

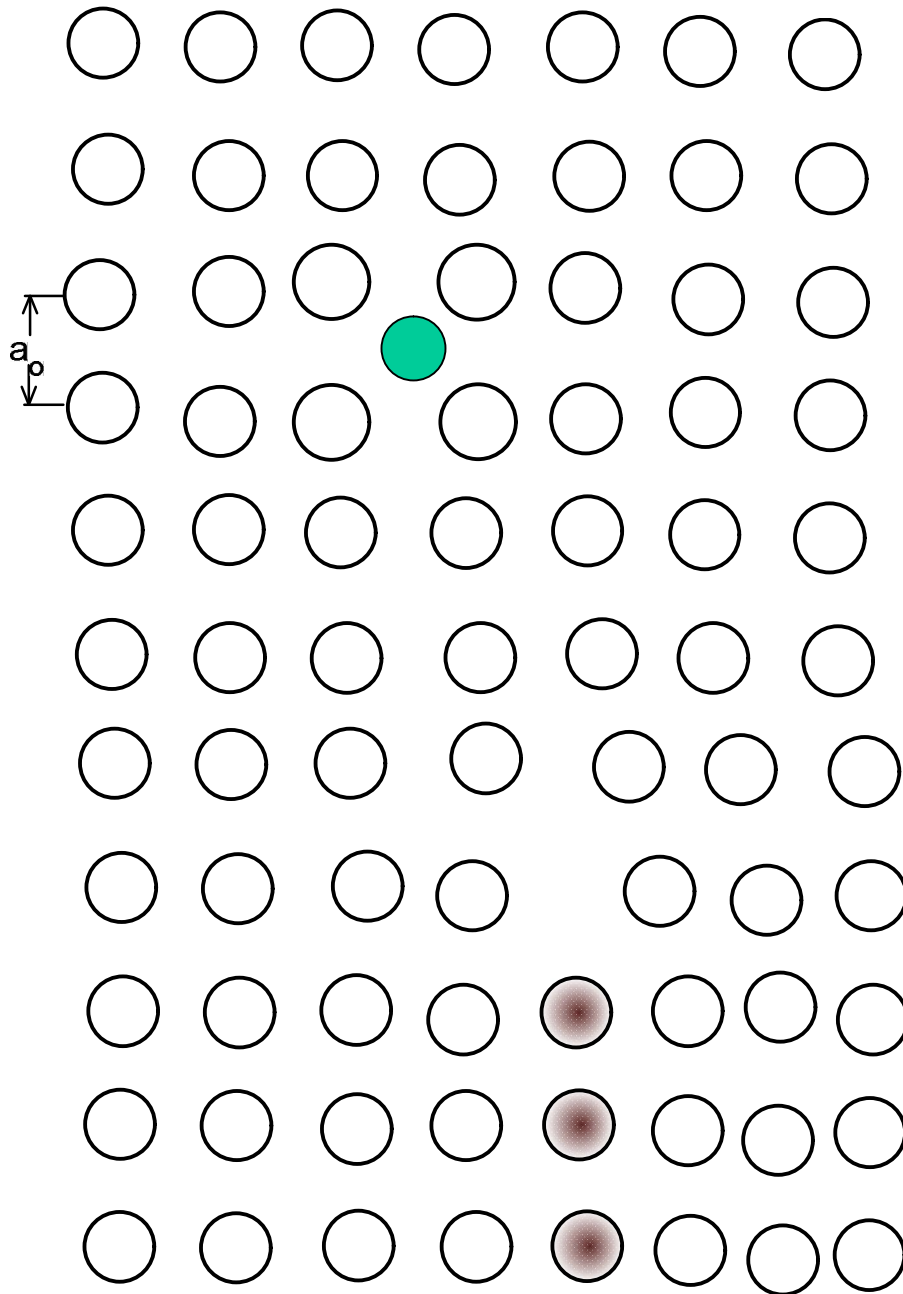
NE 220 Spring 2008

Term Project

(in lieu of a final exam)

Presentations during the last
week of class

Homework load will be
reduced to permit work on the
project



Conventional handling of the Edge dislocation - self-interstitial interaction

- The interstitial is represented as a rigid sphere inserted into a hole of atomic size in the elastic solid. The initial radius of the hole is $R_0 \sim \Omega^{1/3}$
- insertion of the interstitial increases the radius to: $R = (1+\varepsilon)R_0$
- The volume change (for $\varepsilon \ll 1$) is:

$$\Delta V = \frac{4}{3} \pi [(1+\varepsilon)^3 R_0^3 - R_0^3] \cong 4\pi R_0^3 \varepsilon$$

- this expansion does “pdV” work against the hydrostatic component of the stress field of the edge dislocation, which, from (8) of Sect. 3 is:

$$\sigma_h = \frac{1}{3} (\sigma_{rr} + \sigma_{\theta\theta} + \sigma_{zz}) = -\frac{Gb}{3\pi} \left(\frac{1+\nu}{1-\nu} \right) \frac{\sin\theta}{r}$$

The work done in inserting the interstitial increases system energy (1st Law):

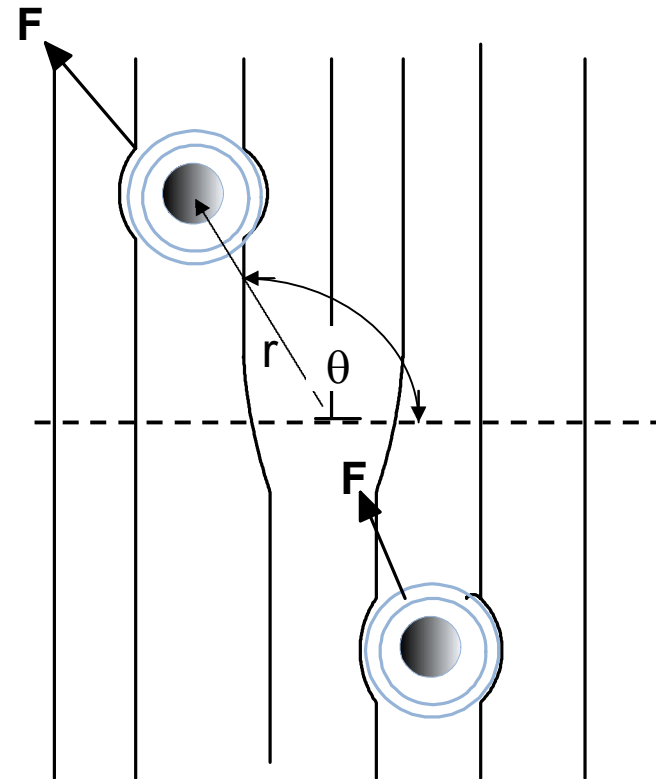
$$E_i = -\sigma_h \Delta V$$

- combining the above equations yields:

$$E_i = \frac{4}{3} \left(\frac{1+\nu}{1-\nu} \right) G \times b \times \varepsilon \times R_o^3 \frac{\sin \theta}{r} \quad (10)$$

- an interstitial in the upper half space of the dislocation is repelled :
 (compressive <-> compressive) $F = -dE_i/dr > 0$

-Below the half-plane of the dislocation the interaction is attractive:
 (tensile + compressive) $F = -dE_i/dr < 0$
(and much stronger than for a vacancy).



- The diffusion equation for the interstitial in the unit cell of the dislocation (sl.4) is solved accounting for the body force exerted by the force F

- To simplify the calculation, the force is assumed cylindrically symmetric by setting $\sin\theta = -1$ in (10) and combining the properties into a single constant, B :

$$E_i = -\frac{B}{r} \quad \text{or} \quad F_i = -\frac{dE_i}{dr} = -\frac{B}{r^2} \quad (11)$$

- F imparts an inward drift velocity to the interstitial: $v_{\text{drift}} = MF_i$, where, by the Nernst-Einstein formula, $M = D_i/kT$ is the mobility of the interstitial. (see text Chap 13, p 238).

- Fick's law is supplemented by the drift velocity term:

$$j_i = -D_i \frac{dC_i}{dr} + C_i v_{\text{drift}} = -D_i \frac{dC_i}{dr} + C_i \frac{D_i}{kT} F_i$$

- The conservation equation for interstitials in the unit cell is:

(as with cavities,
no source term)

$$\frac{1}{r} \frac{d}{dr} (r j_i) = 0$$

substituting j_i into the above equation and using (11) for the force:

$$\frac{d}{dr} \left(r \frac{dC}{dr} \right) - \frac{B}{kT} \left(\frac{C}{r^2} - \frac{1}{r} \frac{dC}{dr} \right) = 0$$

- The boundary conditions and the solution method are the same as those for the vacancy - dislocation in (8) but instead of (8a), Z_i is given by:

$$Z_i = 2\pi \left[\int_{r_0}^{\mathfrak{R}} \exp\left(-\frac{B/kT}{r}\right) \frac{dr}{r} \right]^{-1} \approx 2\pi \left[\ln\left(\frac{\mathfrak{R}}{r_0}\right) - \frac{B/kT}{r_0} \right]^{-1} \approx \frac{2\pi}{\ln(\mathfrak{R}/r_0)} \left[1 + \frac{B/r_0 kT}{\ln(\mathfrak{R}/r_0)} \right]$$

where the integral in the above has been approximated using $B/kT \ll r_0$ (i.e., weak interaction) and $\mathfrak{R} \gg r_0$,

- the coefficient of the bracketed term of the above equation is Z_v (8a), so the *bias factor* for the dislocation to absorb interstitials is:

$$\frac{Z_i - Z_v}{Z_v} = \frac{B/r_0 kT}{\ln(\mathfrak{R}/r_0)} \quad (12)$$

which ranges from 0.02 to 0.05 – however, this small difference has profound consequences on the effect of radiation on metal microstructures

Overall objective of the present analysis: to remove the empiricism from the calculation of the interaction between point defects (V and I) and edge dislocations

4 teams:

- *atomistic/Monte Carlo* – Local strain around point defect; pairwise interaction potential; energy minimization (V team and I team)
- *Elasticity theory* – longer-range stress field around point defects; combine with stress field of edge dislocation to give elastic strain energy between the two defects; compare bias factors for V and I
- *Diffusion analysis* with the *angular variation* of the stress around an edge dislocation accounted for

Teams 1 & 2

- represent the lattice, 2-D, simple cubic structure
 - an interstitial with 5 surrounding shells (next slide)
 - a vacancy with 6 surrounding shells (sl 10)
- Use an interatomic potential consisting of the Born-Mayer function for the repulsive part and a r^{-6} function for the attractive portion:

$$V(r) = Ae^{-r/\rho} - B/r^6$$

- choose shell radii to minimize the total energy of all pair-wise interactions
- this determines the volume change of the solid around the point defect (i.e., strains)

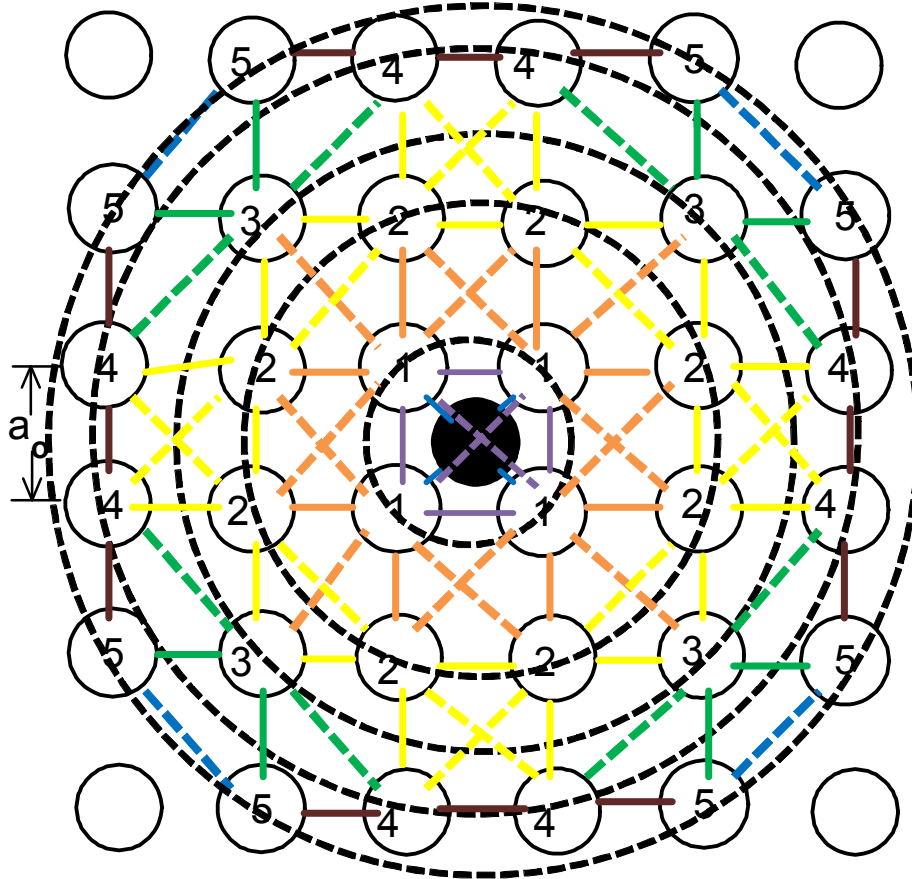
- Identify the circles representing the 1st through 5th nearest neighbors to the point defect (R_1, \dots, R_5)
- Determine the coefficient B in $V(r)$ from the lattice spacing a_0
- Use only dimensionless quantities (e.g., V/A ; r/a_0)

$$\frac{V}{A} = \exp\left(-\frac{r/a_0}{\rho/a_0}\right) - \frac{(B/Aa_0^6)}{(r/a_0)^6} \leftarrow \text{How to determine?}$$

Henceforth, V/A will be denoted by V and the $/a_0$ omitted from all distances

- d_{ij} = distance between nearest-neighbor atoms i and j
- d_{ij} = distance between next-nearest neighbors i and j

(express d_{ij} and d_{ij} in terms of R_1, \dots, R_5)

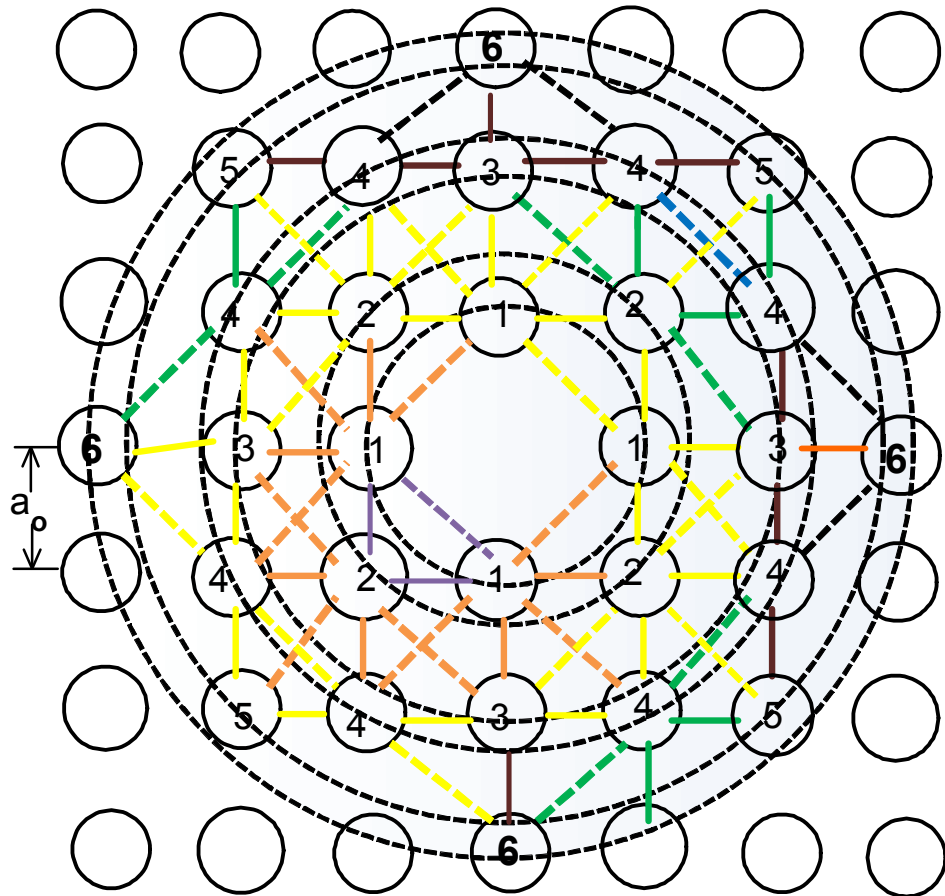


solid lines: nearest neighbors
dashed lines: next-nearest neighbors

Shell No.(k)	R_k^o / a_o	No. of atoms
1	$\sqrt{1} / \sqrt{2}$	4
2	$\sqrt{5} / \sqrt{2}$	8
3	$\sqrt{9} / \sqrt{2}$	4
4	$\sqrt{13} / \sqrt{2}$	8
5	$\sqrt{17} / \sqrt{2}$	8

Interstitial

bond	01	11	11'	12	12'	13'	22	22'	23	24	24'	34'	35	44	45	55'
n_{ij}	4	4	2	8	8	4	4	4	8	8	8	8	8	4	8	4



solid lines: nearest neighbors
dashed lines: next-nearest neighbors

Vacancy

Monte Carlo method

rn = random number between 0 and 1 (different for each k)

$$R_k = R_k^0 + rn \times \Delta R_k$$

ΔR_k = dimensionless interval over which radius of k^{th} shell is varied (> 0 for I; < 0 for V)

Vary rns until:
is a minimum.

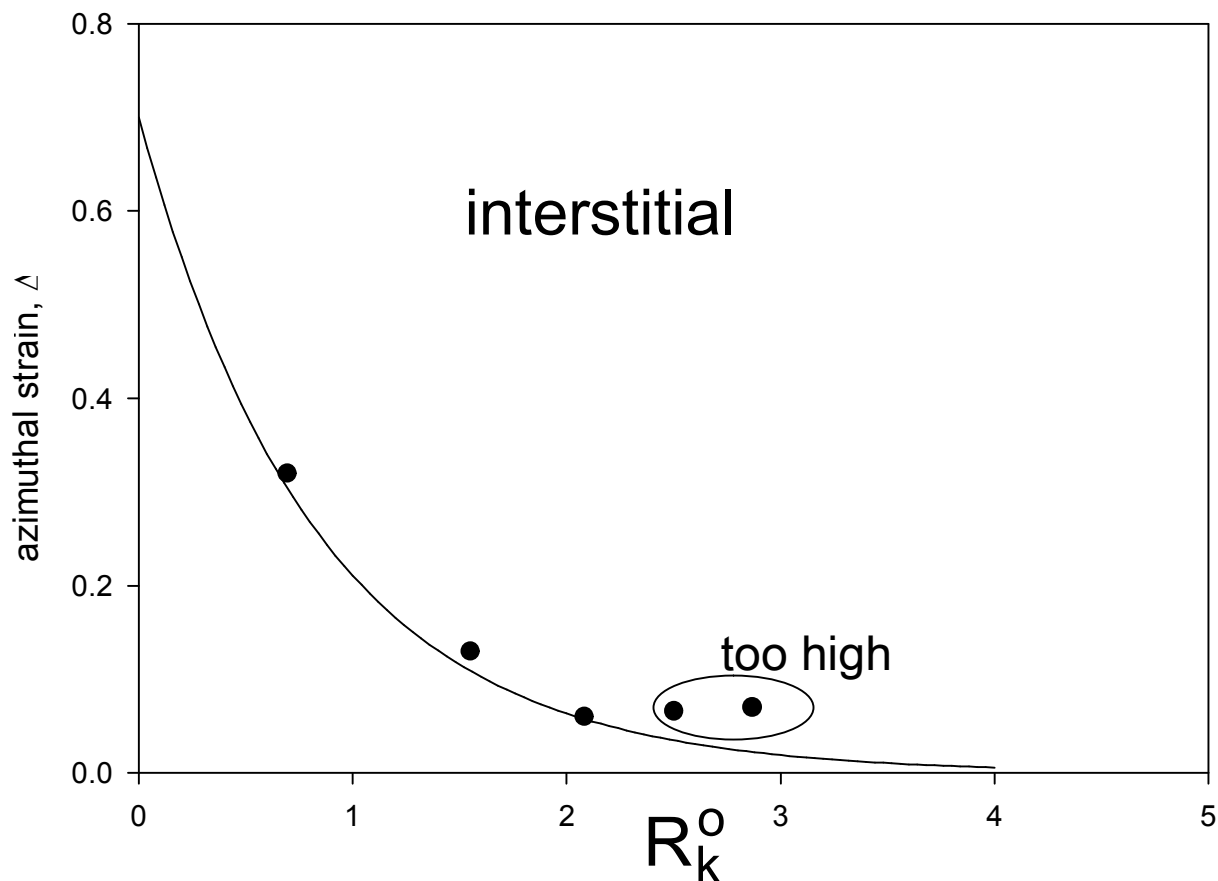
$$E_{\text{tot}} = \sum n_{ij} V(d_{ij})$$

Case 1: Without a point defect (perfect lattice): at the minimum energy configuration: - all distances should be 1 or $\sqrt{2}$
- all shell radii should be R_k^0

- verifies the accuracy of the Monte Carlo method
- provides the reference radii for subsequent calc. of strains

Case 2: With a point defect; select $R_1 \dots R_5$ that minimizes E_{tot} , then calculate strains:

$$\varepsilon_k = \frac{R_k - R_k^0}{R_k^0}$$



R_4 & R_5 are relaxed (ε_4 & ε_5 too large) because restraint due to of atoms outside of shell 5 has been neglected 13

- to represent the missing atoms at shells > 5 , R_5 is reduced (and E_{tot} minimized) until $\varepsilon_1 \dots \varepsilon_5$ form a single monotonically-decreasing curve
- Decreasing R_5 from the restraint-free value (R'_5) requires application of a radial stress σ_r^{ext}
- σ_r^{ext} is computed assuming a 2-D compressibility which responds to the applied radial stress according to:

$$\frac{\Delta A}{A} = \frac{R'^2_5 - R^2_5}{R'^2_5} = \beta \times \sigma_r^{\text{ext}}$$

(use β for Cu)

- σ_r^{ext} becomes the boundary condition for the elastic analysis at $r > R_5$

Elastic Analysis

Objective: to use elasticity theory to determine the stress in the solid for $r > R_5$

$$r \left(\frac{d\sigma_r}{dr} \right) + (\sigma_r - \sigma_\theta) = 0$$

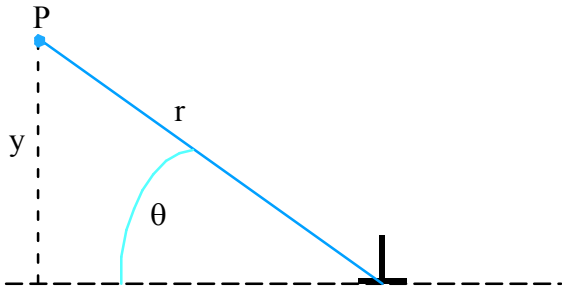
$$\varepsilon_\theta = u/r \quad \varepsilon_r = du/dr$$

$$\varepsilon_r = \frac{1}{E} (\sigma_r - \nu \sigma_\theta) + (\varepsilon_r)_{\text{point defect}} \quad (?)$$

$$\varepsilon_\theta = \frac{1}{E} [\sigma_\theta - \nu \sigma_r] + (\varepsilon_\theta)_{\text{point defect}} \quad (?)$$

Solve for stresses as functions of r using σ_r^{ext} as the bc at $r = R_5$

Stresses in solid around the edge dislocation



$$\sigma_r = \sigma_\theta = -\alpha \frac{\sin \theta}{r};$$

$$\sigma_{r\theta} = \sigma_{\theta r} = -\alpha \frac{\cos \theta}{r}$$

$$\alpha = \frac{Gb}{2\pi(1-\nu)}$$

Add stresses: $\sigma_j = (\sigma_j)_{\text{point defect}} + (\sigma_j)_{\text{dislocation}}$

the r coordinate of $(\sigma_j)_{\text{point defect}}$ must be converted to the r, θ coordinates of the dislocation

Interaction energy (text, p. 601)

$$E_i = \frac{1}{2E} (\sigma_r^2 + \sigma_\theta^2) - \frac{\nu}{E} \sigma_r \sigma_\theta + \frac{1}{2G} \sigma_{r\theta}^2$$

(G = shear modulus) – the above replaces (10) on sl. 4

Because of $\sin \theta$ and $\cos \theta$ terms in $(\sigma_j)_{\text{dislocation}}$, $E_i(r, \theta)$ has a complicated angular dependence

Diffusion analysis

Generalized point-defect flux equation:

$$\vec{J} = -D\nabla C - D\frac{C}{kT}\nabla E_i \quad \text{or} \quad \vec{J} = -D\nabla C - DQC\nabla E_i$$

where Q is a dimensionless parameter:

$Q = A/kT$, A = coefficient of Born-Mayer potential function

E_i is made dimensionless by dividing by A

$$\nabla C = \frac{\partial C}{\partial r}\vec{u}_r + \frac{1}{r}\frac{\partial C}{\partial \theta}\vec{u}_\theta \quad \nabla E_i = \frac{\partial E_i}{\partial r}\vec{u}_r + \frac{1}{r}\frac{\partial E_i}{\partial \theta}\vec{u}_\theta$$

$\vec{u}_r, \vec{u}_\theta =$ unit vectors

Coordinate origin at dislocation

