Modelling of Dislocation Bias in FCC Materials

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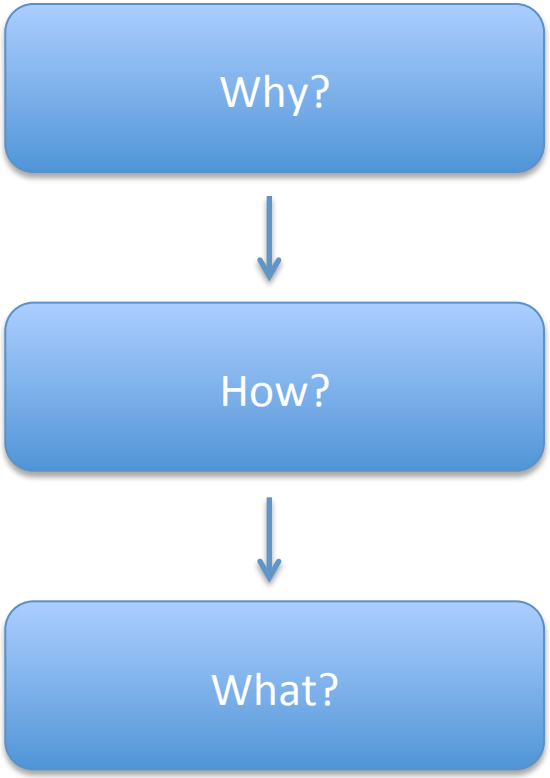
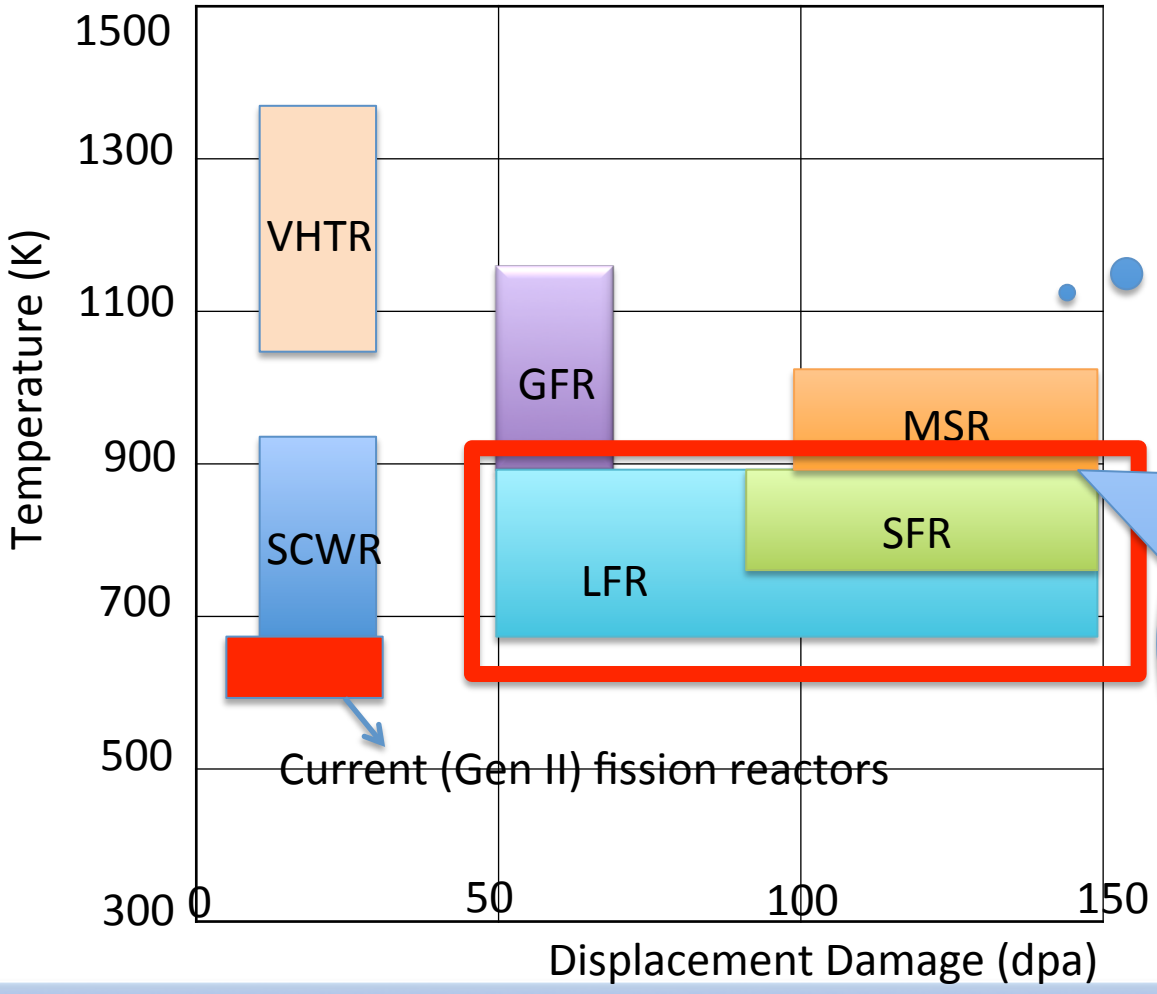


Why? – Gen IV



High burn up;
Low radiotoxity;

✓ Safety;
✓ High power density;

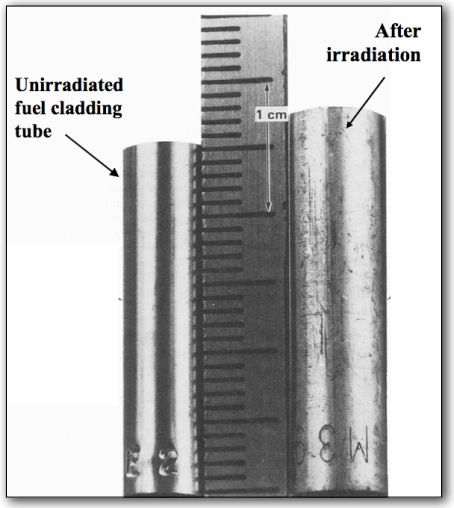
High requirement in materials:
Mechanical properties;
Corrosive environment;
Irradiation conditions;

Why? – Austenitic steel

- Austenitic steel
  - Fe-Cr(15-20%)-Ni(8-15%) FCC
  - Good strength and ductility, fatigue resistance, little or no precipitation, stable parent austenite phase
  - Swelling
    - 260% swelling in 316 during proton irradiation

Properties of 316L Stainless steel

Property	Value
Density	8000 kg/m^3
Melting T	1390-1440 C
Elastic modulus	193 GPa
Shear modulus	82 GPa

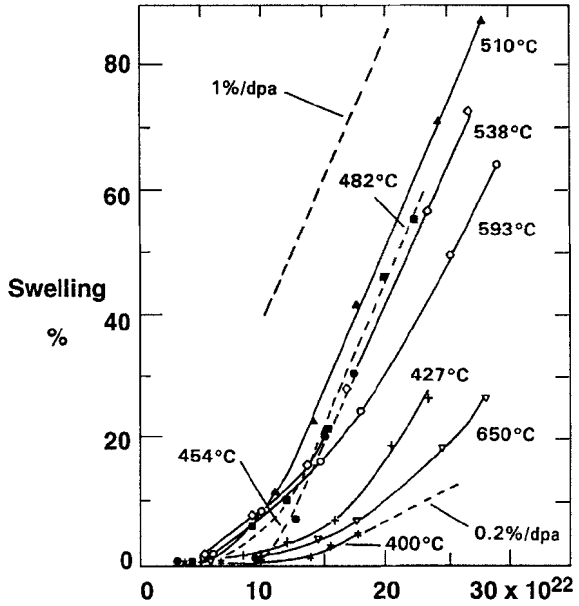


CW316 at 533°C to a fluence of 1.5e23 n/m^2 in the EBR-II.

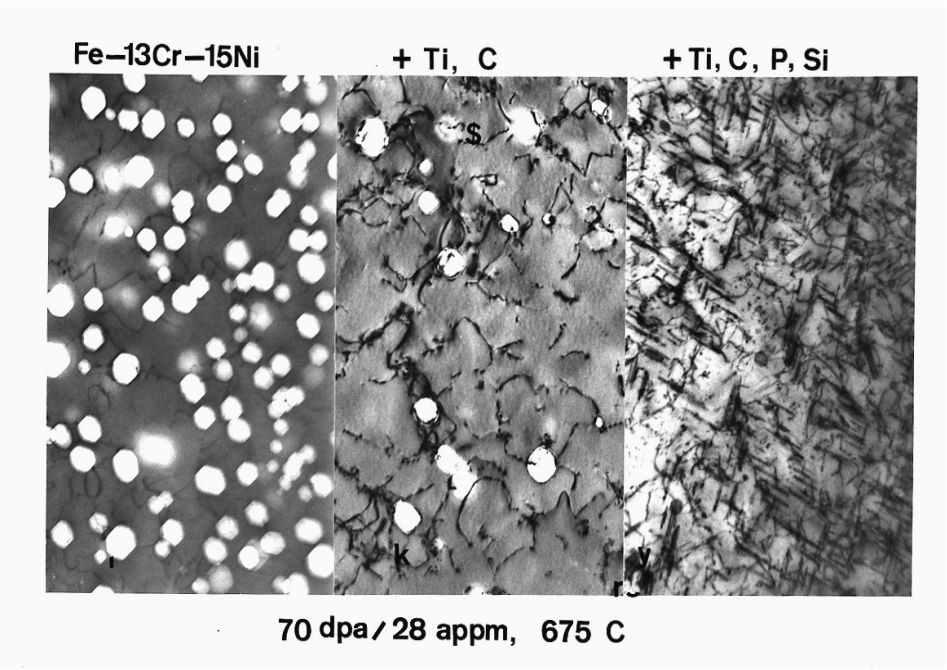
Comprehensive nuclear material
Mansur 1994

Background - Swelling

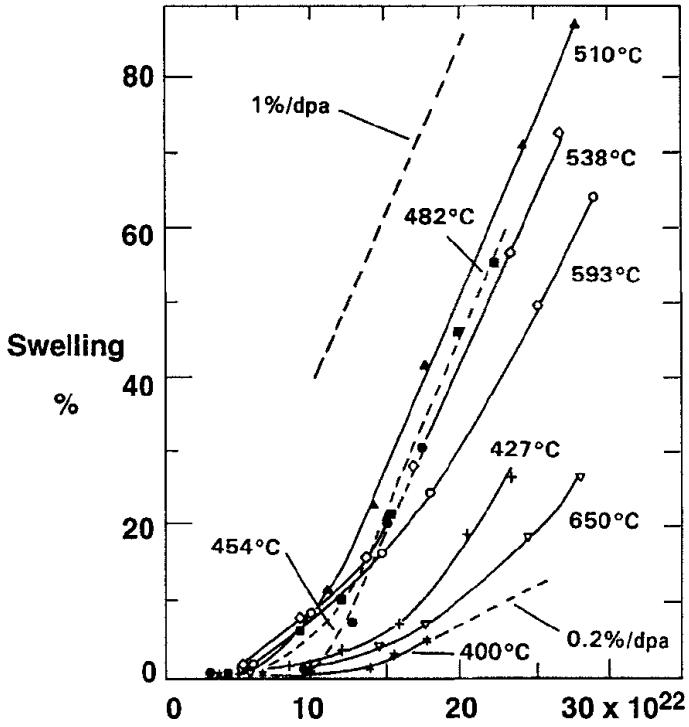
- Dimensional increase of component volume
- Sensitivity to gradients in dose, dose rate an temperature can lead to strong distortions
- Fabricated sizes and shapes not preserved
- May affect particle transport and thermal hydraulics
- Cavity distributions - possible easy paths for fracture
- Limit lifetime



Why? - Swelling



Large reductions in swelling can be attained by alloying additions

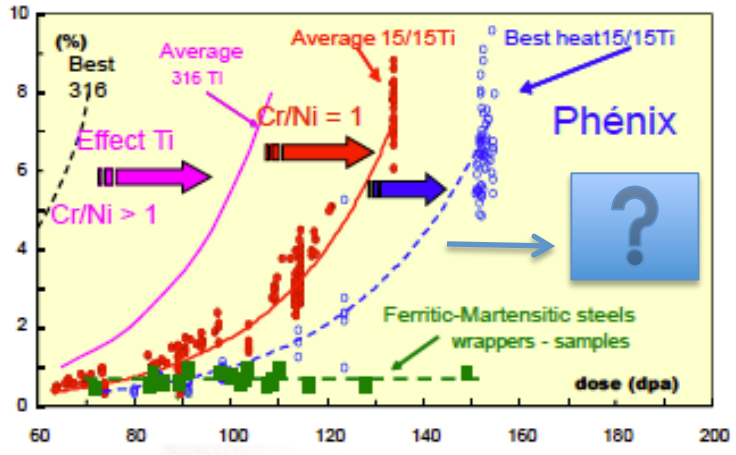


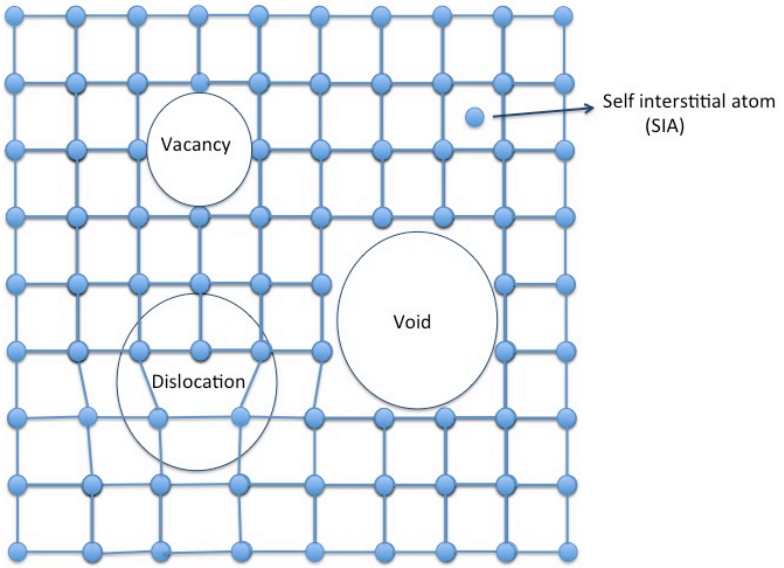
Swelling of 20% CW Austenitic stainless steel in EBR-II

Garner and Gelles, 1990

L. K. Mansur and E. H. Lee 1990

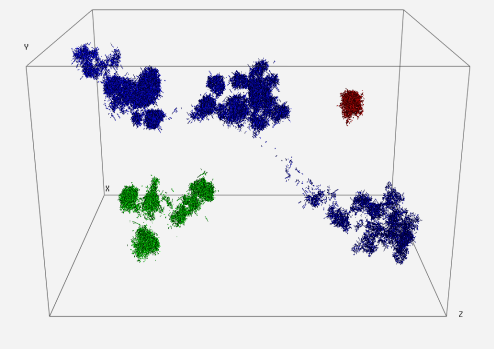
Why? - Swelling





- "Billiard games"

- Primary Knock-on atoms (PKA)
- Collisions in cascades (10^{-13} s)
- Microstructural evolution (10^{6} s)



How? - Standard Rate Theory

- Traditional rate theory approach:

$$\frac{dC}{dt} = Generation - Annihilation$$

Disadvantages: Based on mean field approximation

- Diffusion and recombination take place continuously in time and space – defects are uniformly distributed
- Ignores the inhomogeneous nature of defect production in displacement cascades and formation of defect clusters

Advantages:

- Any time scale
- Void swelling from electron radiation (only Frenkel pairs)

How? - Standard Rate Theory

$$\frac{dC_v}{dt} = G - k_v^2 D_v C_v - \mu_r D_i C_i C_v \qquad \frac{dC_i}{dt} = G - k_i^2 D_i C_i - \mu_r D_i C_i C_v$$

Assumptions: Only voids and dislocations are present, recombination is negligible:

$$G - k_C^2 D_v C_v - k_{Dv}^2 D_v C_v = 0 \qquad G - k_C^2 D_i C_i - k_{Di}^2 D_i C_i = 0$$

Void is a neutral sink, swelling rate is the net flux of vacancies to voids:

$$\frac{ds}{d\phi} = k_C^2 (D_v C_v - D_i C_i) = B_D \frac{k_C^2 k_{Dv}^2}{(k_C^2 + k_{Dv}^2)(k_C^2 + k_{Di}^2)}$$

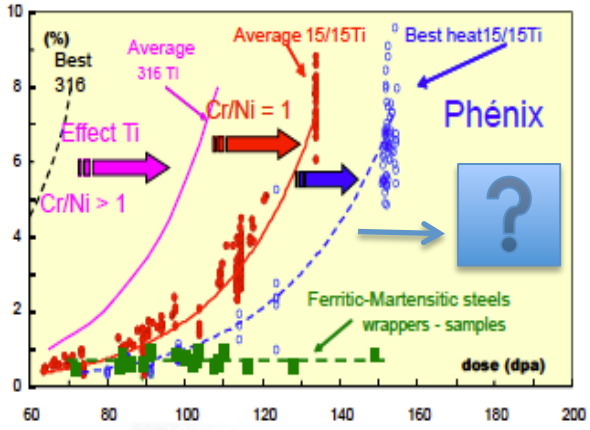
Sink strength for voids: $k_C^2 = 4\pi \bar{R} N$

Bias factor: $B_D = \frac{k_{Di}^2 - k_{Dv}^2}{k_{Dv}^2}$

S total volume of voids; Φ irradiation dose; $k^2_{v/i}$ sink strengths for vacancy / interstitial

Golubov 2001

How? – Bias



Standard Rate Theory (SRT)

Sink bias: different absorption rates of interstitials and vacancies

$$\frac{ds}{d\phi} = B_d \frac{k_c^2 Z_v^d \rho}{(k_c^2 + Z_v^d \rho)(k_c^2 + Z_i^d \rho)}$$

- Analytically
  - Elasticity theory
  - Fick's law with drift term solve diffusion equation

Some analytical values:

B_D =25% for Cu

B_D =34% for Ni

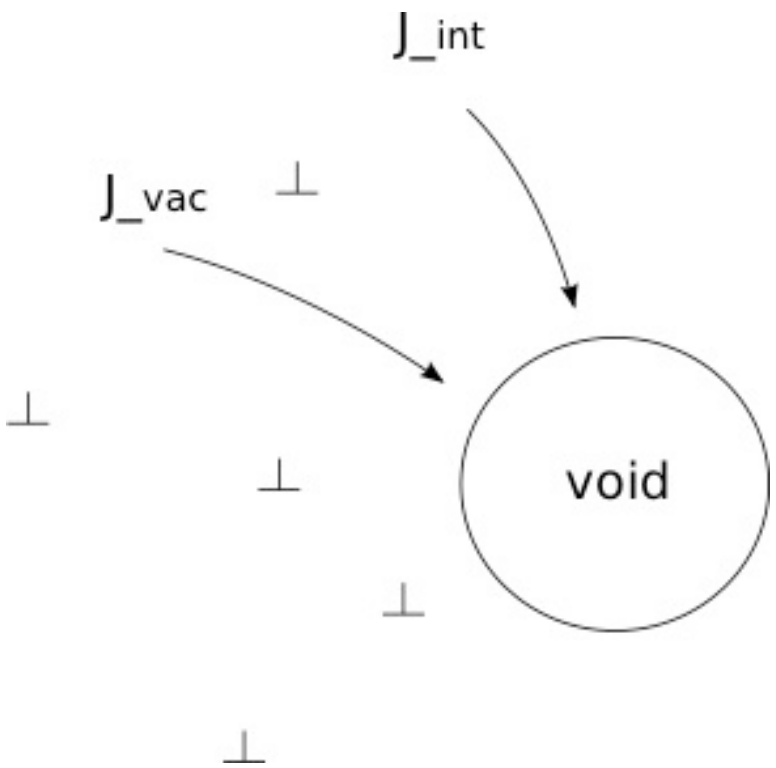
- Experimentally
  - Parameter fitting

Some experimental values:

B_D =2-4% for Cu

B_D =2% for pure Fe-Cr-Ni alloy

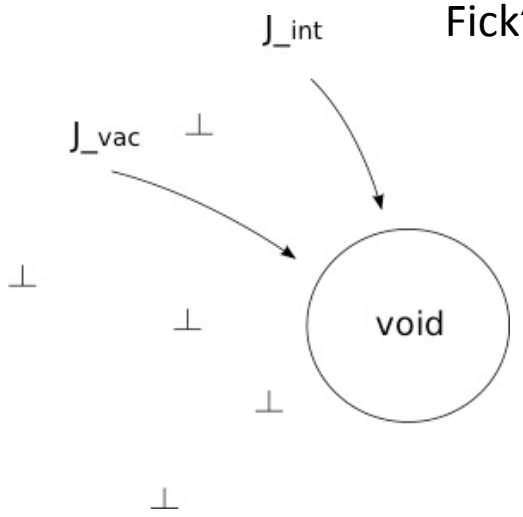
How? – Simplest SRT Model



1. Incident particle produces only FPs
2. Both SIAs and vacancies migrate in 3D
3. Dislocations "prefer" SIAs to vacancies.
   - SIAs have stronger interaction energy with dislocation
   - SIAs have larger interaction range

FP =Frenkel pair, SIA=self interstitial atom

How? - Theoretical approach



Fick's law with drift term: $J = -\nabla(DC) - \beta DC\nabla E$

Steady state: $\nabla J = 0$

$$\nabla^2 U = \beta(\nabla U)(\nabla E) \quad \text{with} \quad U = DCe^{\beta E(r)}$$

$$J = -e^{\beta E(r)} \cdot \nabla U$$

J_{tot} is the total flux around the dislocation core

Sink strength: $k^2 = \dfrac{J_{tot}}{U_\infty - U_0}$

Capture efficiency: $Z = \dfrac{k^2}{k_0^2} = \dfrac{J_{tot}}{J_0}$

Bias factor: $B_D = \dfrac{Z_i - Z_v}{Z_v}$

How? - Analytical Interactions

- 1st order size interaction (long range interaction)

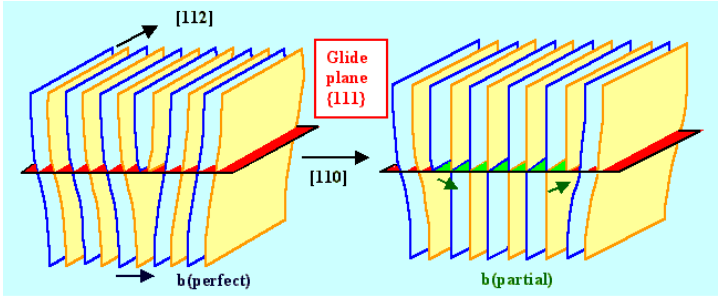
$$E(r,\theta) = -\frac{A\sin\theta}{r}$$

$$A = \frac{\mu b}{3\pi}\frac{1+\nu}{1-\nu}\Delta\Omega$$

- Crystal: elastic medium
- PD: elastic inclusion

μ shear modulus; b Burges vector
ν Poisson ratio; ΔΩ dilatation volume

- Assumptions:
  - Isotropic system
  - Exact spherical form of PD
  - Non-split dislocation core



PD=point defects

Bullough 1970

How? - Analytical Interactions

➢ Anisotropic

$$E(x,y) = \frac{b(1+\nu)I\Delta\Omega}{6\pi}\frac{(2x^2y + Hx^2y + 2y^3)}{(x^2+y^2)^2 + Hx^2y^2}$$

$$I = (c_{11}+c_{12})\left[\frac{c_{66}(c_{11}-c_{12})}{c_{11}(2c_{66}+c_{11}+c_{12})}\right]^{1/2}$$

$$H = \frac{(c_{11}+c_{12})(c_{11}-c_{12}-2c_{66})}{c_{11}c_{66}}$$

- Crystal: anisotropic elastic medium
- PD: elastic inclusion

- Assumptions:
  - ~~Isotropic system~~
  - Exact spherical form of PD
  - Non-split dislocation core

b Burges vector; c_{ij} elastic constants;
v Poisson ratio; ΔΩ dilatation volume;

Chang 1962

How? - Calculation Methods

- Analytically
  - Elasticity theory
  - Fick's law with drift term solve diffusion equation analytically

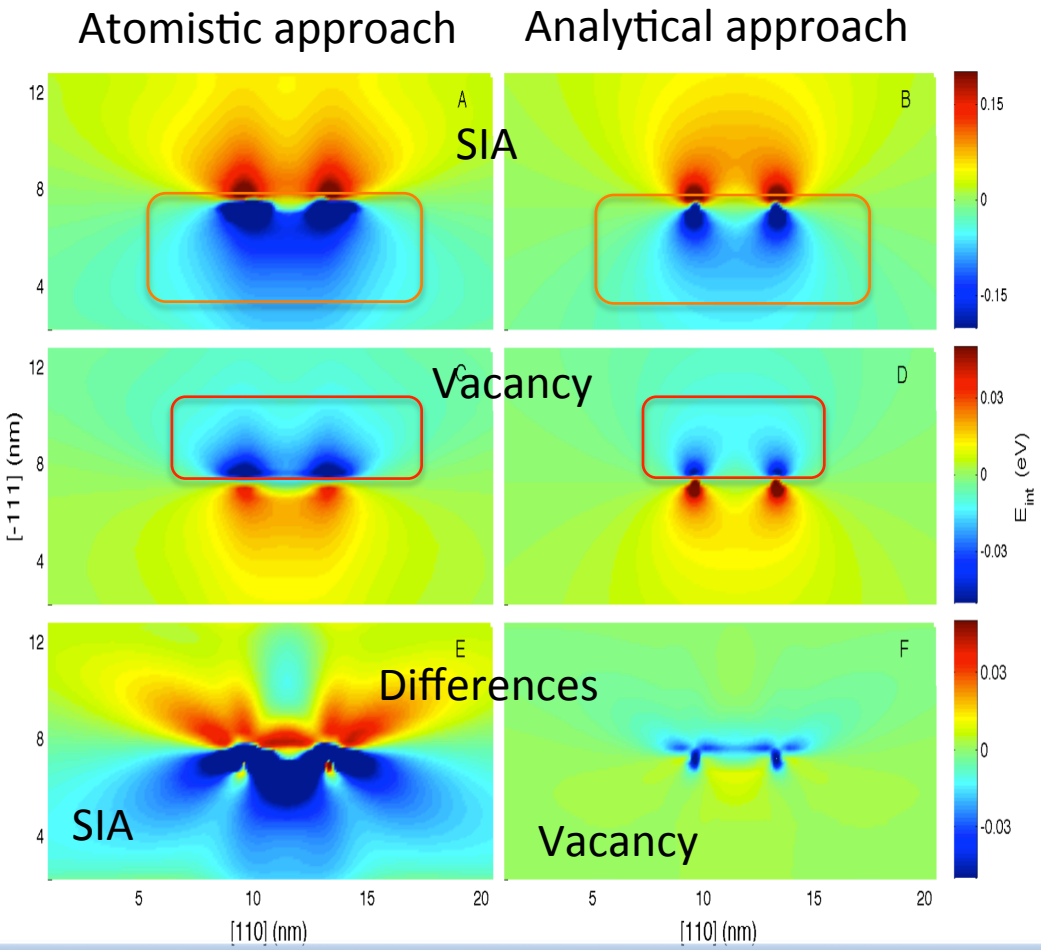
- Realistically
  - Atomistic model
  - Fick's law with drift term solve diffusion equation numerically

Parameter	Cu	Ni
X(a_0) [110]	70	70
Y(a_0) [-11-2]	7	7
Z(a_0) [-111]	41	76
Number of atoms	85980	157572
ρ_d (m^{-2})	$2.8*10^{15}$	$1.5*10^{15}$

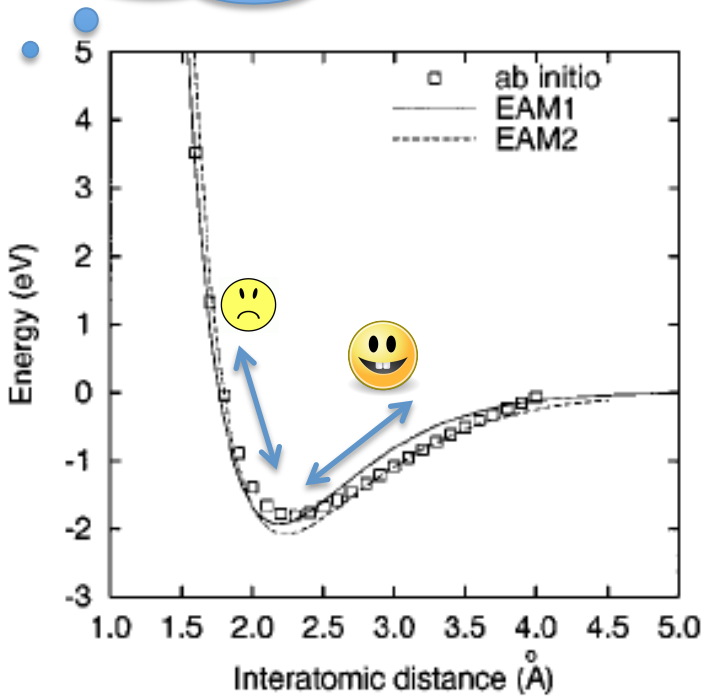
- Set up the correct dislocation system
  - Periodic array of dislocation
- Atomistic calculations
  - DYMOKA package
  - EAM interatomic potential
    - Cu potential from Y. Mishin 2001
      - Stacking fault energy 44 mJ/m²
      - Dilatation volume of vacancy: -0.3Ω; of SIA: 1.8Ω
    - Ni potential from G.Bonny 2011
      - Stacking fault energy 113 mJ/m²
      - Dilatation volume of vacancy: -0.07Ω; of SIA: 1.16Ω
- MATLAB PDE toolbox
  - Finite element method, numerical solutions

Mishin 2001;
Bonny 2011

What? – Interaction energies Cu



Core structures are different!

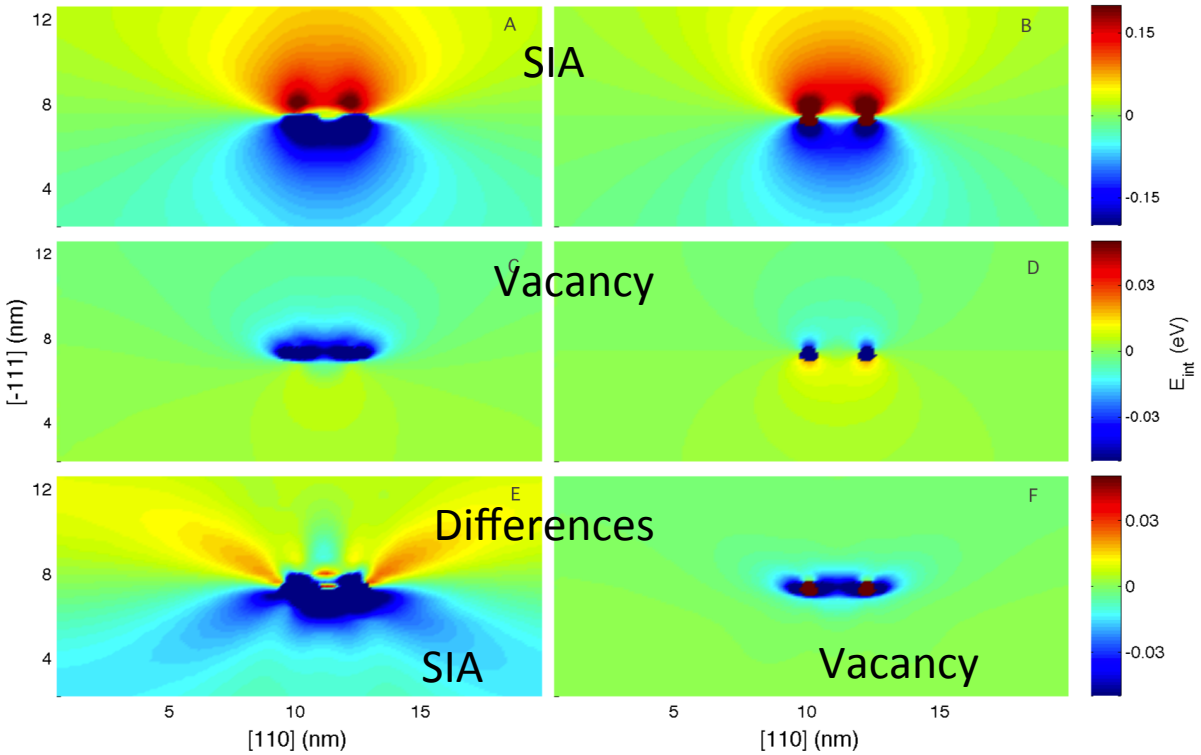


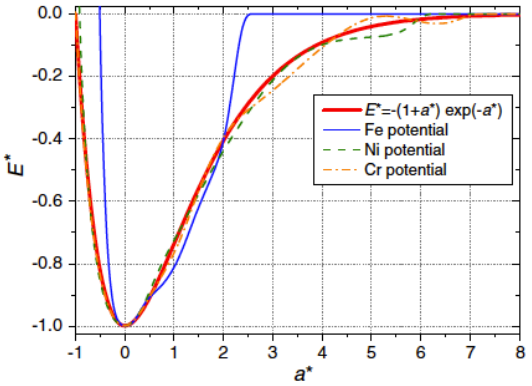
E_{SF}= 44.4 mJ/m^2 ; d=37.6 Å

Anisotropy: 3.22

What? – Interaction energies Ni

Atomistic approach Analytical approach

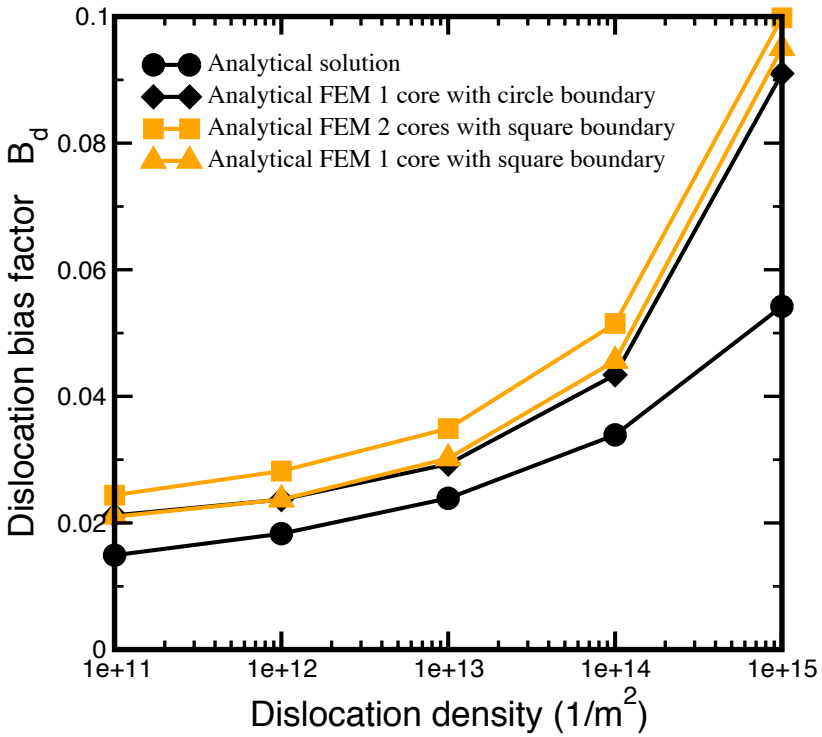




E_{SF}= 113 mJ/m^2
d=22 Å
Anisotropy: 2.5

Anisotropic effects;
Non-linear elasticity;
First order size interaction;

What? – Method analysis



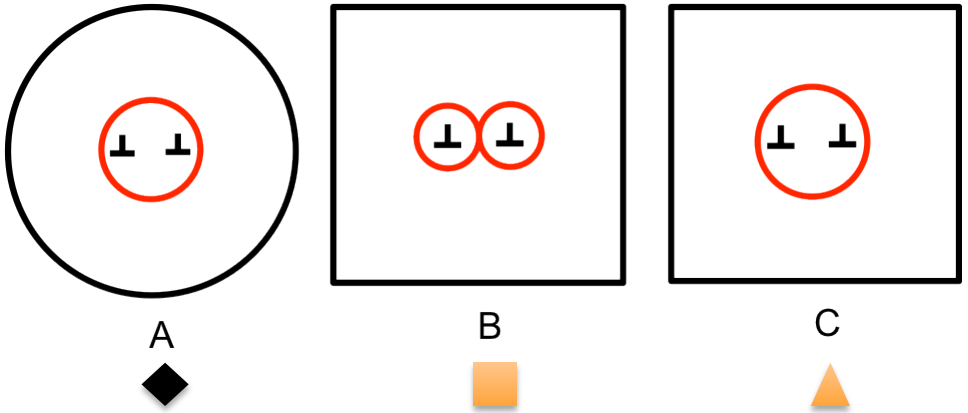
- Analytical solution:

$$Z_{str} = \frac{2\pi I_0(L/2r_0)}{K_0(L/2R_{ext})I_0(L/2r_0) - K_0(L/2r_0)I_0(L/2R_{ext})}$$

- FEM solutions:

$$z = \oint_{core} \frac{j(\vec{r})}{j_0} d\vec{r}$$

- Different configurations:



Heald 1975

What? – Bias factors

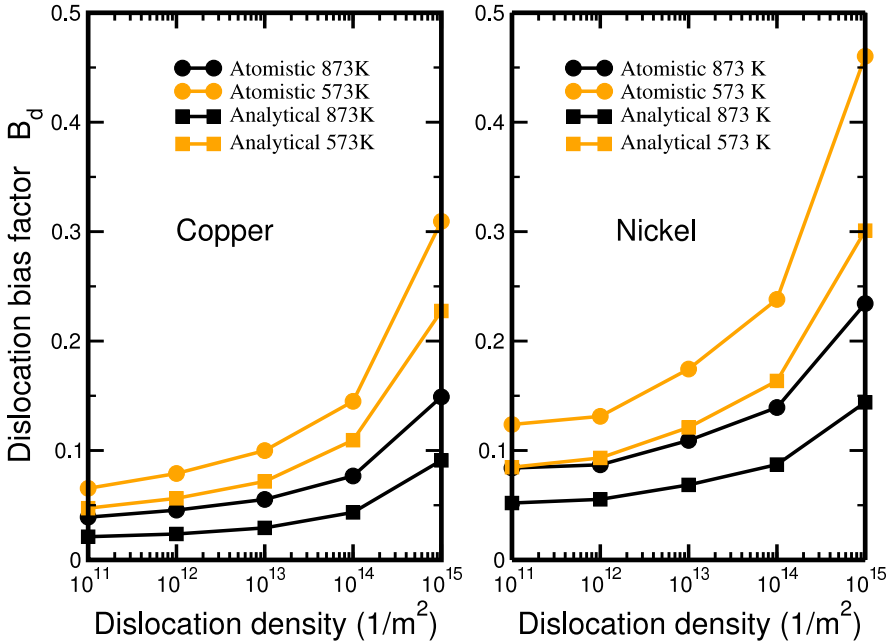
- Cu, Ni @ T=873 K, ρ_d=1.5*10^{15} m^{-2}
- Z_v^d ~ 1.00, Z_i^d determine
- $Bd_{Ni} > Bd_{Cu}$
- $Bd_{atom} > Bd_{analytic}$

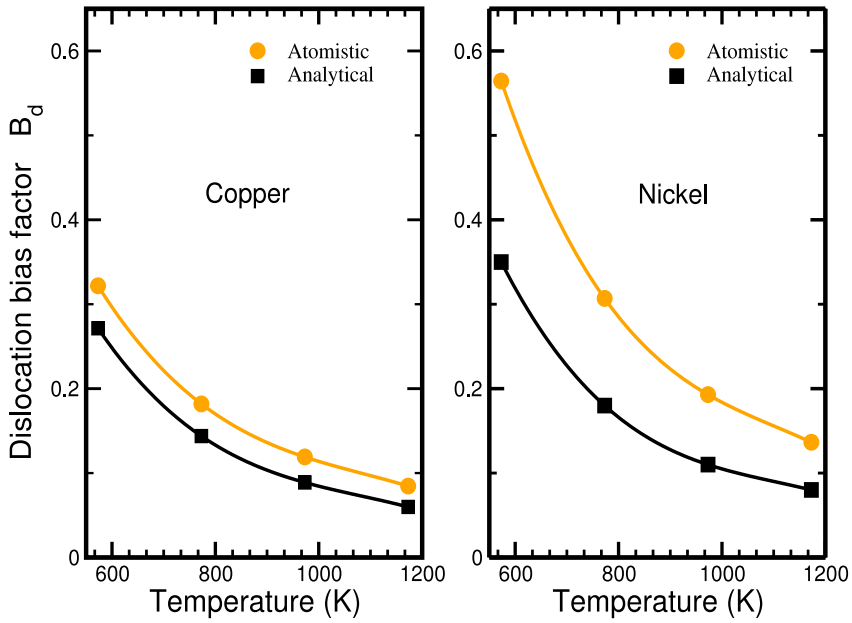
$$B_D = \frac{Z_i - Z_v}{Z_v}$$

@ 873 K, dislocation density =1.5*10^{15} m^{-2}

	Cu			Ni		
	Z_i^d	Z_v^d	B_d	Z_i^d	Z_v^d	B_d
Atomistic	1.16	1.01	0.15	1.28	1.02	0.25
Analytical	1.12	1.00	0.12	1.16	1.00	0.16

What? – Bias factors

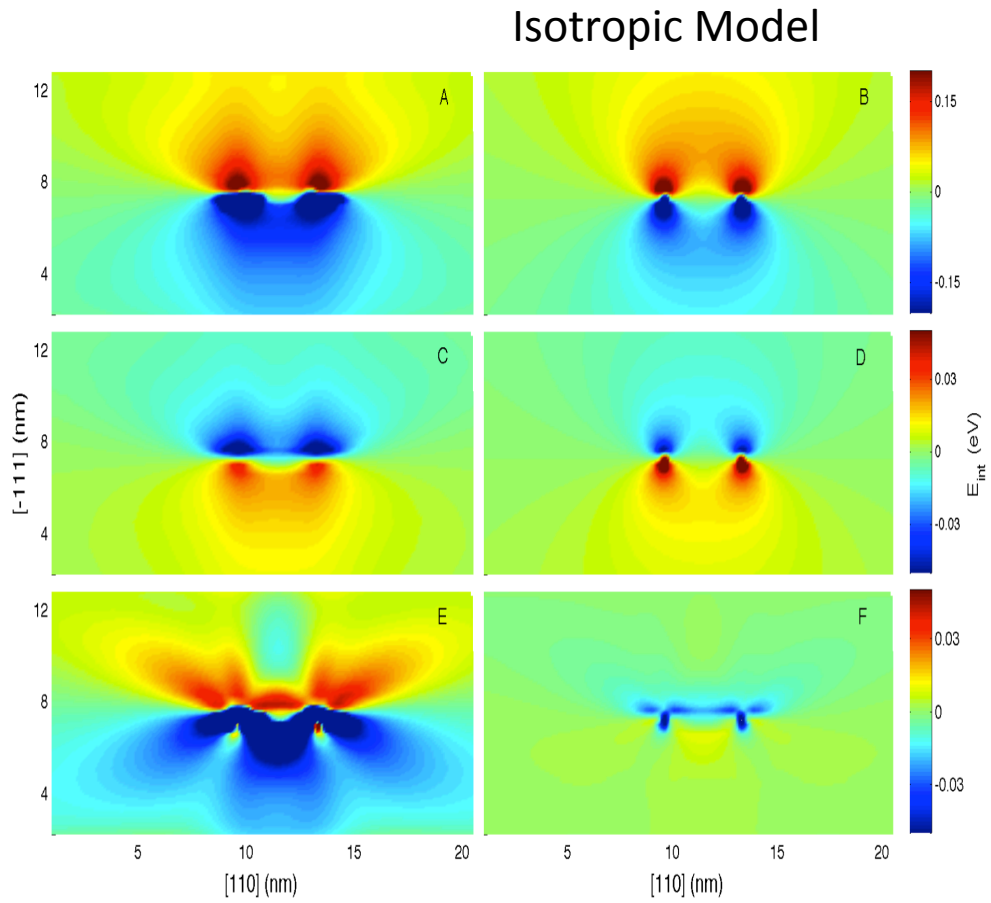


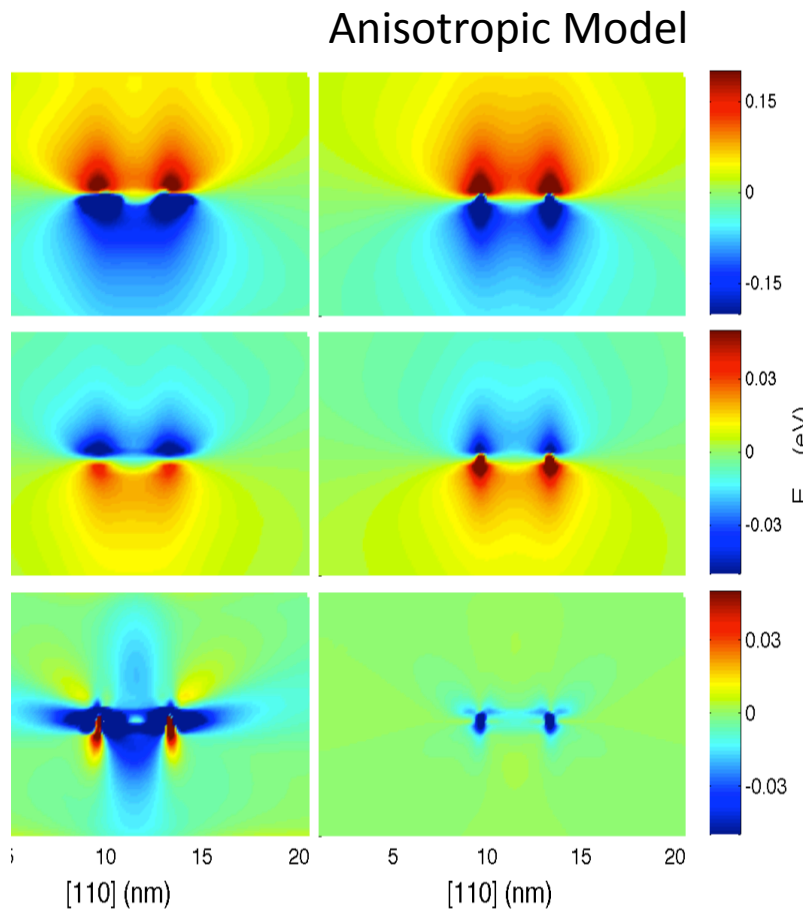


- Density increase, Bd increase;
- Higher T, lower Bd
- $Bd_{Ni} > Bd_{Cu}$
- $Bd_{atomistic} > Bd_{analytic}$

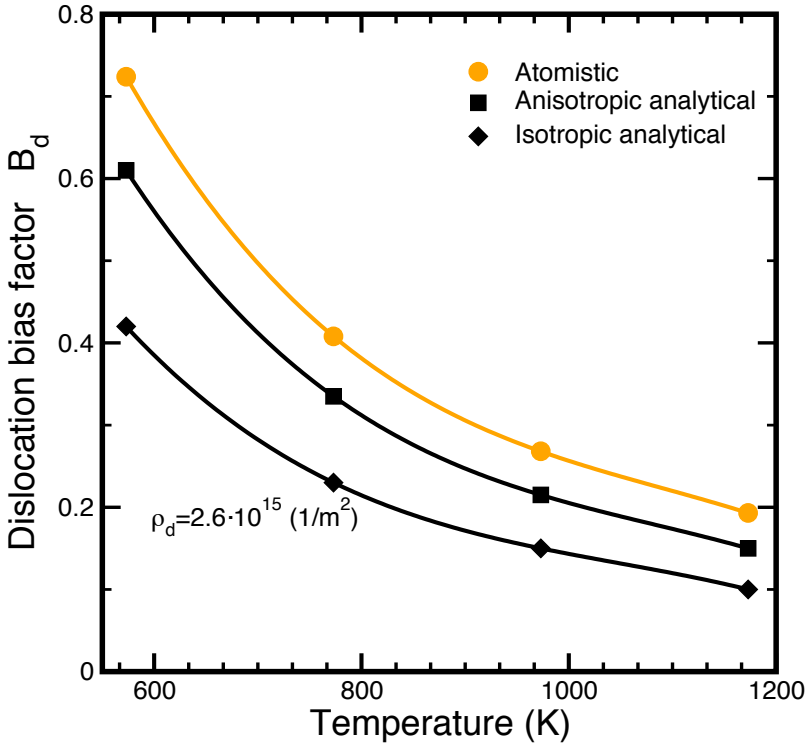
- Low density, high T, atomistic and analytical results tend to converge – Diffusion is dominant.
- High density, low T – core is important.

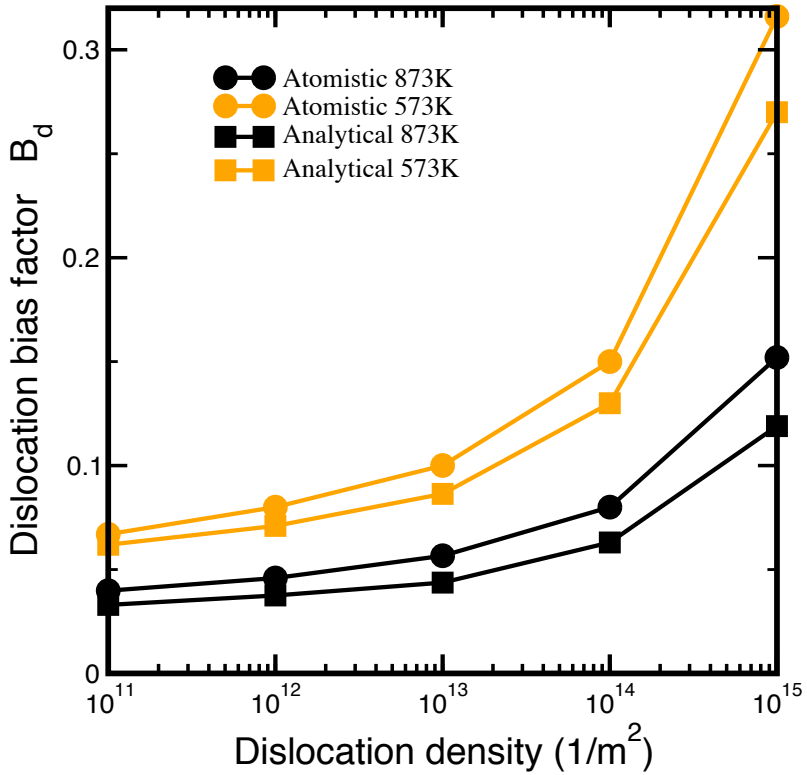
What? – Interaction energies Cu





What? – Anisotropic model in Cu





- Anisotropic contribution in Cu

What? - Comparison

- Cu @ T=520 K, ρ_d=1*10^{11} m^{-2}
- Reference calculation: experimental fitting, void size distribution, transient period.
- Atomistic calculation: FEM numerical calculation, mean void size, steady state.

$$\frac{ds}{d\phi} = k_C^2(D_v C_v - D_i C_i) = B_D \frac{k_C^2 k_{Dv}^2}{(k_C^2 + k_{Dv}^2)(k_C^2 + k_{Di}^2)}$$

Projectile particle	Dose (dpa)	Void density (m^{-3})	Void diameter (nm)	Reference swelling (%)	Calculated swelling (%)
2.5 MeV Electron	0.013	0.2-1.2 *10^{19}	13.8	0.2 - 1 * 10^{-3}	5.8 * 10^{-3}
3 MeV Proton	0.002	9.2*10^{19}	3.9	2.8 * 10^{-4}	5.1 * 10^{-4}
3 MeV Proton	0.008	1.3*10^{20}	6.5	1.9 * 10^{-3}	0.91 * 10^{-3}

Singh 2000

Conclusions

- Atomistic calculation of interaction energy combined with FEM numerical solvation to obtain $B_{d.}$
- SIA has higher interaction energy with dislocation than vacancy, the difference is more significant in atomistic approach than in analytical approach.
- In low T and high dislocation density region, atomic description of dislocation core is in need.
- Atomistic approach predict higher dislocation bias than elasticity theory.
- Anisotropic effect is important.
- Ni is predicted to have larger swelling rate than Cu.
- Bd >> 2%, not reconcile with the common presumption that dislocation bias is the main driving force for swelling in electron irradiation conditions.

Thank you!