformáció görbék

2D & 3D

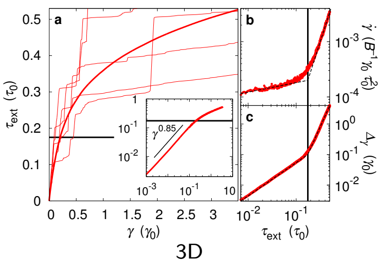

a
b
c
τ_{ext} (MPa)
γ (%)
$\gamma^{0.75}$
$\dot{\gamma}$ (1/s)
$\Delta\gamma$ (%)
τ_{ext} (MPa)


a
b
c
τ_{ext} (τ_0)
γ (γ_0)
$\gamma^{0.85}$
$\dot{\gamma}$ ($B^{-1}\gamma_0\tau_0^2$)
Δ_γ (γ_0)
τ_{ext} (τ_0)

2D & 3D

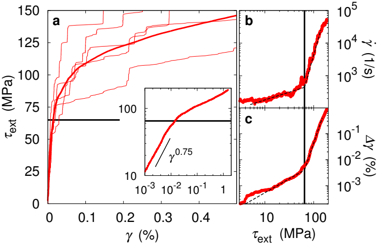


a
b
c
150
125
100
75
50
25
0
0
0.1
0.2
0.3
0.4
γ (%)
τext (MPa)
10
100
2D



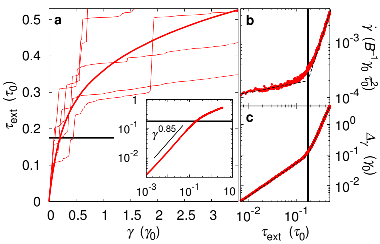
a
b
c
0.5
0.4
0.3
0.2
0.1
0
0.5
1
1.5
2
2.5
3
γ (γ0)
τext (τ0)
3D

2D & 3D



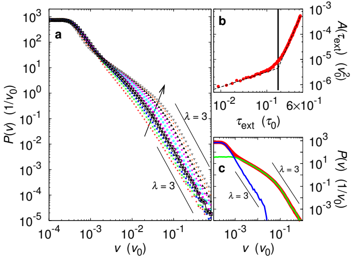
a
b
c
τ_{ext} (MPa)
γ (%)
$\dot{\gamma}$ (1/s)
$\Delta\gamma$ (%)
$\gamma^{0.75}$
τ_{ext} (MPa)

2D



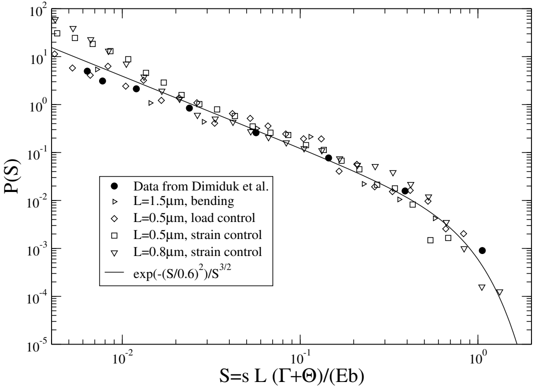
a
b
c
τ_{ext} (τ_0)
γ (γ_0)
$\dot{\gamma}$ ($B^{-1}\gamma_0\tau_0^2$)
Δ_γ (γ_0)
$\gamma^{0.85}$
τ_{ext} (τ_0)

3D



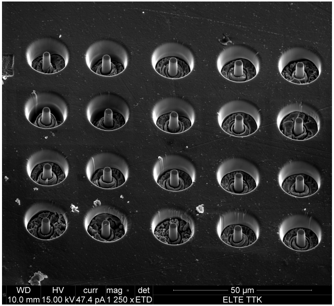
a
b
c
$P(v)$ ($1/v_0$)
v (v_0)
$\lambda = 3$
$A(\tau_{ext})$ (v_0^2)
τ_{ext} (τ_0)

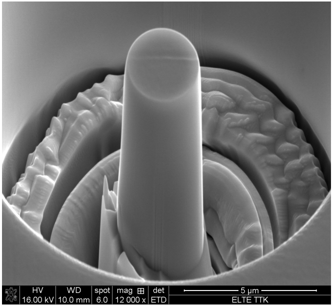
Lavinák



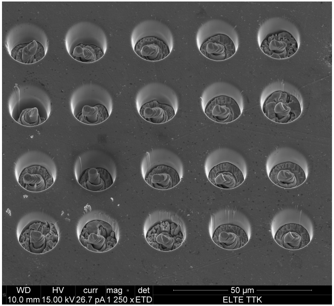
P(S)
S=s L (Γ+Θ)/(Eb)
Data from Dimiduk et al.
L=1.5µm, bending
L=0.5µm, load control
L=0.5µm, strain control
L=0.8µm, strain control
exp(-(S/0.6)^2)/S^3/2

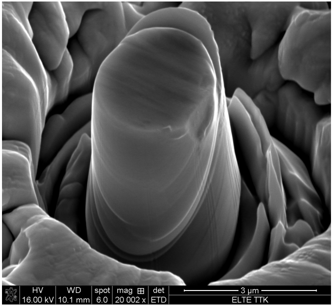
Kísérlet

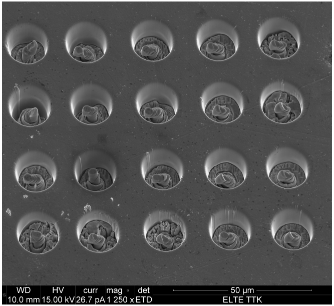

WD HV curr mag det 50 µm
10.0 mm 15.00 kV 47.4 pA 1 250 x ETD ELTE TTK

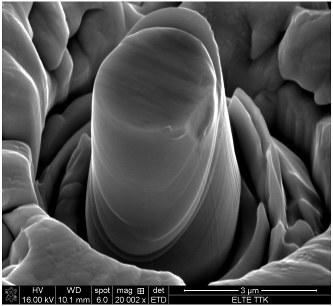

HV WD spot mag det 5 µm
16.00 kV 10.0 mm 6.0 12 000 x ETD ELTE TTK

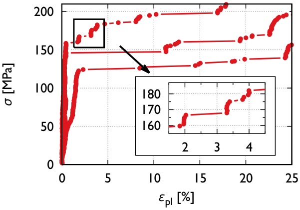
Kísérlet


WD
10.0 mm
HV
15.00 kV
curr
26.7 pA
mag
1 250 x
det
ETD
50 µm
ELTE TTK

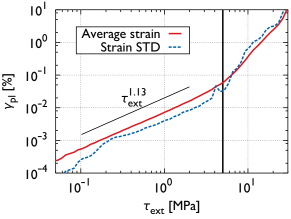

HV
16.00 kV
WD
10.1 mm
spot
6.0
mag
20 002 x
det
ETD
3 µm
ELTE TTK

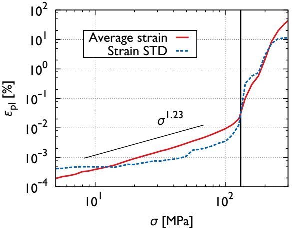

WD 10.0 mm
HV 15.00 kV
curr 26.7 pA
mag 1 250 x
det ETD
50 μm
ELTE TTK

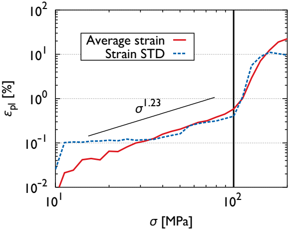

HV 16.00 kV
WD 10.1 mm
spot 6.0
mag 20 002 x
det ETD
3 μm
ELTE TTK

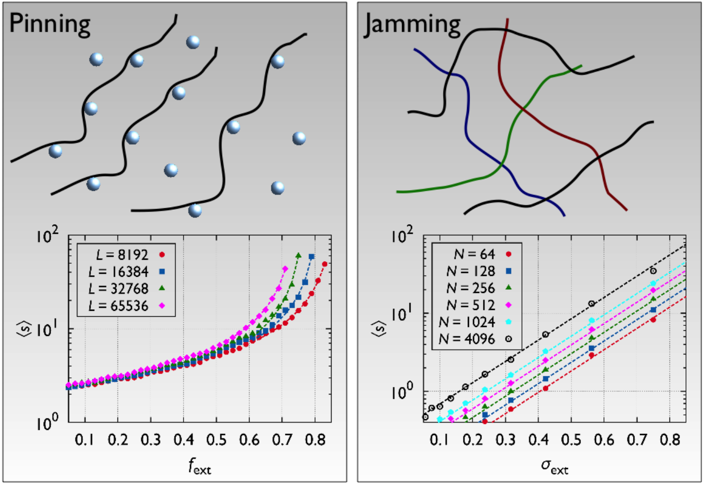

σ [MPa]
ε_pl [%]
0
50
100
150
200
5
10
15
20
25
180
170
160
2
3
4

Összehasonlítás








Pinning
L = 8192
L = 16384
L = 32768
L = 65536
⟨s⟩
f_ext
Jamming
N = 64
N = 128
N = 256
N = 512
N = 1024
N = 4096
⟨s⟩
σ_ext