Local Lattice Instability at Mode I Crack Tip: Emergence of High Stiffness Zone in Si

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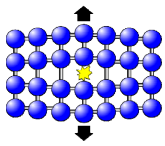
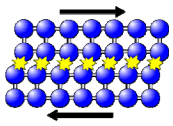
Local lattice instability analysis

Original concept: bond-breaking and re-bonding necessarily happens in inelastic deformation



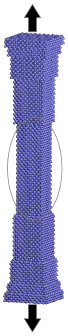
Cleavage cracking



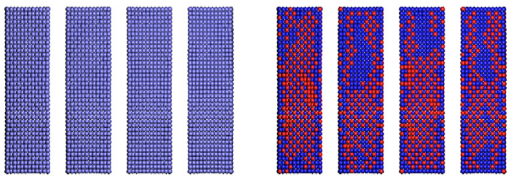
Slip deformation

Discuss local deformation by "local lattice instability" in MD simulation

Example: deformation process of Ni nanospecimen



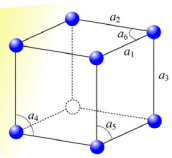
Movie: deformation process of four surface from perfect crystal to disordered one by slip



left: atom motion
right: colored by "local lattice instability", blue is stable, red unstable

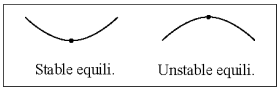
Born's stability criteria for perfect lattice

Discuss crystal stability by the positivity of Hessian, explicitly counting the interatomic potential assuming ideal uniform lattices in continuum body



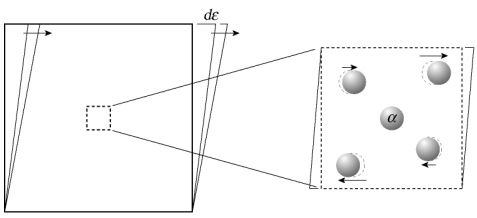
$$\left.\frac{\partial^2 U}{\partial a_i \partial a_j}\right|_{\{a_i\}} > 0 \quad \text{Stable}$$

$$\left.\frac{\partial^2 U}{\partial a_i \partial a_j}\right|_{\{a_i\}} < 0 \quad \text{Unstable}$$



Max Born (1882-1970)

Instability analysis by elastic stiffness coefficients



Elastic stiffness coefficients for whole the system

$$B_{ijkl} = \frac{\partial \sigma_{ij}}{\partial \varepsilon_{ij}}$$

Stability criteria for whole crystal (Wang 1993)

Elastic stiffness coefficients for an atom

$$B^{\alpha}_{ijkl} = \frac{\partial \sigma^{\alpha}_{ij}}{\partial \varepsilon_{ij}}$$

Local stability at each atom point (Yashiro 2001)

Stress, elastic coefficients, elastic stiffness coefficients

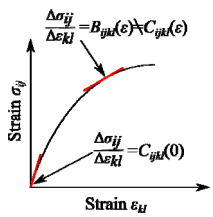
Elastic stiffness can be evaluated with the stress and elastic coefficients

$$B_{ijkl} = \frac{\Delta \sigma_{ij}}{\Delta \varepsilon_{kl}} = C_{ijkl} + (\sigma_{il}\delta_{jk} + \sigma_{jl}\delta_{ik} + \sigma_{ik}\delta_{jl} + \sigma_{jk}\delta_{il} - \sigma_{ij}\delta_{kl} - \sigma_{kl}\delta_{ij})/2$$

Stress and elastic coefficients are defined as 1st and 2nd order derivatives of internal energy

$$\sigma_{ij} = \frac{1}{V}\frac{\partial U}{\partial \varepsilon_{ij}}$$

$$C_{ijkl} = \frac{1}{V}\frac{\partial^2 U}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}}$$



Atomic stress and elastic coefficients in Tersoff potential

In the Tersoff potential, energy contribution of atom α is expressed as

$$E^{\alpha} = \sum_{\beta \neq \alpha} \frac{1}{2} \left\{ f_R(r^{\alpha\beta}) + b^{\alpha\beta} f_A(r^{\alpha\beta}) \right\}$$

Thus we can define atomic stress and atomic elastic coefficients as

$$\sigma^{\alpha}_{ij} \equiv \frac{1}{\Omega} \frac{\partial E^{\alpha}}{\partial \varepsilon_{ij}} = \sum_{\beta \neq \alpha} \left\{ \left[f'_R(r^{\alpha\beta}) + b^{\alpha\beta} f'_A(r^{\alpha\beta}) \right] \frac{r^{\alpha\beta}_i r^{\alpha\beta}_j}{r^{\alpha\beta}} + \boxed{\frac{\partial b^{\alpha\beta}}{\partial \varepsilon_{ij}}} f_A(r^{\alpha\beta}) \right\} / 2\Omega$$

$$C^{\alpha}_{ijkl} \equiv \frac{1}{\Omega} \frac{\partial^2 E^{\alpha}}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} = \sum_{\beta \neq \alpha} \left\{ \left[f''_R(r^{\alpha\beta}) + b^{\alpha\beta} f''_A(r^{\alpha\beta}) - \frac{f'_R(r^{\alpha\beta}) + b^{\alpha\beta} f'_A(r^{\alpha\beta})}{r^{\alpha\beta}} \right] \frac{r^{\alpha\beta}_i r^{\alpha\beta}_j r^{\alpha\beta}_k r^{\alpha\beta}_l}{(r^{\alpha\beta})^2} \right.$$
$$\left. + \boxed{\frac{\partial b^{\alpha\beta}}{\partial \varepsilon_{kl}}} f'_A(r^{\alpha\beta}) \frac{r^{\alpha\beta}_i r^{\alpha\beta}_j}{r^{\alpha\beta}} + \boxed{\frac{\partial b^{\alpha\beta}}{\partial \varepsilon_{ij}}} f'_A(r^{\alpha\beta}) \frac{r^{\alpha\beta}_k r^{\alpha\beta}_l}{r^{\alpha\beta}} + \boxed{\frac{\partial^2 b^{\alpha\beta}}{\partial \varepsilon_{kl} \partial \varepsilon_{ij}}} f_A(r^{\alpha\beta}) \right\} / 2\Omega$$

On the derivatives for three body bond order term, please see
Yashiro, Com. Mat. Sci. 112 (2016) 120–127
(for 1988 Tersoff potential, however, 1989 Tersoff is rather simple so that
I would like to recommend the later version)

Atomic elastic stiffness and eigenvalue analysis

Taking the Voigt symmetry into account, we represents the atomic elastic stiffness with 6x6 matrix B^{α}_{ij} instead of 4th tensor B^{α}_{ijkl}

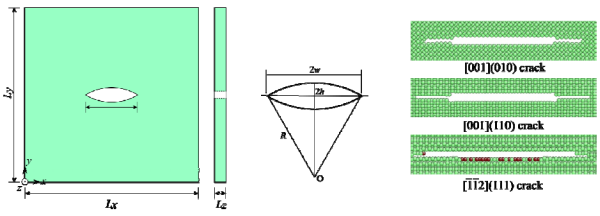
$$[B^{\alpha}_{ij}] = \begin{vmatrix} C^{\alpha}_{11} + \sigma^{\alpha}_1 & C^{\alpha}_{12} - (\sigma^{\alpha}_1 + \sigma^{\alpha}_2)/2 & C^{\alpha}_{13} - (\sigma^{\alpha}_1 + \sigma^{\alpha}_3)/2 & C^{\alpha}_{14} - \sigma^{\alpha}_4/2 & C^{\alpha}_{15} + \sigma^{\alpha}_5/2 & C^{\alpha}_{16} + \sigma^{\alpha}_6/2 \\ & C^{\alpha}_{22} + \sigma^{\alpha}_2 & C^{\alpha}_{23} - (\sigma^{\alpha}_2 + \sigma^{\alpha}_3)/2 & C^{\alpha}_{24} + \sigma^{\alpha}_4/2 & C^{\alpha}_{25} - \sigma^{\alpha}_5/2 & C^{\alpha}_{26} + \sigma^{\alpha}_6/2 \\ & & C^{\alpha}_{33} + \sigma^{\alpha}_3 & C^{\alpha}_{34} + \sigma^{\alpha}_4/2 & C^{\alpha}_{35} + \sigma^{\alpha}_5/2 & C^{\alpha}_{36} - \sigma^{\alpha}_6/2 \\ & & & C^{\alpha}_{44} + (\sigma^{\alpha}_2 + \sigma^{\alpha}_3)/2 & C^{\alpha}_{45} + \sigma^{\alpha}_6/2 & C^{\alpha}_{46} + \sigma^{\alpha}_5/2 \\ & \text{sym.} & & & C^{\alpha}_{55} + (\sigma^{\alpha}_3 + \sigma^{\alpha}_1)/2 & C^{\alpha}_{56} + \sigma^{\alpha}_4/2 \\ & & & & & C^{\alpha}_{66} + (\sigma^{\alpha}_1 + \sigma^{\alpha}_2)/2 \end{vmatrix}$$

Negative eigenvalue implies the existence of unstable deformation path

$$\Delta\sigma^{\alpha}_i = B^{\alpha}_{ij} \Delta\varepsilon_j = \eta^{\alpha} \Delta\varepsilon_i$$

We evaluate all the eigenvalue and eigenvector at each atom point
by using LAPACK math library

Tensile simulation of center crack in Si

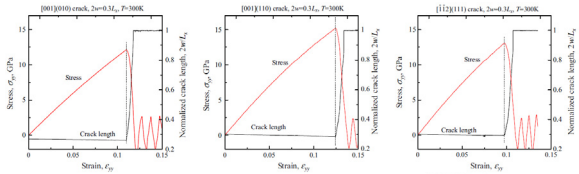


(a) simulation cell (b) dimensions of crack (c) atom configuration around crack after relaxation

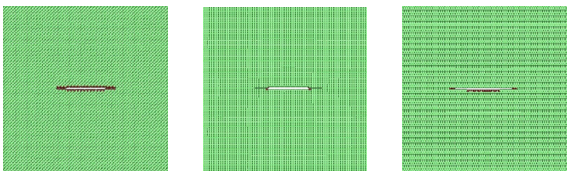
Simulation conditions
Potential function: Tersoff
Periodic boundary condition
Tempterature: 300K
Tensile speed: $\varepsilon_{yy} = 1.0 \times 10^{-6}$/fs

crack width: 0.3Lx
10000fs initial relaxation
Number of atoms: about 120,000

Stress strain curves and movie of crack propagation

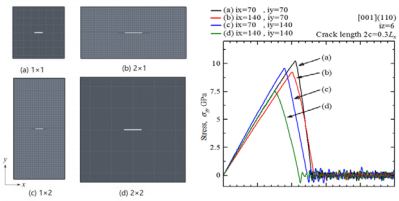


(a) [001](010) crack (b) [001](110) crack (c)[$\bar{1}\bar{1}$2](111) crack



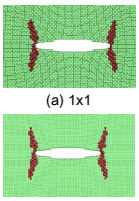
Red atom: negative 1st eigenvalue

Results in bcc-Fe ([001](110) crack)



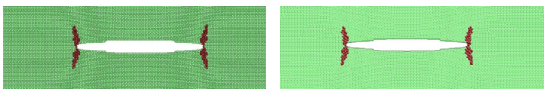
Change the cell size
(different crack array)

Different max. strain



(a) 1x1

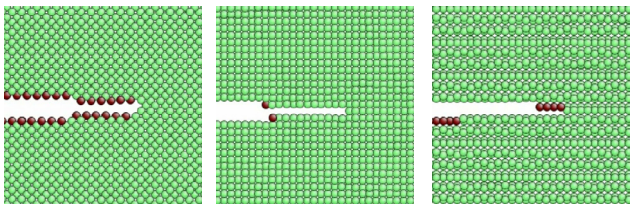
(b) 1x2



(c) 2x1 (d) 2x2

Same distribution of unstable atoms before crack propagation

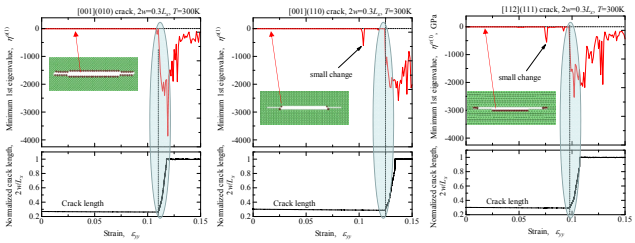
Magnified view of the crack tip



[001](010) [001](110) [$\bar{1}\bar{1}$2](111)

Movies are made with position data at every 1000fs
Unstable domain is relatively small even at the crack propagation

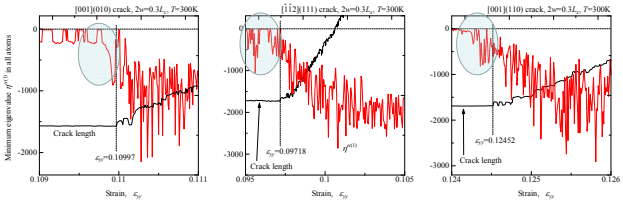
Change in the minimum eigenvalue and crack length



The minimum eigenvalue is selected from all the atom for each time step
The eigenvalue and crack length are evaluated at every 1000fs position data ($\Delta\varepsilon_{yy}$=0.001)

- surface "negative" eigenvalues are almost zero

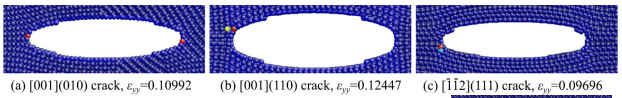
Detail change just at the unstable propagation



The eigenvalue and crack length are evaluated at every 10fs position data ($\Delta\varepsilon_{yy}$=0.00001)

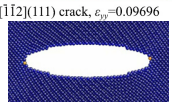
- large negative eigenvalue emerges before crack propagation

Position of large negative eigenvalue and eigenvector



(a) [001](010) crack, ε_{yy}=0.10992 (b) [001](110) crack, ε_{yy}=0.12447 (c) [1̄1̄2](111) crack, ε_{yy}=0.09696

Warm color atoms have large negative eigenvalue
They are symmetrically located at crack tip

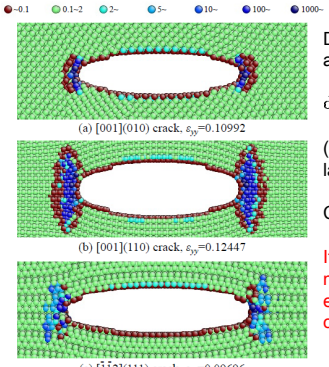


■components of eigenvector

	$\varepsilon_1(\varepsilon_{xx})$	$\varepsilon_2(\varepsilon_{yy})$	$\varepsilon_3(\varepsilon_{zz})$	$\varepsilon_4(\varepsilon_{yz})$	$\varepsilon_5(\varepsilon_{zx})$	$\varepsilon_6(\varepsilon_{xy})$
[001](010)	-0.56	0.69	-0.12	0.41	-0.05	0.13
[001](110)	-0.59	-0.50	0.40	0.40	-0.03	0.25
[112](111)	0.30	-0.55	-0.35	-0.09	0.61	-0.33

The largest components suggest
[001](010) crack is mode I (yy), [001](110) mode II (xx)
and [112](111) mode III (zx)

High stable area at crack tip



(a) [001](010) crack, ε_{yy}=0.10992
(b) [001](110) crack, ε_{yy}=0.12447
(c) [1̄1̄2](111) crack, ε_{yy}=0.09696

Determinant of 6x6 matrix of atomic elastic stiffness

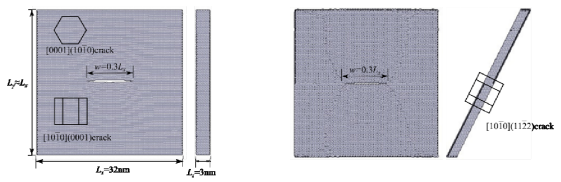
$$\det B^{\alpha}_{ij}(=\eta^{\alpha(1)}\eta^{\alpha(2)}\eta^{\alpha(3)}\eta^{\alpha(4)}\eta^{\alpha(5)}\eta^{\alpha(6)})$$

(Normalized by that in perfect lattice, i.e. $\det B^{\alpha}_{ij}=1$ in bulk)

Cold color: high stable atom

It is never seen in Fe, and may prevent dislocation emission and give brittle character to Si?

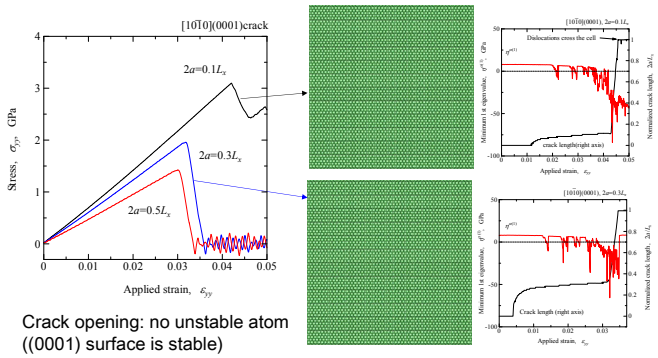
Recent application: Ideal crack in Mg



(a) periodic cell in Cartesian coordinate (b) periodic cell in non-Cartesian coordinate

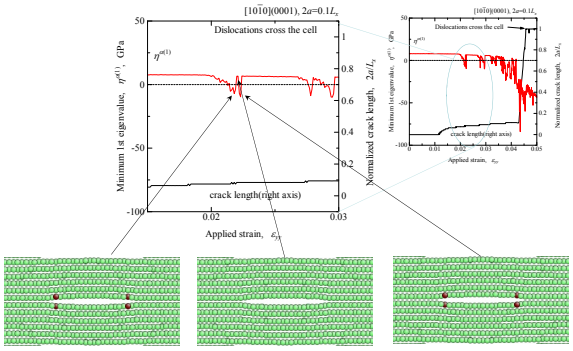
Simulation conditions
Potential function: EAM (Liu, 1996) crack width: 0.1Lx, 0.3Lx, 0.5Lx
Periodic boundary condition Ideal crack: virtual force shield
Temperature: 0.1K Number of atoms: about 120,000~130,000
Tensile speed: $\Delta\varepsilon_{yy}=1.0\times10^{-7}/\mathrm{fs}$

Results in the basal plane crack



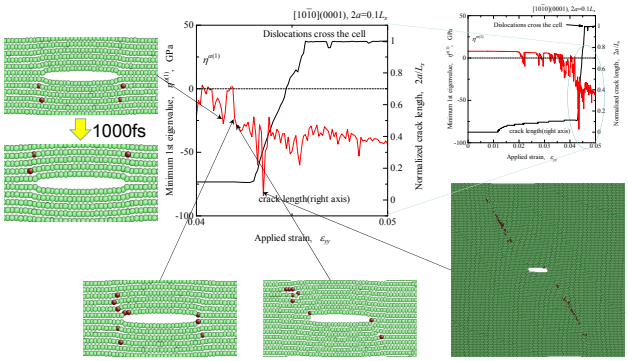
Crack opening: no unstable atom
((0001) surface is stable)
Dislocation emission and crack propagation:
burst of unstable atoms

Early stage in the crack tip instability (basal plane crack, 0.1Lx)

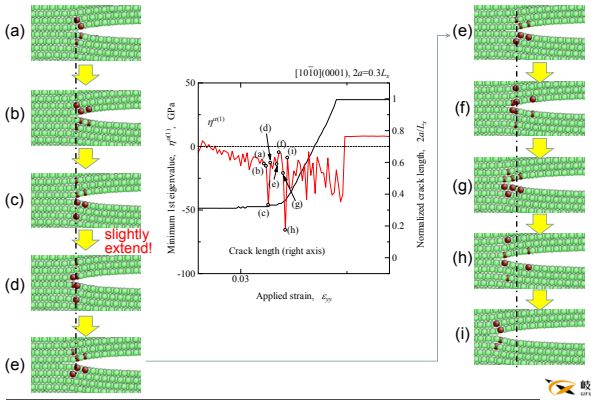


Symmetrical distribution in the negative atom lines

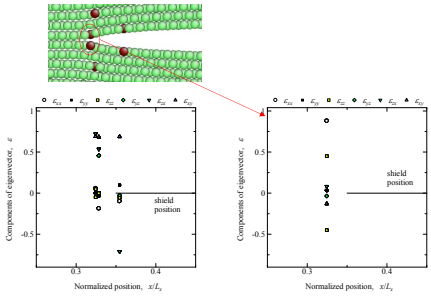
Dislocation emission process (basal plane crack, 0.1Lx)



Crack propagation process (basal plane crack, 0.3Lx)



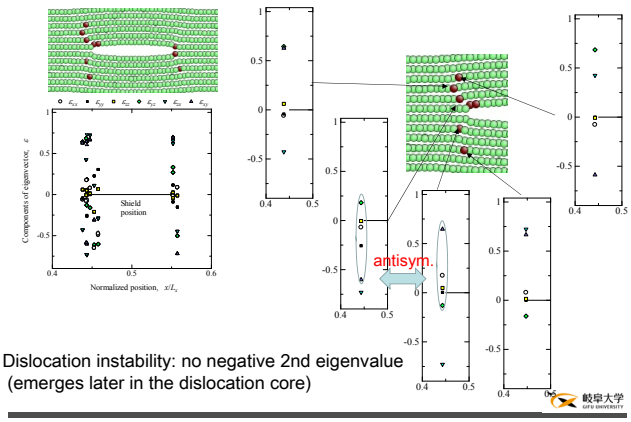
Eigenvector for crack propagation



negative 1st eigenvalue negative 2nd eigenvalue

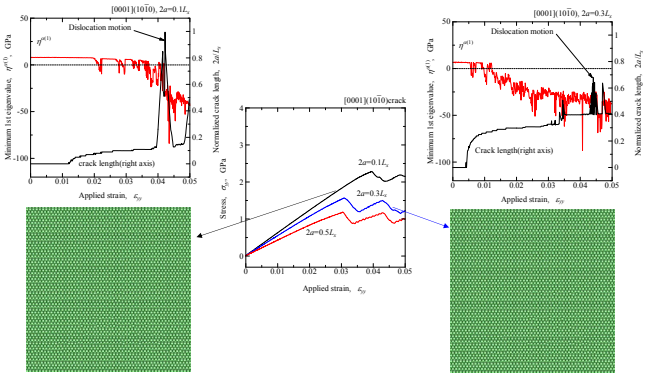
Crack instability: large normal component ε_{xx} and ε_{zz} in the 2nd eigenvector

Eigenvector for dislocation emission



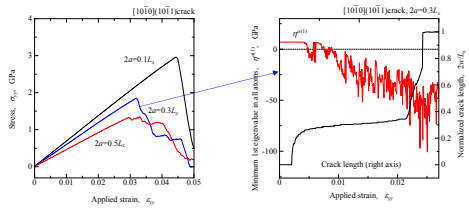
Dislocation instability: no negative 2nd eigenvalue
(emerges later in the dislocation core)

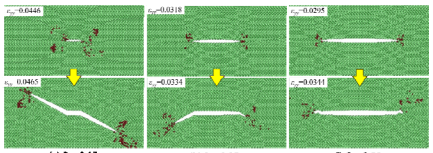
Results in the prismatic plane crack



Dislocation emission rely on the unstable area?(loop like area)

Results in the pyramidal plane crack





(g) $2a$=0.1L_x (h) $2a$=0.3L_x (i) $2a$=0.5L_x

[10$\bar{1}$0](10$\bar{1}$1) crack (cracking in multiple basal plane)

Summary

Atomic elastic stiffness (AES) could be a powerful tool, such as central symmetry parameter, to find out local deformation

The eigenvalue of the AES always shows preceding instability before local deformation

The normalized determinant of the AES also reveals that highly stable zone emerges at the crack tip in Silicon.
It is never seen in metallic system.