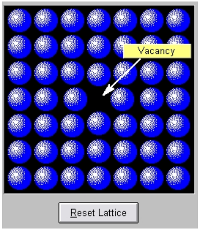
Anyagfizika
Kristályhibák

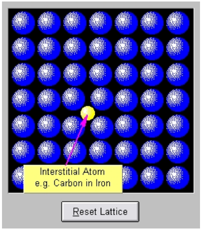
Groma István

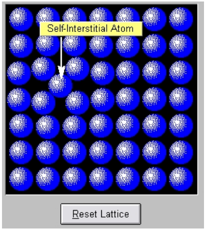
ELTE

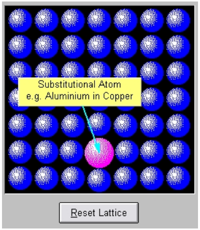
March 10, 2022

Ponthiba


Vacancy
Reset Lattice


Interstitial Atom
e.g. Carbon in Iron
Reset Lattice


Self-Interstitial Atom
Reset Lattice


Substitutional Atom
e.g. Aluminium in Copper
Reset Lattice

Szabadenergia

$$S(U, V, N) \longrightarrow F(T, V) = U - TS$$

$$dU = TdS - pdV$$
$$dF = SdT - pdV$$

Rendszer + termosztat= zárt

$$dS_r + dS_t \geq 0$$
$$dU_r + dU_t = 0$$
$$dS = \frac{dU}{T} + \frac{p}{T} dV$$

innen mivel itt $dV = 0$

$$dS_s - \frac{dU_s}{T} \geq 0 \longrightarrow dU_s - TdS_s \leq 0$$
$$dT = 0, \qquad dF = dU - TdS - SdT \leq 0$$

Vakancia

Egyensúlyi vakanciakoncentráció
Gibbs potenciál

$$G(T,p) = U - TS + pV$$

n vakancia N atom

$$\triangle U = \epsilon_0 n$$

$$\triangle V = v_0 n$$

Entrópia

$$S^{config} = k_B \ln \begin{pmatrix} N+n \\ n \end{pmatrix} = k_B \ln \frac{(N+n)!}{N!n!}$$

Stirling-formula

$$\ln n! \approx n \ln n$$

Így

$$S^{config} = k_B \left[(N+n)\ln(N+n) - N\ln N - n\ln n\right]$$

Innen

$$\triangle G = \epsilon_0 n + p v_0 n - k_B T \left[(N+n)\ln(N+n) - N\ln N - n\ln n\right]$$

Vakancia

Egyensúly koncentráció

$$\frac{\partial \triangle G}{\partial n} = 0$$

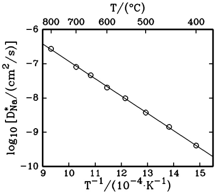
$$\epsilon_0 + pv_0 - k_B T[\ln(N+n) - \ln n] = 0$$

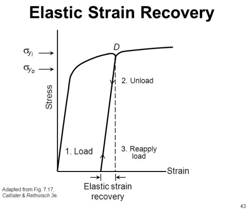
$$\frac{n}{N+n} = e^{-\frac{\epsilon_0 + pv_0}{k_B T}}$$

$N >> n$

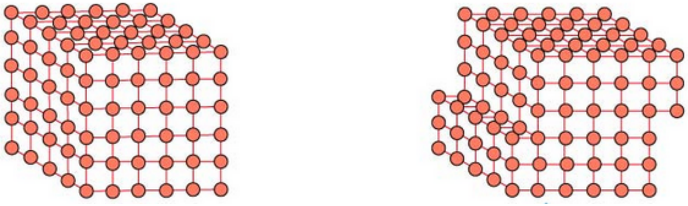
$$n = Ne^{-\frac{\epsilon_0 + pv_0}{k_B T}}$$

Arrhenius plot (nátrium)





Ideális nyírás



Plasztikus deformáció

Ideális nyírás

$$F(x) = F_0 \left| \sin\left(\frac{\pi}{a}x\right) \right| = \sigma a^2$$

Kis deformáció

$$\gamma = \frac{x}{a}, \qquad \sigma = \mu \frac{x}{a}$$

Így

$$F_0 = \mu \frac{a^2}{\pi}$$

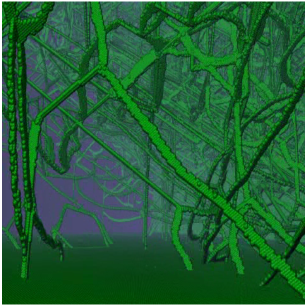
Innen

$$\sigma_f \cong \frac{\mu}{\pi} \cong 30 GPa$$

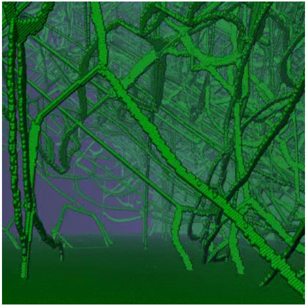
Kísérlet

$$\sigma_f \cong 100 MPa$$

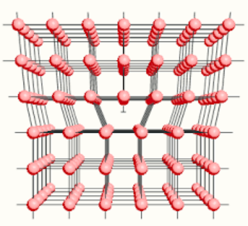
MDD

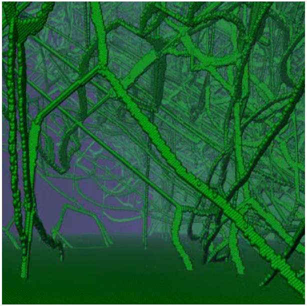


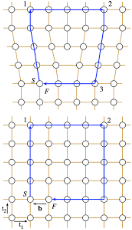
MDD



Polányi, Orován, Taylor (1934)

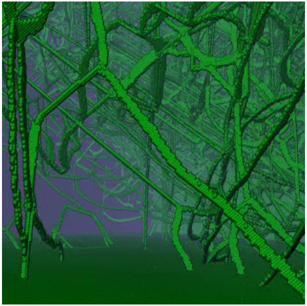


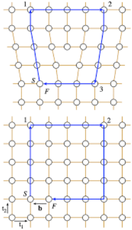




Burgers vector

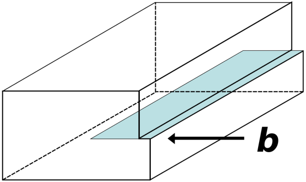
MDD





Burgers vector

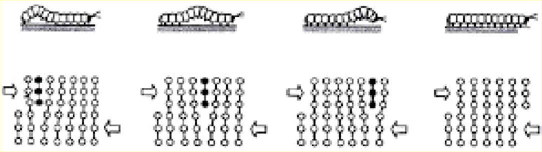
Vito Volterra (1905)



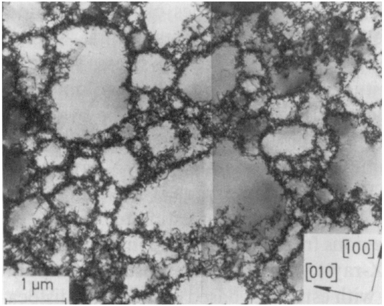
Diszlokáció

Az elcsúszás nem egyszerre megy végbe

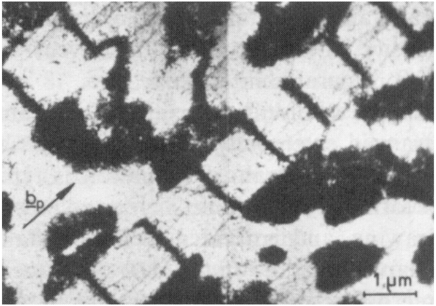
Ez csak akkor lehetséges, ha a kristály tartalmaz egyméretű rácshibákat, diszlokációkat.



Csúszás: atomok száma megmarad
Mászás: atomok száma nem marad meg, magas hőmérséklet kell



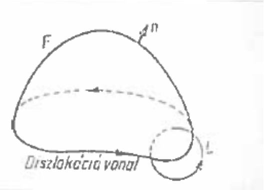
Cella szerkezet



PSB szerkezet

diszlokáció sűrűség $\rho = 10^{14} m^{-2}$

Diszlokáció



Diszlokációk térelmélete

$$\partial_i u_j := \beta_{ij} = \beta^p_{ij} + \beta^e_{ij} \qquad \frac{d\underline{u}}{d\underline{r}} := \hat{\beta} = \hat{\beta}^e + \hat{\beta}^p$$

Diszlokáció sűrűség tensor

$$\alpha_{ij} = e_{ikl}\partial_k \beta^p_{lj} = -e_{ikl}\partial_k \beta^e_{lj} \qquad \hat{\alpha} = \nabla \times \hat{\beta}^p = -\nabla \times \hat{\beta}^e$$

$$b_j = \int_A \alpha_{ij} dA_i$$

$$b_j = -\int_A e_{ikl} \frac{\partial}{\partial r_k} \beta^e_{lj} dA_i = -\oint \beta^e_{ij} ds_i = -\oint du_j.$$

Diszlokáció

Egyedi diszlokáció

$$\alpha_{ij} = l_i b_j \delta(\xi) \qquad (\hat{\alpha} = \underline{l} \circ \underline{b}\delta(\xi))$$

Plasztikus disztorzió

$$\beta_{ij}^{p}(\vec{r}) = n_i b_k \delta(\zeta)$$

Szorozzuk meg a rugalmas állandóval és vegyük a div-jét

$$\frac{\partial}{\partial r_i} C_{ijkl} \frac{\partial u_k}{\partial r_l} = \frac{\partial}{\partial r_i} C_{ijkl} \beta_{kl}^{p} = f_j \left(div\ \hat{C} \frac{d\underline{u}}{d\underline{r}} = div\ \hat{C} \hat{\beta}^{p} = \underline{f} \right)$$

Csavardiszlokáció elmozdulástere

$$u_3 = \frac{b}{2\pi} \varphi$$

Egyenes diszlokáció feszültségtere $\sigma \propto b/r$

$$\sigma_{11} = \frac{\mu b}{2\pi(1-\nu)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2}$$

$$\sigma_{22} = \frac{\mu b}{2\pi(1-\nu)} \frac{y(x^2-y^2)}{(x^2+y^2)^2}$$

$$\sigma_{12} = \frac{\mu b}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

Diszlokáció energiája

$\sigma \propto b/r$ így $E \propto b^2$

$$2\left(\frac{b}{2}\right)^2 < b^2$$

$\underline{b} = \underline{a}_i$

Fcc $\underline{b} = \frac{1}{2}(1,1,0)$
Bcc $\underline{b} = \frac{1}{2}(1,1,1)$

Diszlokációk kölcsönhatása

Rugalmas energia

$$E = \frac{1}{2}\int \sigma_{ij}\partial_i u_j dV$$

Legyen

$$\sigma_{ij} = \sigma_{ij}^{ext} + \sigma_{ij}^{disl}$$
$$u_i = u_i^{ext} + u_i^{disl}$$

Ekkor

$$E = \frac{1}{2}\int \left[\sigma_{ij}^{ext}\partial_i u_j^{ext} + \sigma_{ij}^{ext}\partial_i u_j^{disl} + \sigma_{ij}^{disl}\partial_i u_j^{ext} + \sigma_{ij}^{disl}\partial_i u_j^{disl}\right] dV$$

Mivel

$$\sigma_{ij} = C_{ijkl}\partial_i u_j$$

$$E = E_{ext} + E_{disl} + \int \sigma_{ij}^{ext}\partial_i u_j^{disl} dV$$

Diszlokációk kölcsönhatása

$$E_{int} = \int \sigma_{ij}^{ext} \partial_i u_j^{disl} dV$$

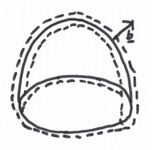
Parciális integrálással

$$E_{int} = \int \partial_i (\sigma_{ij}^{ext} u_j^{disl}) dV - \int (\partial_i \sigma_{ij}^{ext}) u_j^{disl} dV$$

Mivel

$$\partial_i \sigma_{ij}^{ext} = 0$$

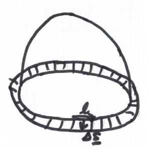
$$E_{int} = \int \partial_i (\sigma_{ij}^{ext} u_j^{disl}) dV = \int (\sigma_{ij}^{ext} u_j^{disl}) dn_i$$



$\underline{u}$-nak $\underline{b}$ ugrása van a vágási felületen!

$$E_{int} = b_j \int_f \sigma_{ij}^{ext} dn_i$$

Ha a vonal megmozdul az vonal által húzott övre



$$\triangle E_{int} = b_j \oint_v \sigma_{ij}^{ext} (\triangle \underline{r} \times \underline{dl})_i$$

Diszlokációk kölcsönhatása

$$\triangle E_{int} = \oint_{v} (\underline{dl} \times (\hat{\sigma}^{ext}\underline{b}))_i \triangle r_i$$

Peack Koehler erő

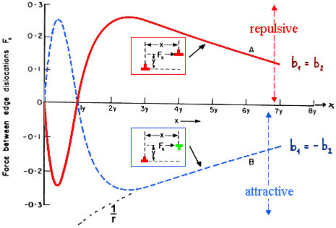
$$\underline{f} = (\hat{\sigma}^{ext}\underline{b}) \times \underline{l}$$

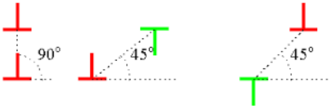
Kúszásnál csak a csúszósíkra eső vetület számít

$$f_{glide} = [(\hat{\sigma}^{ext}\underline{b}) \times \underline{l}]\frac{\underline{b}}{b} = \underline{n}\hat{\sigma}^{ext}\underline{b} = \tau b \ \text{ ahol } \ \underline{n} = \frac{\underline{b}}{b} \times \underline{l}$$

Éldiszlokációk

$$f = b_1 b_2 \frac{\mu}{2\pi(1-\nu)} \frac{x(x^2-d^2)}{(x^2+d^2)^2}$$

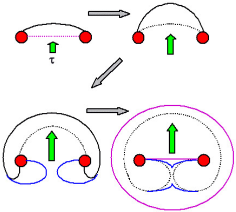




Possible equilibrium configurations

Diszlokációk sokszorozódása

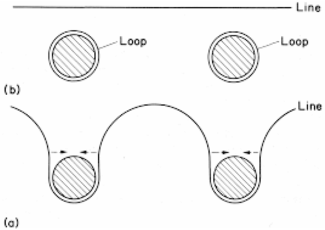
Frank-Read forrás



Folyáshatár (Taylor reláció)

$$\tau_f = \alpha \mu \boldsymbol{b} \sqrt{\rho}$$

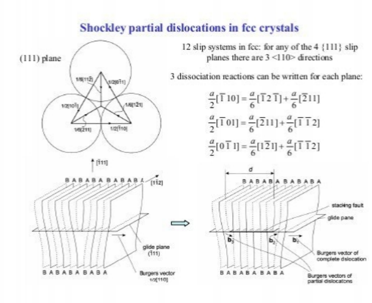
Vonalfeszültség $\tau_l = E_l/R$

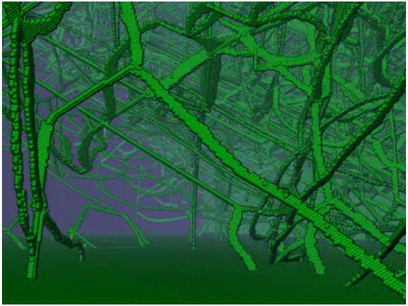


Kritikus feszültség

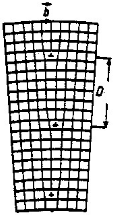
$$\tau_c = \propto \frac{1}{l}$$

Parciális diszlokáció

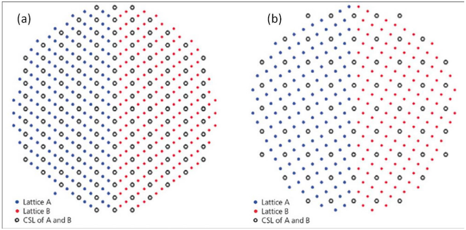




Szemcsehatár

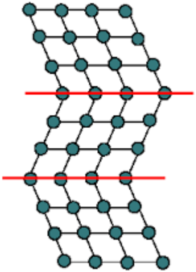


Kisszögű szemcsehatár



Koincidencia rács (Σn)

Ikerhatár



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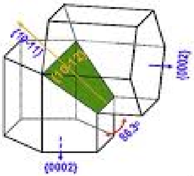

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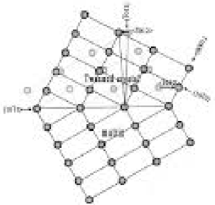

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