Computer Simulation for Understanding of CMP Process

April 11, 2019

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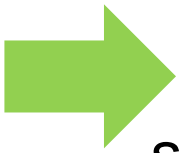
   - Our concept to control RRs
   - Function of chemical additives
   - Validity of the present model
   - Application of the present model

3. Novel polishing simulator
   - Mechanical polishing of SiO_2 patterned film
   - Implementation of chemical effects and its validation

4. Summary & Future plan

Introduction

Further understanding of CMP process



Predictions of
removal rates (RR)
surface morphology of wafers

What we should validate

Roles of chemical additives in CMP

Relation of individual step* in CMP with RR and surface morphology

(*)adsorption / desorption / diffusion of abrasive particles, removal of substrate

Our approach by using computer simulations

Novel modeling of RRs from the viewpoints of atoms and molecules**

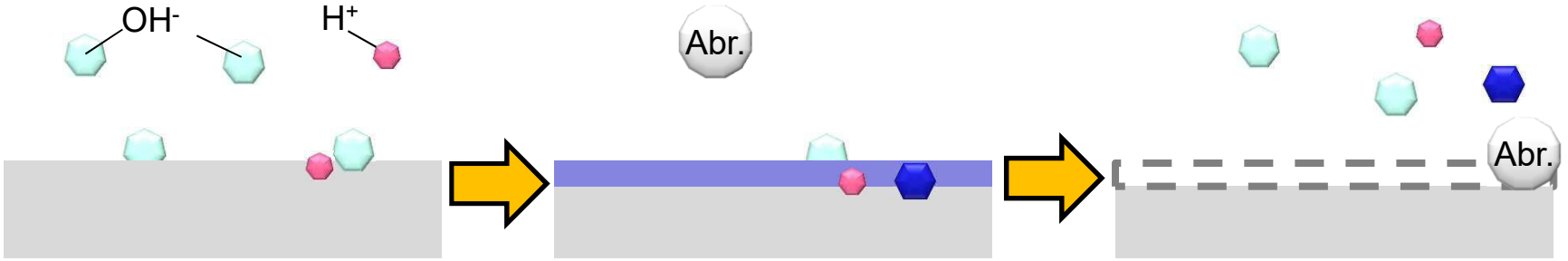
Novel polishing simulator from the viewpoint of particles***

(**)Endou et al., ISSM 2014, PO-46; Shinoda et al., ISSM 2018, PC-O-7.

(***)Endou et al., ISSM2016, PO-O-4.

Brief introduction of our modeling activities

CMP mechanism considered so far



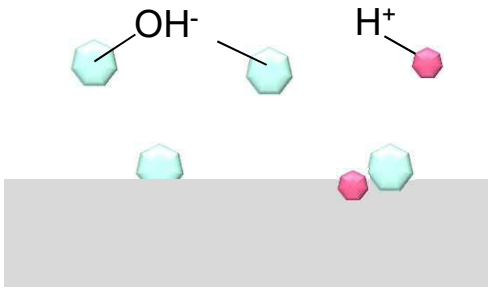
Chemicals (ex. H^+, OH^-) in a slurry react with a substrate surface

Embrittlement of substrate surface due to chemical reactions (ex. hydrolysis)

Removal of brittle layer by (a)mechanical action of abrasive particles and (b)dissolution of the surface

*H. Prigge, P. Gerlach, P. O. Hahn, A. Schnegg, and H. Jacob, *J. Electrochem. Soc.*, **138** (1991) 1388.

Our concept to control RRs



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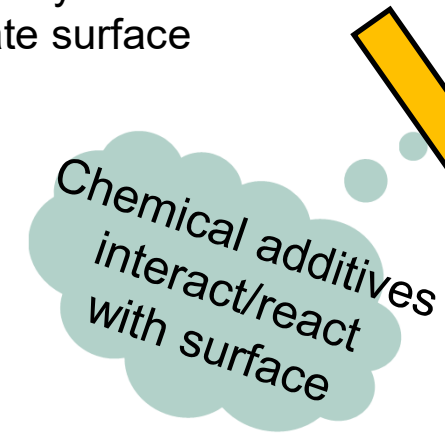
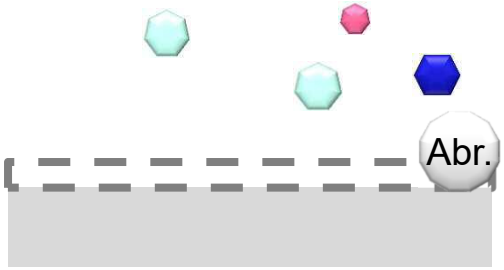


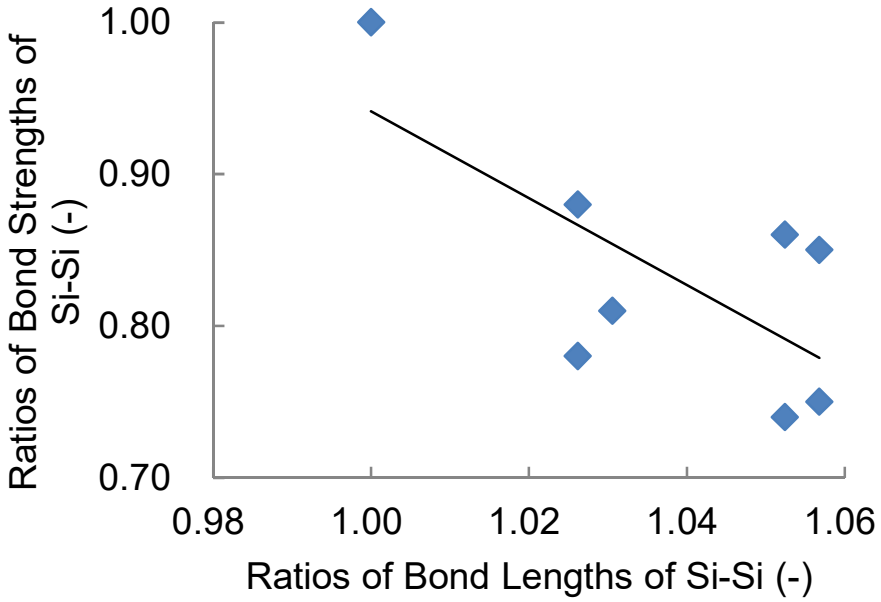
By using chemical additives,
some modification of the surface will be expected to form weaker surface layer

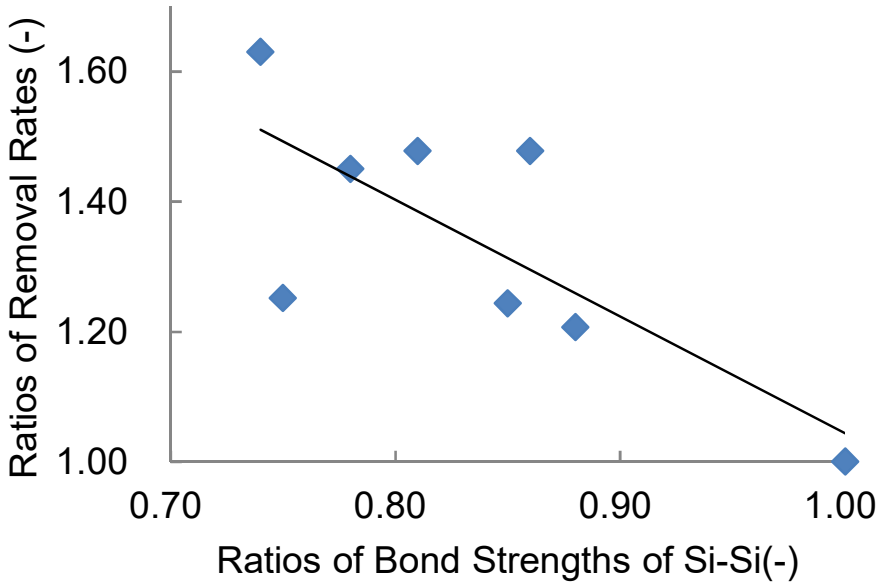


Easier removal of the surface with mechanical action of abrasive particles
and
attack of chemicals (ex. H^+, OH^-)

Validate the function of chemical additives by using computer simulations

Validation of the function of chemical additives : (ex.)bare-Si





A linear correlation between strengths and lengths for Si-Si

Longer Si-Si bonds correspond to weaker ones.

Higher RRs can be realized with weaker bonds

... Weaker chemical bonds can be easily broken.

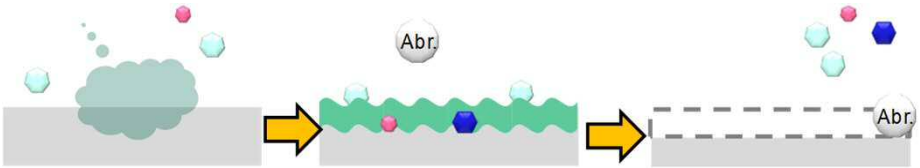
Expected function of chemical additives was validated.

Published model of CMP
+ our computer simulations

Borst model (*)

(*) Borst et al., J. Electrochem. Soc., 149 (2002) G118-G127.

(1)Chemical effects :
Substrate + nR $\rightarrow$ Substrate*; rate = k_1



(2)Mechanical effects :
Substrate* $\rightarrow$ Removed !; rate = k_2

$$RR \propto \frac{k_1}{1 + \frac{k_1}{k_2}}$$

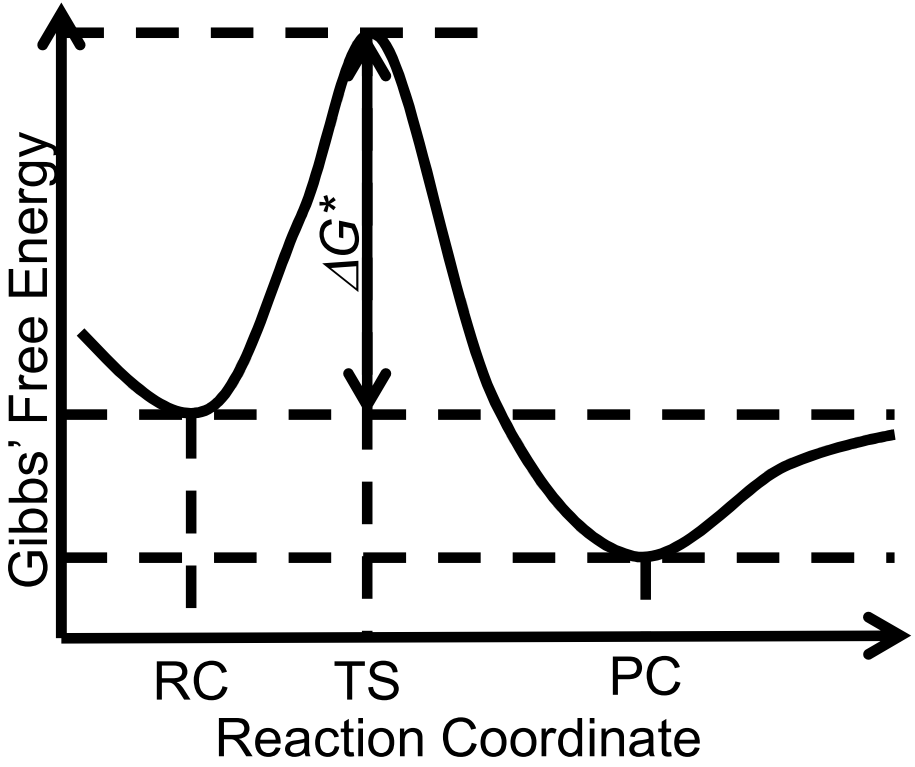
Necessary parameters

Parameter A : ratios of values of k_1
Parameter B : averages of ratios of terms related to k_2

Both A and B were led from the results obtained with our computer simulations

What is ‘Parameter A’ ?

Chemical reactions
be invoked via formation of
reaction complex (RC)



Easy to interact with substrate surface

⇩

RC will be easily formed

⇩

Increasing freq. of chemical reaction

⇩

Surface modification with chemical additive will be easily occurred

⇩

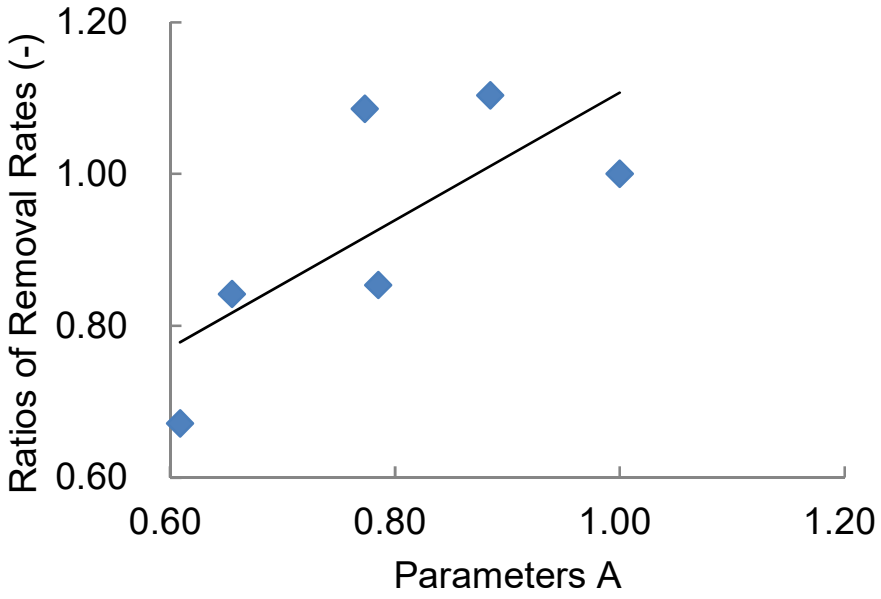
Modified parts of substrate surfaces will be easily removed with abrasive particles

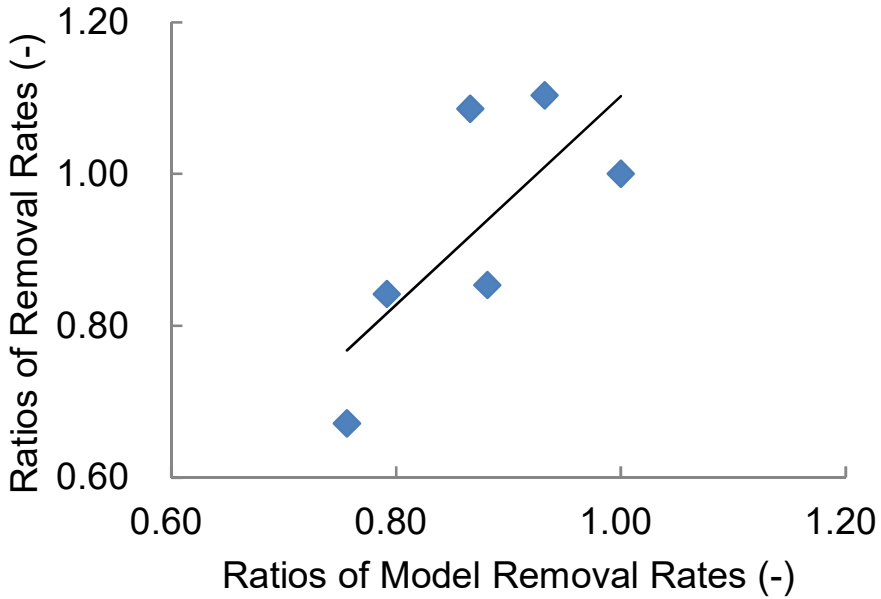
⇩

Increasing RRs for substrate

Easiness of interaction of additive with substrate surface
= Driving force of chemical reactions (parameter A)

Validity of the present model : (ex.)bare-Si



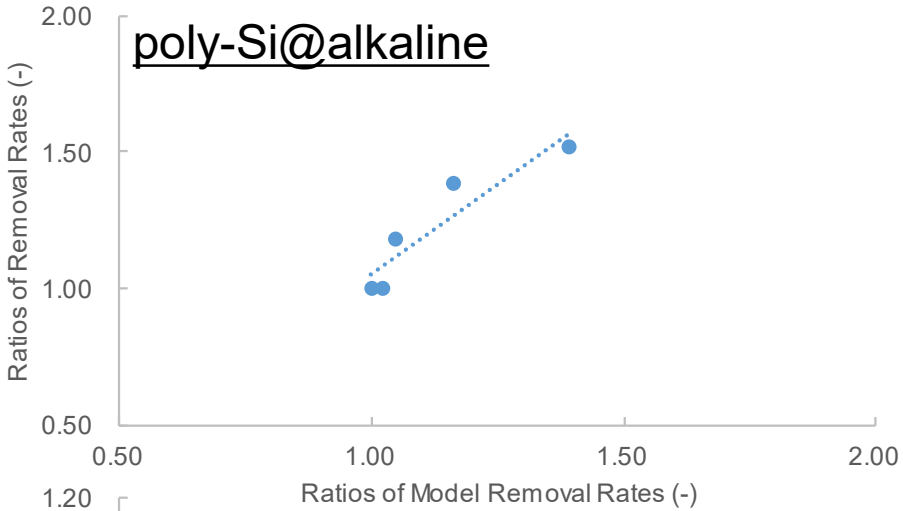


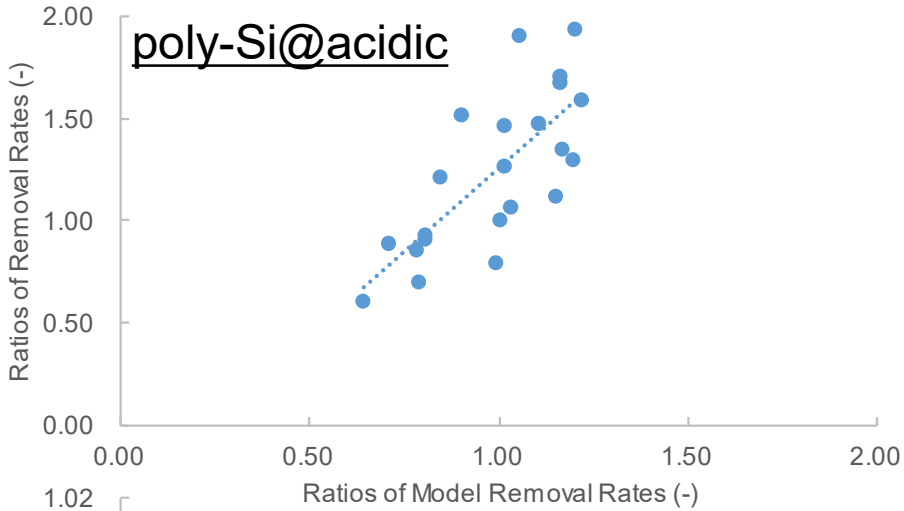
Importance of parameter A in describing RRs

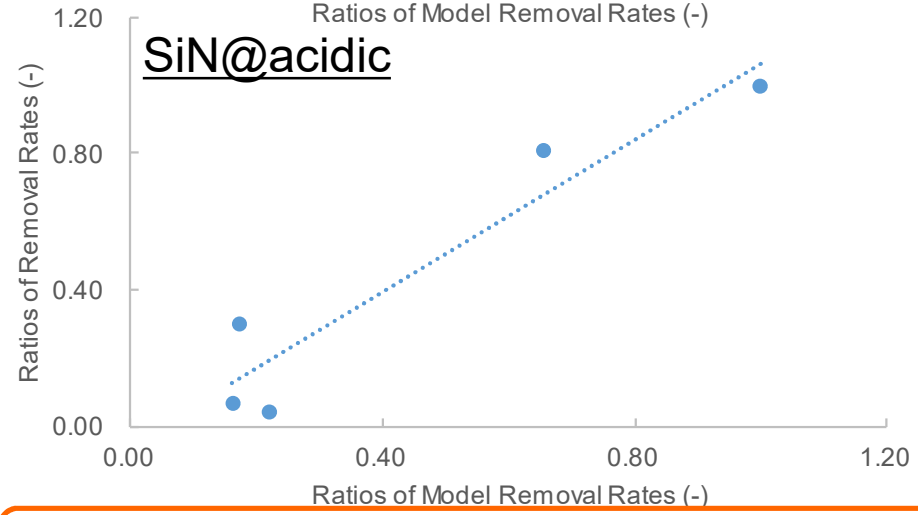
Model ratios correlate with experimental ones

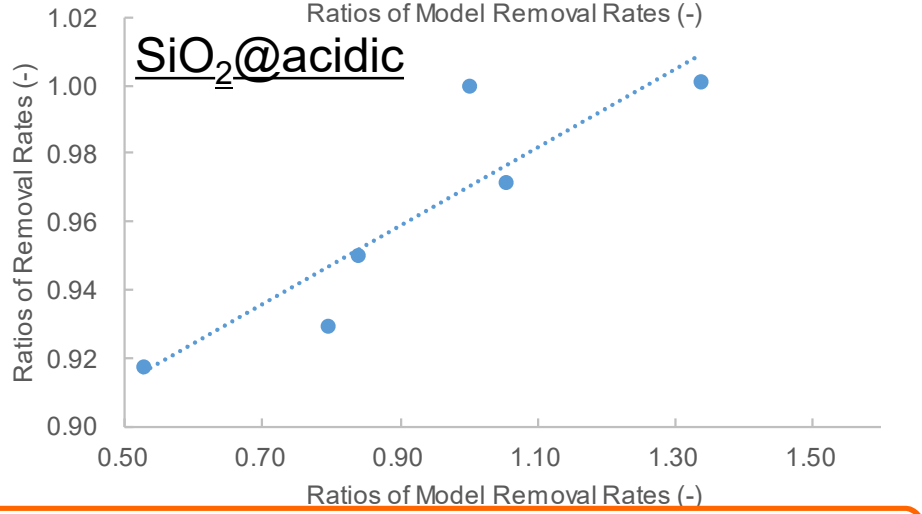
Validate our concept

Application of the present model



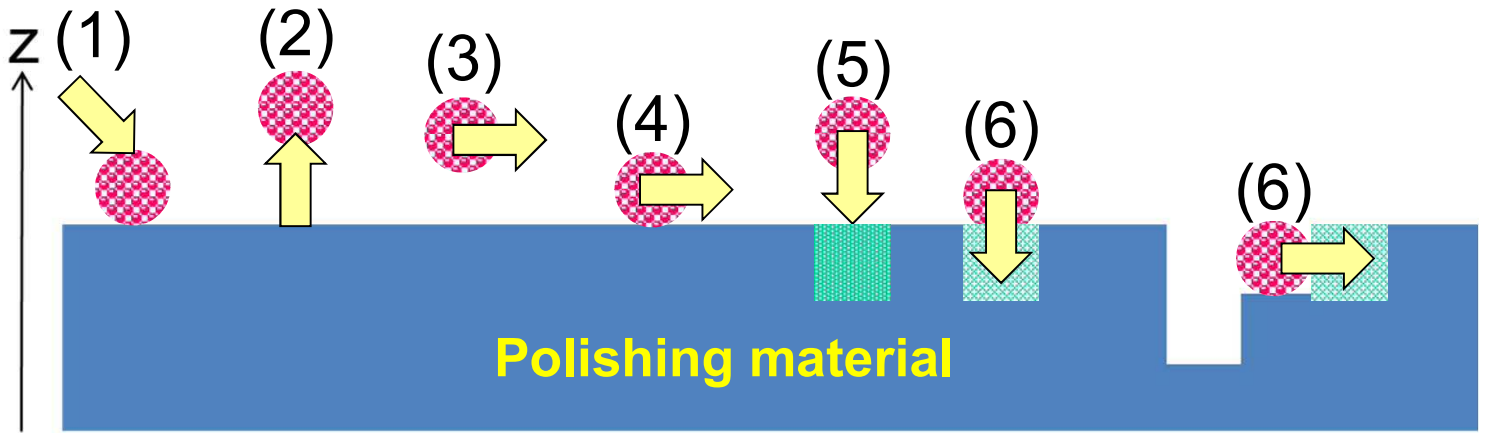






Modeling of RRs for various substrates has been succeeded.

Development of novel polishing simulator (1): mechanical effects



Considered effects in mechanical polishing:

(1)Adsorption of abrasive particle on polishing surface
(2)Desorption of abrasive particle from polishing surface
(3)Diffusion of free abrasive particle without adsorption
(4)Diffusion of abrasive particle on polishing surface
(5)Nano-indentation of abrasive particle on polishing surface
(6)Removal of polishing surface by abrasive particle (vertical or horizontal)

They are selected with the assigned probabilities and random numbers.

Input parameters and output data

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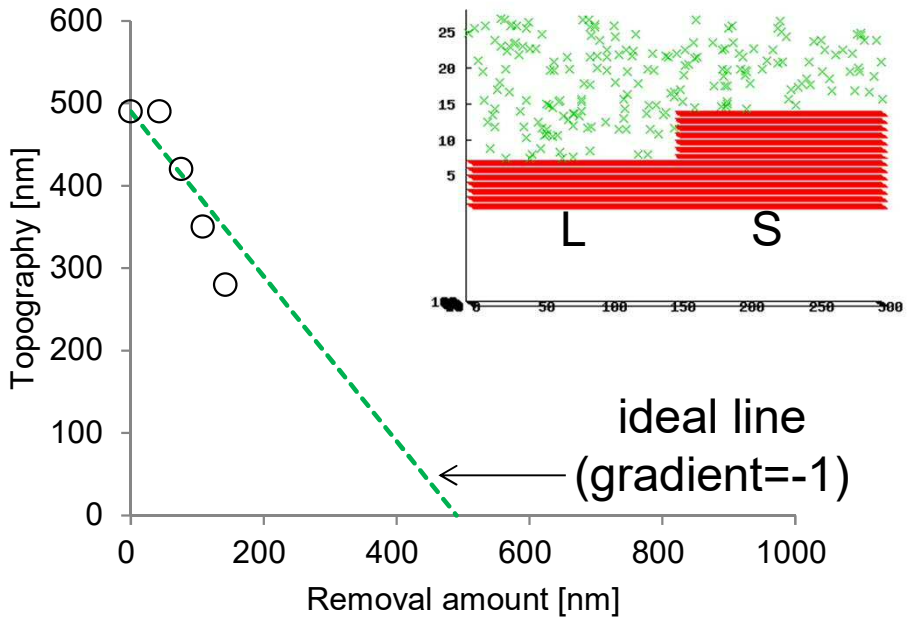
Input

- Pressure adding to the substrate
- Linear velocity of abrasive particles
- Temperature
- Diameters of abrasive particles
- Easiness of removal of polishing materials
- Probabilities for the mechanical effects and chemical ones

Output

- Total elapsed time
- Removal amount per time (RAPT)
  - = (number of the removed lattice points) / total elapsed time

Mechanical polishing of patterned SiO_2 (under 1 psi and at room temperature)



L/S = 10.5 μm/10.5 μm

Gradient of PE plot

Simulation : -1.57

Experiment : -1.69

Obtained theoretical tendency agrees with the experimental one.

Development of novel polishing simulator (2): chemical effects

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Adsorption of RR modifier (enhancers or suppressors)

Desorption of RR modifier

Oxidation of polishing surface

Hydrolysis of polishing surface

Dissolution of polishing surface

Deposition of dissolved polishing surface

*They are selected with the assigned probabilities and random numbers.

*An arbitrary combination of the above is available.

Implementation of chemical effects

Ratio of deviation of RAPT

$$Y = 100 \times \left(\frac{y_C}{y_M} - 1\right)$$

RAPT : Removal amount per time

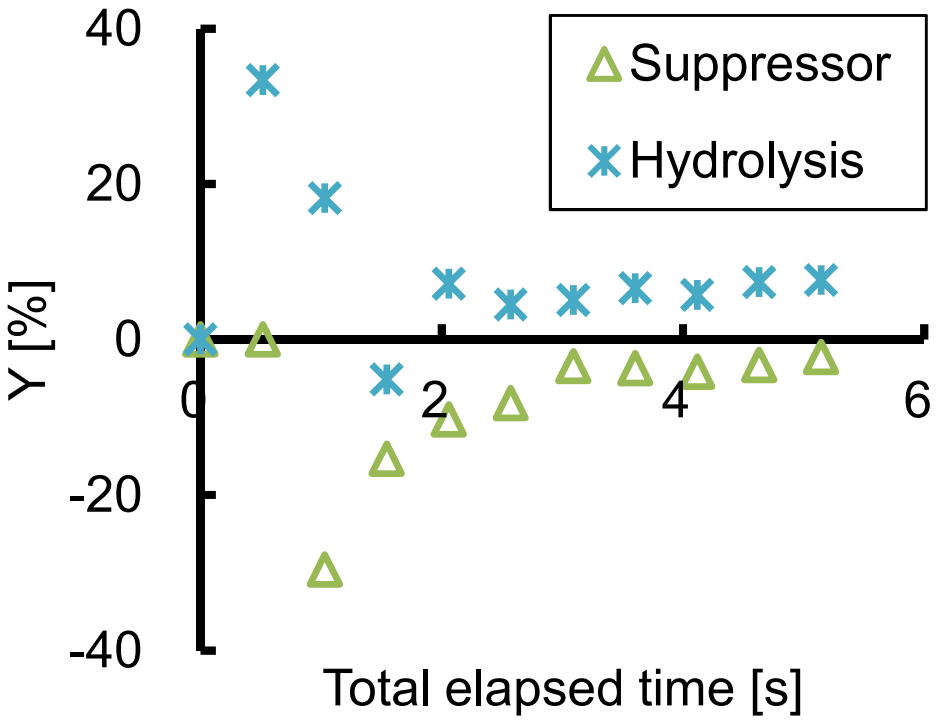
Y : Ratio of deviation of RAPT

y_M : RAPT with only mechanical effects

y_C : RAPT with mechanical + chemical effects

Larger Y ... $y_C > y_M$

Result for SiO_2 substrate



Adsorption and desorption of RR suppressor : 0 or smaller than y_M

Hydrolysis : larger than y_M

The chemical effects implemented in the simulator on RAPT worked as expected.

Summary

Novel modeling of RRs in atomic and molecular levels

*Function of chemical additives which interact/react with substrate surface was considered to change the surface state of substrate.

→ Justified with both computer simulations and experiments

→ Effectiveness of the chemical additives on controlling RRs

*Combination of published model on RRs and computer simulations results

→ Good correlation with the ratios of experimental RRs

→ Available to not only bare-Si but also poly-Si, SiN, and SiO_2

Novel polishing simulator in particle level

*It is applicable to both blanket and patterned wafers.

→ PE curve can be obtained.

*This simulator can use 6 kinds of chemical effect.

→ Chemical effects on removal amount per time work as expected.

→ Be useful to model mechanical and/or chemical effects in CMP.