

T. Hoshi, Y. Iguchi, and T. Fujiwara, PRB72, 075323 (2005)

T. Hoshi, JPCM19, 365243, 7pp, (2007)

T. Hoshi, M. Tanikawa, A. Ishii, Physica E 42, 2784 (2010)

(1)

(2)

工学的視点:破壊研究=材料強度研究 (半導体「疲労」→MEMSデバイスなど) 理学的視点:perfect (dislocation-free) Si crystal→理想的な脆性 cf. 蕪木英雄・寺倉 清之「破壊・フラクチャの物理」岩波(2007)のp.115



Pioneering work (1) : Griffith theory for crack propagation



Energy of a crack with the crack length of 2c

$$U = -\frac{\pi c^2 \sigma^2}{E} L_z + 4\gamma c L_z$$
(1)  
*E*: Yong modulus (in 2D)  
 $\gamma$ : surface energy

A. Griffith, Philos. Trans. R. Soc. London Ser. A 221, (1920).

(1st term):energy gain of stress relaxzation(2st term):energy loss of surface creation

Condition for crack propagation

$$0 = \frac{dU}{dc} = -\frac{\pi\sigma^2}{E} 2cL_z + 4\gamma L_z$$
 (2)

 $\rightarrow$  Critical crack length for propagation

$$c = c_{\rm G} \equiv \frac{2}{\pi} \frac{\gamma E}{\sigma^2} \tag{3}$$

### Pioneering work (2): Mott theory for fracture propagation velocity

N. F. Mott, Engeering 165, 16 (1948).



Introducing the kinetic energy term as

$$K = \frac{\rho}{2} k v^2 c^2 \frac{\sigma^2}{E^2} L_z \tag{4}$$

*v* : fracture propagation velocity *ρ* : density *k* : small numerical factor

Condition for crack propagation

$$\frac{d}{dc}\left(U+K\right) = 0\tag{5}$$

→ Fracture propagation velocity

$$v = \sqrt{\frac{2\pi}{k}} \sqrt{\frac{E}{\rho}} \left(1 - \frac{c_{\rm G}}{c}\right)^{1/2}$$

$$\rightarrow \sqrt{\frac{2\pi}{k}} \sqrt{\frac{E}{\rho}} \quad (c \gg c_{\rm G})$$
(6)
(7)

## Atomistic viewpoints of fracture

### Cleavage as non-equillibrium dynamics

- Two **comparable** timescales : Tprop ( propagation ) Trecon ( reconstruction )
  - $\rightarrow$  Local reconstruction mechanism
  - ex. Si(111)-(2x1) structure
    = nearest neighbor coupling in the propagation direction
    = quantum mechanical feature



# Silicon cleavage simulation with (111)-2x1 reconstruction

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Technical details 10<sup>4</sup>-10<sup>5</sup> atoms Dynamics in ~10 ps External load for cleavage Quantitative agreement with experiments  $K_{\rm C}$  : critical stress intensity factor  $V_{\rm p}$  : crack propagation velocity



\* Spence, et al., Acta Metall. Mater. 41, 2815 (1993). \*\* Hauch, et al., PRL82, 3823 (1999) Application : Si(111)-(2x1) cleavage simulation

Hoshi, Iguchi, Fujiwara, PRB72, 075323 (2005)

 $\rightarrow \pi$ -bonded (Pandey) structure with tilting Steps are formed in large (10-nm-scale) samples

В

[111]

→[211]

14 nm [211] 0.7 nm STEP 5 6 5 7 7 5 5 5 5

Surface ( $\pi$  -bonding) state



Example of STM experiment



# Silicon cleavage simulation with electronic structure

Which plane ( index ) appears ?Plane with small surface energy ?Plane with small number of dangling bonds ?

Missing viewpoints
 (a) reconstruction with energy gain
 (b) non-equillibrium dynamics

Si:surfac	e energie order of 1 eV	es [J/m <sup>2</sup> ] // surf. atom )
(111)	1.44 (2x1)	1.82 ideal
(110)	1.70 buckled	2.04 ideal
(001)	1.41 c(4x2)	2.39 ideal

Cleavege planes in macro samples (111) plane in metastable (2x1) str. (110) plane (less favorable)

 $\rightarrow$  (001) plane is impossible ?



Bending of cleavage path into favorite planes

( as a size effect on 10-nm-scale or larger )

→ Experimentally observed planes
: (111) or (110) plane [less favarable]



Bending of cleavage path into favorite planes

Artificial cleavage 'seed': (001) plane  $\rightarrow$  Experimentally observed planes

: (111) or (110) plane [less favarable]



![](_page_9_Figure_0.jpeg)

Si(111)-(2x1) surface : LDOS and bias-dependent STM

STM image of flat (unstepped) surface area

→ The spot positions are different for different signs of voltage bias, as expected.

![](_page_10_Figure_3.jpeg)

![](_page_10_Picture_4.jpeg)

Stepped Si(111)-2x1 surface formed in clevage dynamics

→ Stability Bias-dependent STM image

→A hierarchical research
(a) Prediction by the large-scale
(10nm-scale) calculation
(b) (c) Confirmation by
the DFT-PW calculation
with a small system

![](_page_11_Figure_3.jpeg)

Conclusion

# Si cleavage simulation with electronic struture calculations

- Preference of (111) and (110) cleavage surface is shown (a) dynamical theory (b) bending of cleavage planes
- Appearance of (111)-2x1 (Pandey) surface prediction of steps with bias-dependent STM image
   → consistent to experimental STM images