Computer-Simulation Studies of Plasma-Surface Interactions

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Topics of my talk:

- reviews, from material's point of view, of codes used for plasma-surface interactions
- main results obtained with these codes
- data-fitting formulae
- future subjects

Becoming more important because of long pulse / steady-state operations are such issues of plasma-surface interactions as:

- physical/chemical erosion of plasma-facing materials
- retention of D, T, He and impurities
- T co-deposition with eroded carbon
- lifetimes of materials
- deterioration of materials
- formation of mixed-materials
- dust formation

Frequently used simulation codes are classified into:

according to the treatment manners of atomic collisions In solids,

(1) BCA codes (slowing-down process by Binary Collision Approximation)

(2) Dynamic MC codes with no thermal process

(3) Dynamic MC codes with thermal process

(4) MD codes (both processes by Classical/Quantum Molecular Dynamics)

BCA codes and data-fitting formulae

Codes: TRIM, TRIM.SP, SRIM, ACAT for amorphous targets

Main different features:

- TRIM.SP→ uses a mean free-path for collisions.
- ACAT→ employs the "cell model" where a target atom is randomly selected in a simple cubic cell

Difference of calculated sputtering yields: ?

- very small, generally.

Calculated sputtering yield data:

- TRIM.SP→IPP 9/82 (1993), IPP 9/132 (2002).
- ACAT→ADNDT 62 (1996) 149, NIFS-DATA-23.

Fitting formulae for sputtering yield data

mono-atomic targets (for normal incidence):

- **revised Bohdansky's formula**
- **Yamamura's formula**

$$Y(E) = 0.042 \frac{Q\alpha^*(M_2/M_1)}{U_S} \frac{S_n(E)}{1+\Gamma k_e^{0.3}} \left[1 - \sqrt{\frac{E_{th}}{E}}\right]^s \quad (1),$$

- **Unified analytic formula**

E : projectile energy

ε : LSS reduced energy

$\Gamma = W/(1+(M_1/7)^3)$

k_e : Lindhard inelastic energy loss

M_1, M_2 : masses of projectile and target atoms; $S_n(E)$: nulear stopping cross-section

$\alpha^*(M_1/M_2)$: best-fit function of M_1/M_2 ; Q, W, s : fitting parameters ;

U_S : surface binding energy; E_{th} : threshold energy and a function of M_1, M_2 and U_S.

multi-component targets (for normal incidence):

- **eq. (1) is applicable by replacing**

$< Z_2 >= \Sigma c_i Z_i$; $< M_2 >= \Sigma c_i M_i$; $< U_S >= \Sigma c_i U_{S,i}$; c_i : atomic fraction of ith component

; $< E_{th,i} >= \max\{E_{th,i}\}$; $< E_{th,i} >= \Sigma c_i E_{th,i}$ for O projectile.

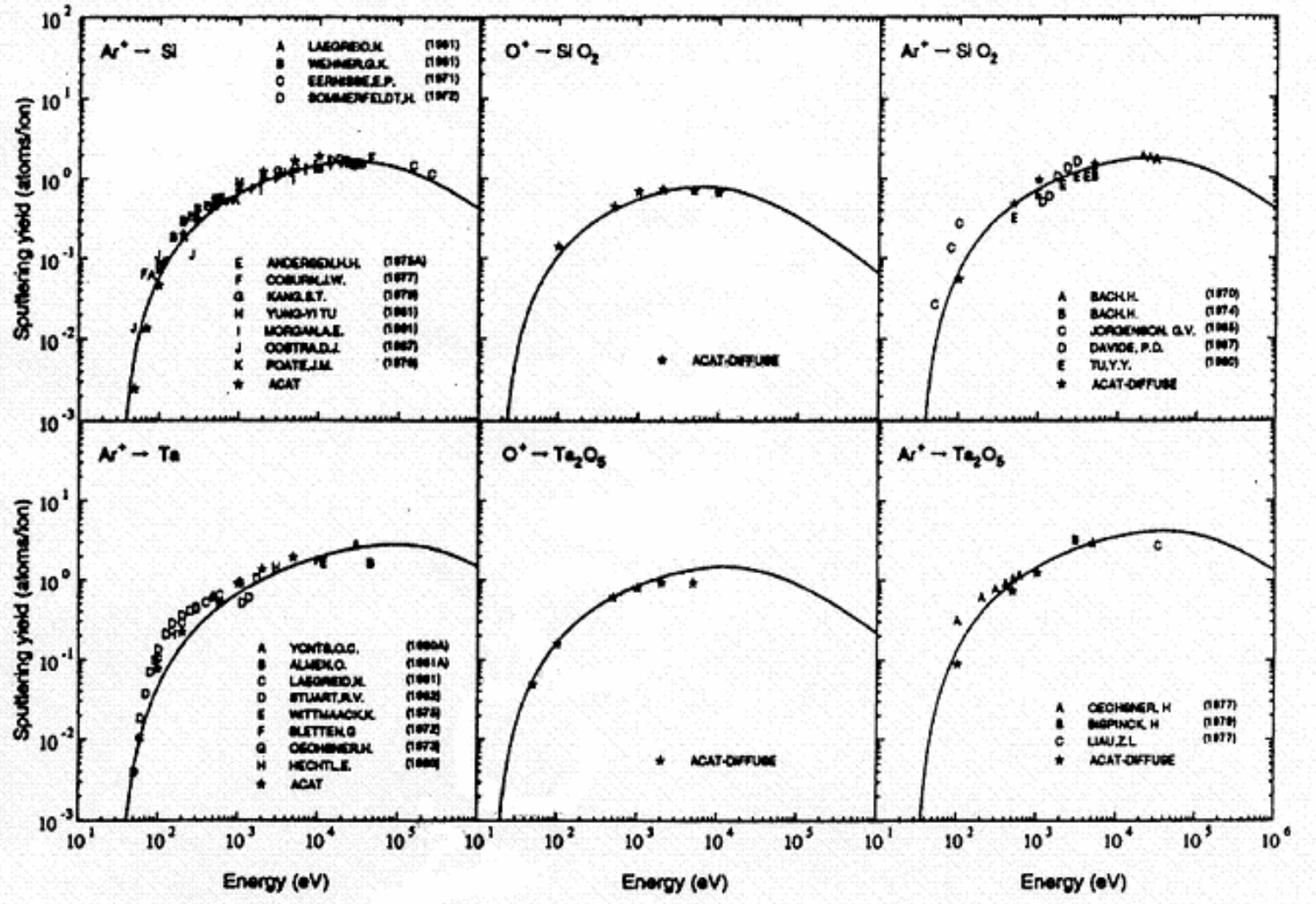

Fig. 1. Energy dependence of the sputtering yield of Si, Ta, SiO_2, and Ta_2O_5 for argon and oxygen ion bombardment, where the solid lines correspond to the empirical formula eq. (1) and experimental data of monatomic solids are from Ref. [15] and those of oxide from Ref. [12]. (Y. Yamamura, M. Ishida, Appl. Surf. Sci. 9202 (2002) 1.)

Fitting formulae for energy of sputtered atoms

Energy formulae（without normalization factors）

Our formula; $E_1(E_1+U)^{-5/2}\cdot\ln\left[(B+E_{inc}^{1/2})/(B+(E_1+U)^{1/2}/(\gamma(1-\gamma))^{1/2})\right]$

Thompson/ *truncated*; $E_1(E_1+U)^{-3}\cdot\left[1-((E_1+U)/(\gamma E_{inc}))^{1/2}\right]$

Thompson/ *untruncated*; $E_1(E_1+U)^{-3}$

Falcone ; $E_1(E_1+U)^{-5/2}\cdot\ln((\gamma E_{inc})/(E_1+U))$

Kenmotsu ; $E_1(E_1+U)^{-8/5}\cdot\left\{\ln\left[(\gamma(1-\gamma)E_{inc})/(E_1+U)\right]\right\}^2$

- **Kenmotsu and our formulae are fit to the energy spectra of sputtered atoms due to low-energy incident light ions.**

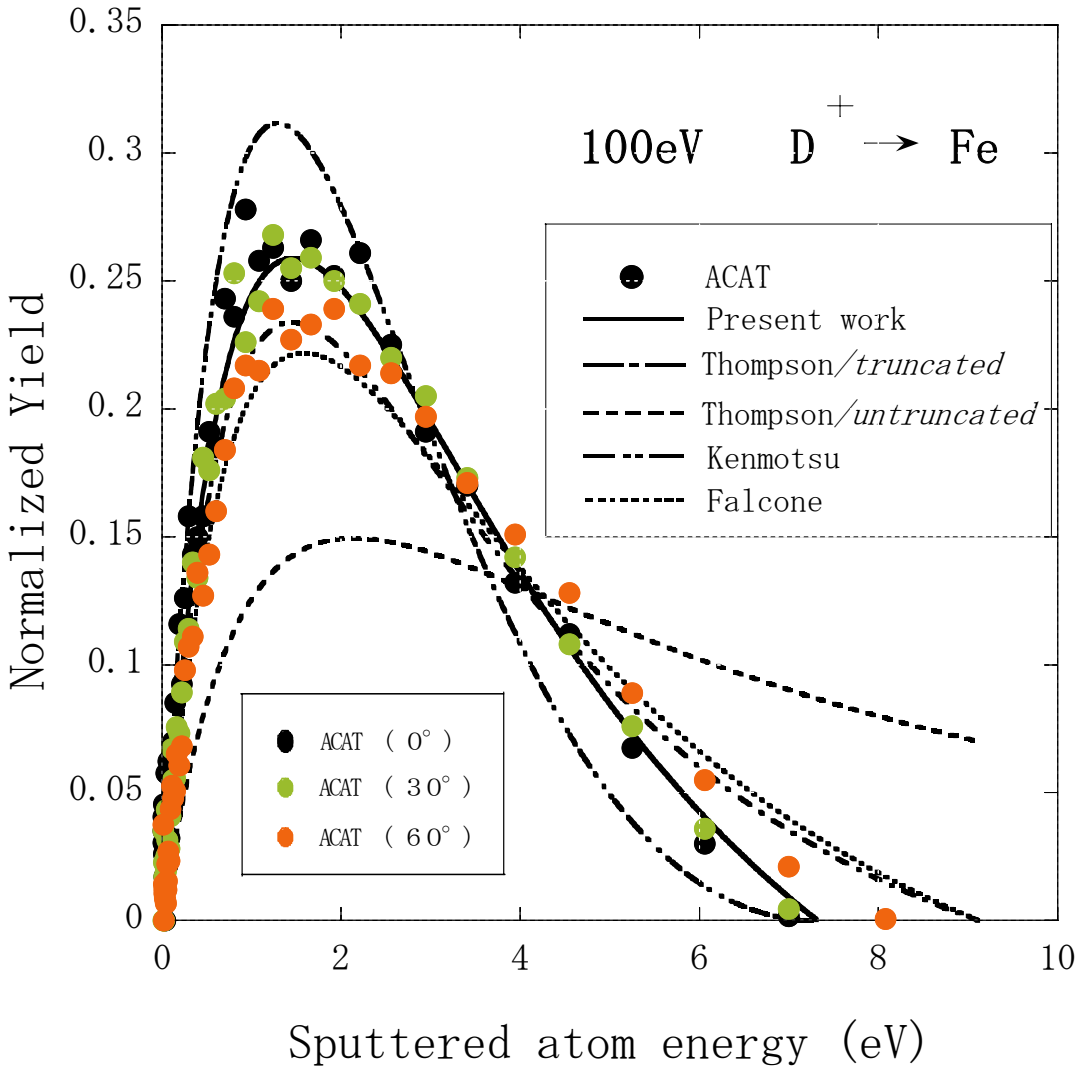

Fig.2. Normalized yields of atoms sputtered from a Fe material irradiated by 100eV D ions at incidence angles of 0º, 30º and 60º vs. sputtered atom energy in eV. The legend shows the curves obtained with the different formulas. (T. Ono, Y. Aoki, T. kawamura, J. Nucl. Mater. 337-339 (2005) 975.)

Dynamic MC codes with no thermal process

code: TRIDYN

Main features:

- **Outputs: surface composition, surface recession/growth and other irradiation-related effects as a function of the fluence of incident projectiles**

- **Each projectile = ' pseudo-particle' ←→**

$$\Delta\Phi = \Phi_{\mathrm{tot}} / N_{\mathrm{H}}, (\Phi_{\mathrm{tot}} : \mathrm{total\ fluence}, N_{\mathrm{H}} : \mathrm{number\ of\ incident\ pseudo\text{-}projectile's\ histories})$$

- **Relaxation ←→ local partial densities of the constituents are rearranged according to their atomic volumes.**

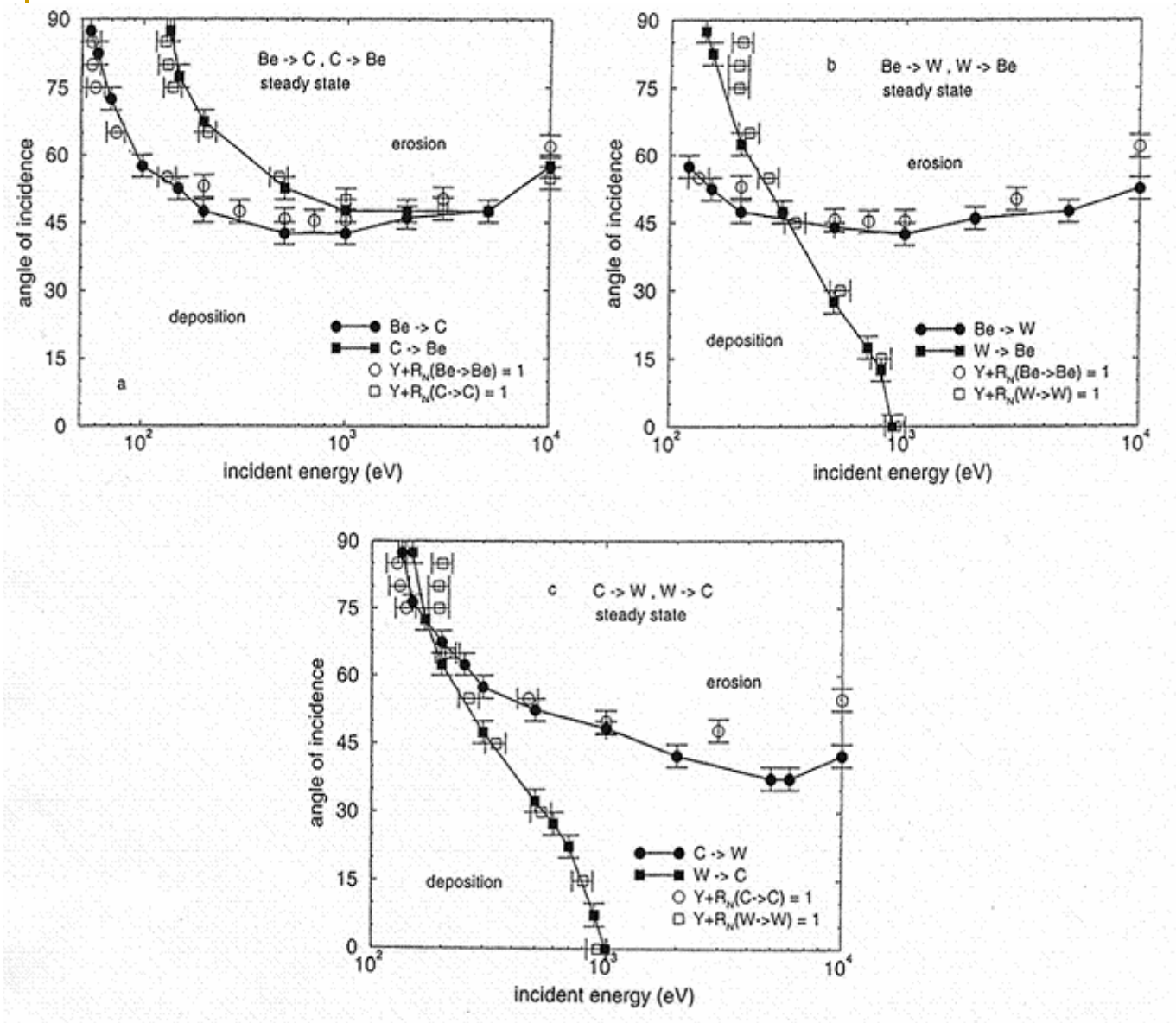

Fig.3.Regions of deposition and erosion versus the incident energy and incidence angle at steady-state conditions for the bombardment of: (a) C with Be and of Be with C, (b) W with Be and of Be with W and (c) W with C and of C with W. For both examples, the region below each curve belong to the deposition regime, the region above each curve to the erosion regime. Lines drawn to guide the eye. (W. Eckstein, J. Nucl. Mater. 281 (2000) 195.)

TRIDYN results

Dynamic MC codes with diffusion (1)

codes: ACAT-DIFFUSE, TRIDYN + PIDAT, TRIDYN + DIFFUSEDC /+ YCEHM, EDDY, TMAP4

Main features of ACAT-DIFFUSE:

- collisions /previously trapped projectiles, target atoms
- thermal process: implanted projectiles, recoil atoms
- calculates: radiation-enhanced diffusion, segregation, chemical erosion, ...
- consists of: ACAT routine + DIFFUSE routine

ACAT routine → slowing-down process

DIFFUSE routine → thermal process (via diffusion eq.)

Dynamic MC codes with diffusion (2)

Main features : TRIDYN + PIDAT, TRIDYN + DIFFUSEDC + YCEHM, EDDY, TMAP4

- PIDAT : diffusion code/ 6 traps, varying exponential mesh grids
- DIFFUSEDC: diffusion code
- TRIDYN+DIFFUSEDC: temperature-dependent erosion & deposition due to bombardment of W by C
- YCEHM: chemical erosion module
- TRIDYN+DIFFUSEDC +YCEHM : simultaneous bombardment of W by C and D
- EDDY: ion reflection from & physical & chemical erosion of materials & local transport of released particles
- TMAP4: no slowing-down process, T retention & loss, 1-d thermal- & mass-diffusive transport & trapping , 0-d fluid transport between enclosures & across the interface between enclosures & structures

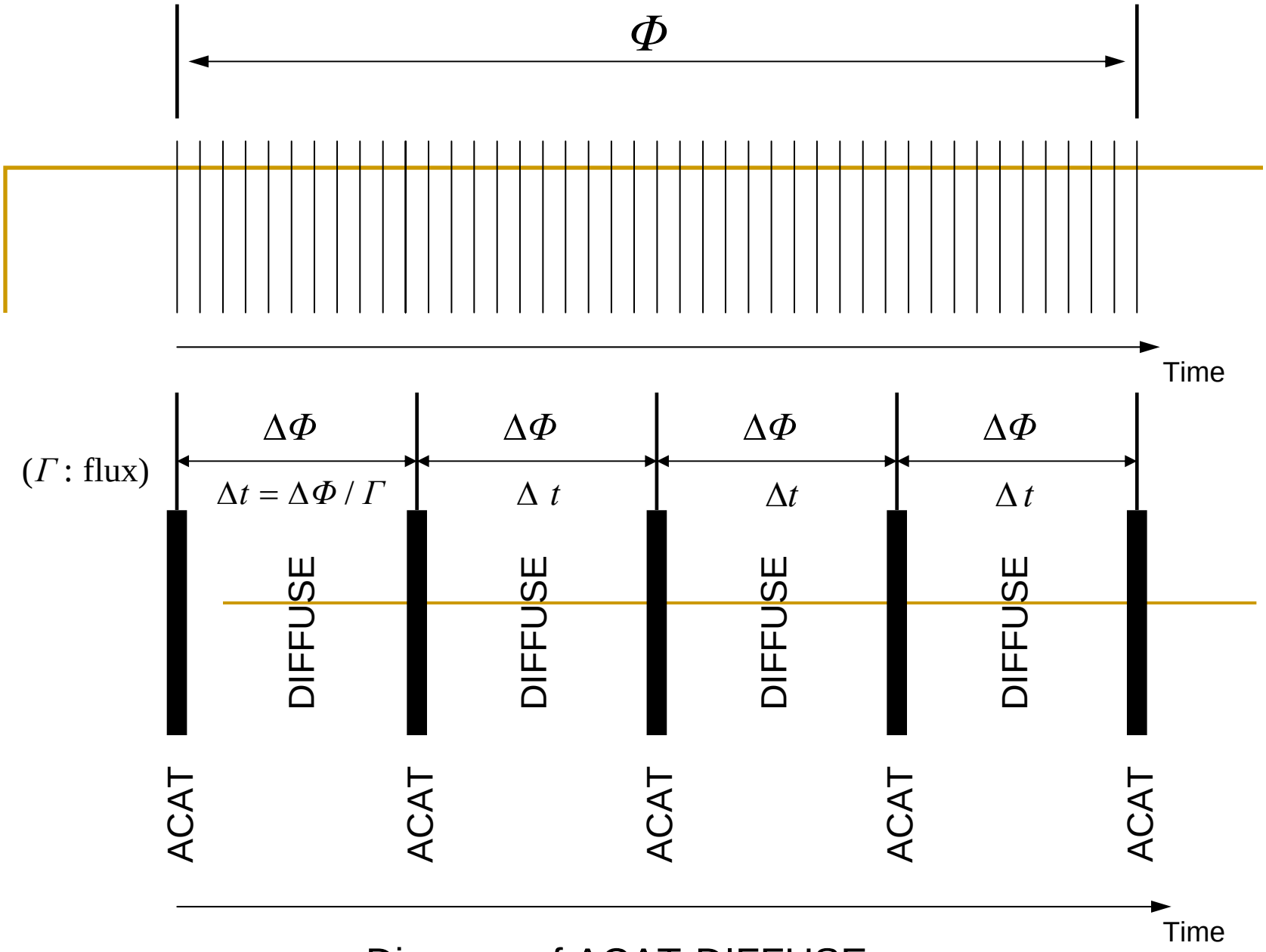

Diagram of ACAT-DIFFUSE run

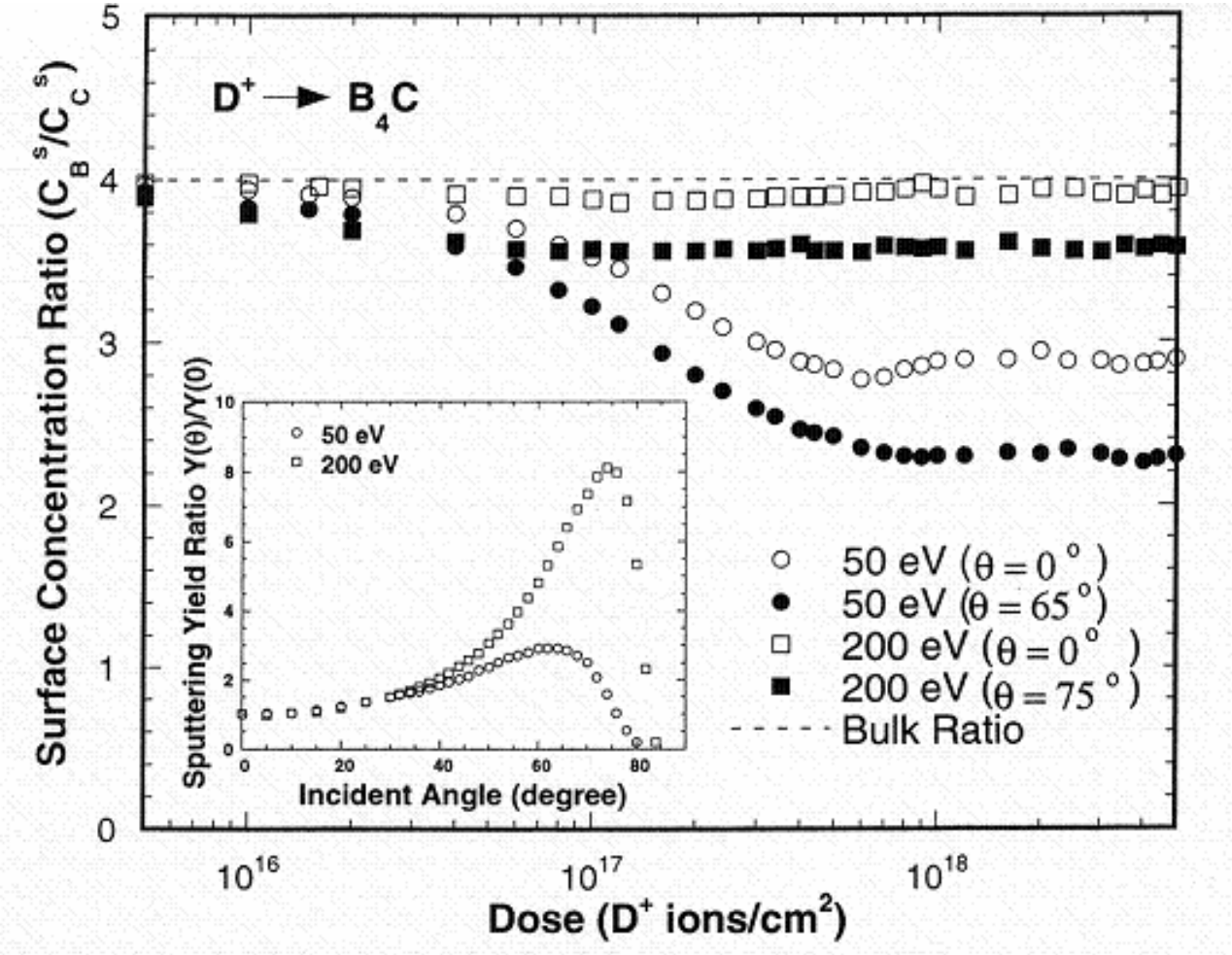

Fig.4. Dose dependence of the surface concentration ratio C^s_B / C^s_C during 50 and 200 eV D ion bombardment on B_4C at normal and grazing incidence, where the grazing angles are 65° for 50 eV and 75° for 200 eV. The inset shows the normalized sputtering yield, $Y(\Theta)/Y(0^\circ)$, as a function of incident angle for 50 and 200 eV D ion bombardment on B_4C material bombarded by Φ_0 of D ions. (T. Kenmotsu, T. Kawamura, T. Ono, Y. Yamamura, J. Nucl. Mater. 258-263 (1998) 729.)

ACAT-DIFFUSE results

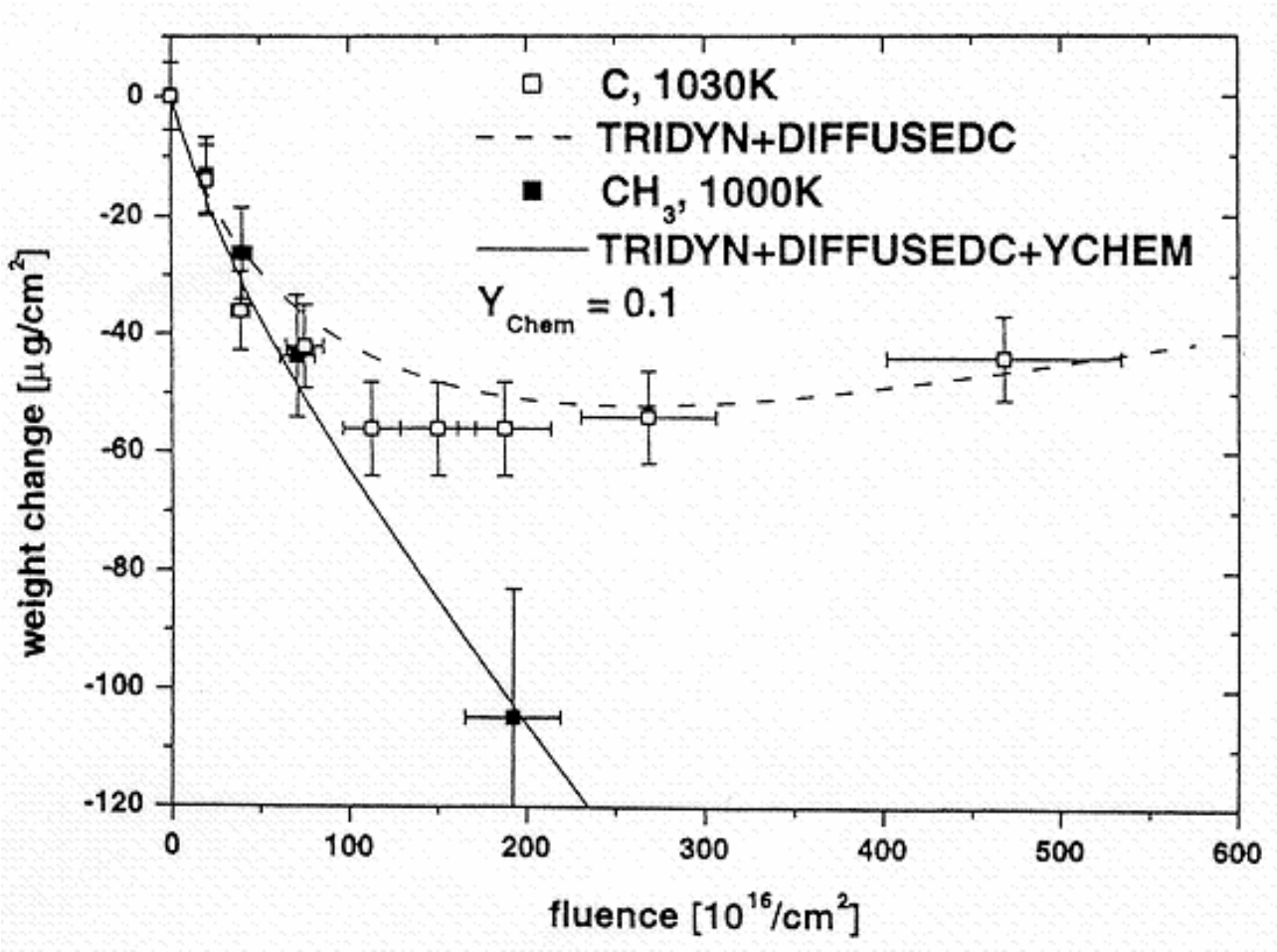

Fig.5 Comparison between experimental and simulated data of the bombardment of W with 2.4 keV C at 1030 K and 3.0 keV CH_3 at 1000 K. (K. Schmid, J. Roth, J. Nucl. Mater. 313-316 (2003) 302.)

TRIDYN+DIFFUSEDC & TRIDYN+DIFFUSEDC+YCHEM results

MD codes & results

- Method of MD: solve eq.s of motion of a many-body system to determine time-evolutionally states of the system, using an empirical potential (classical) or determining potential of the system from 1^s principle (quantum)- Car & Parrinello method with density functional.

- calculate: (1) dynamic properties (reflection (R_E, R_N, atomic state, ...), sputtering, chemical reaction, adsorption/desorption, diffusion coefficient, viscosity coefficient, electric conductivity, ...)

  (2) thermodynamic properties (internal energy, specific heat, ...)

- restrictions: (1) time ... (time step to solve eq. of motion) ~10^{-15}s x (number of steps) ~10^6 = 10^{-9}s in real time

  (2) size of a system ... ~10^8 atoms ←→cubic space with 100 nm sides in bcc structure (classical) / ~100 atoms (quantum)

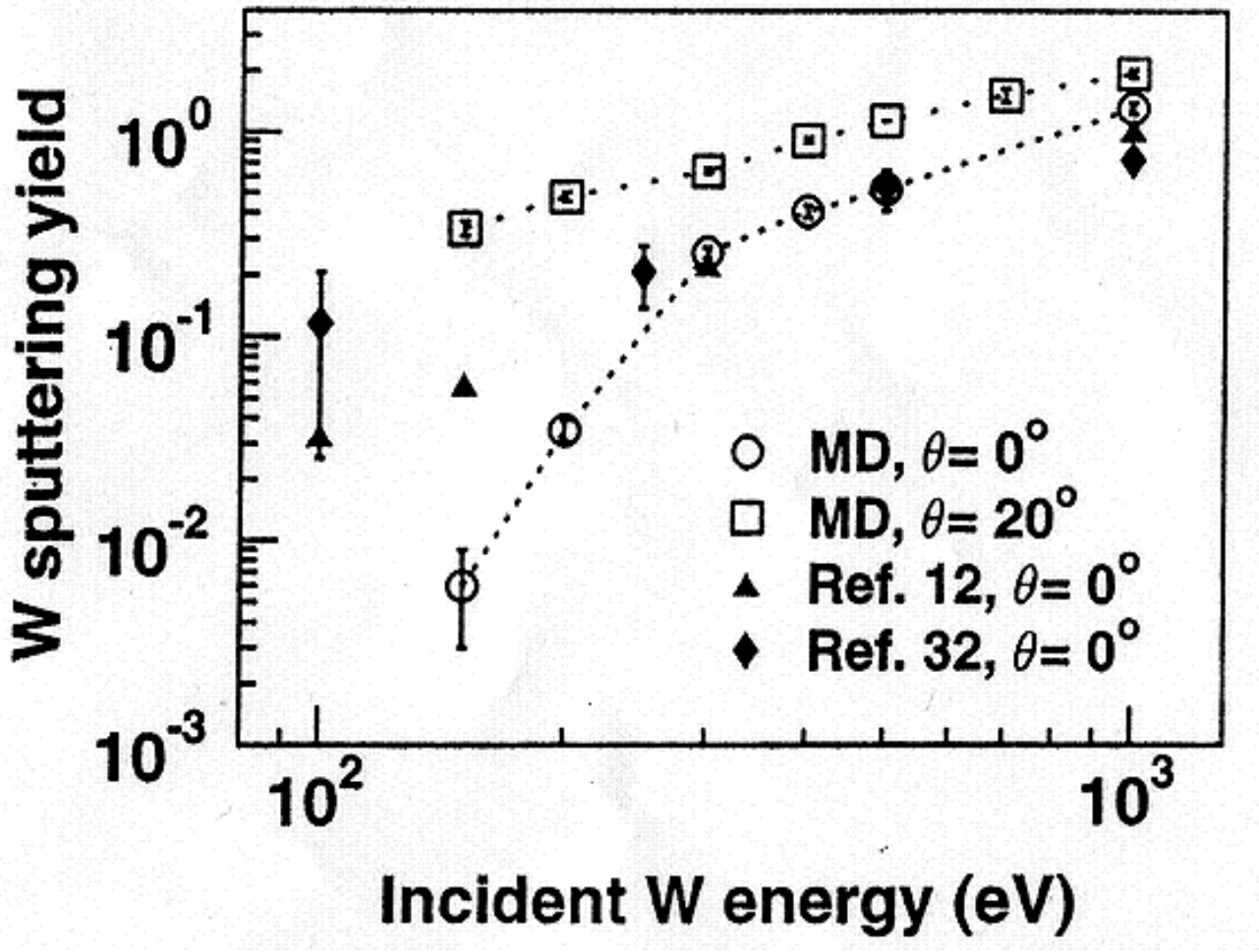

Fig. 13. Self-Sputtering yields of W for off-normal impact angles of 0° (open circles) and 20° (open squares). Experimental data for normal incidence [12,32] are also shown. Some of our data are from Ref. [34]. (E. Salonen, K. Nordlund, J. Keinonen, J. Nucl. Mater. 313-316 (2003) 404.)

Classical MD at 300 K, with Finnis-Sinclair potential for W

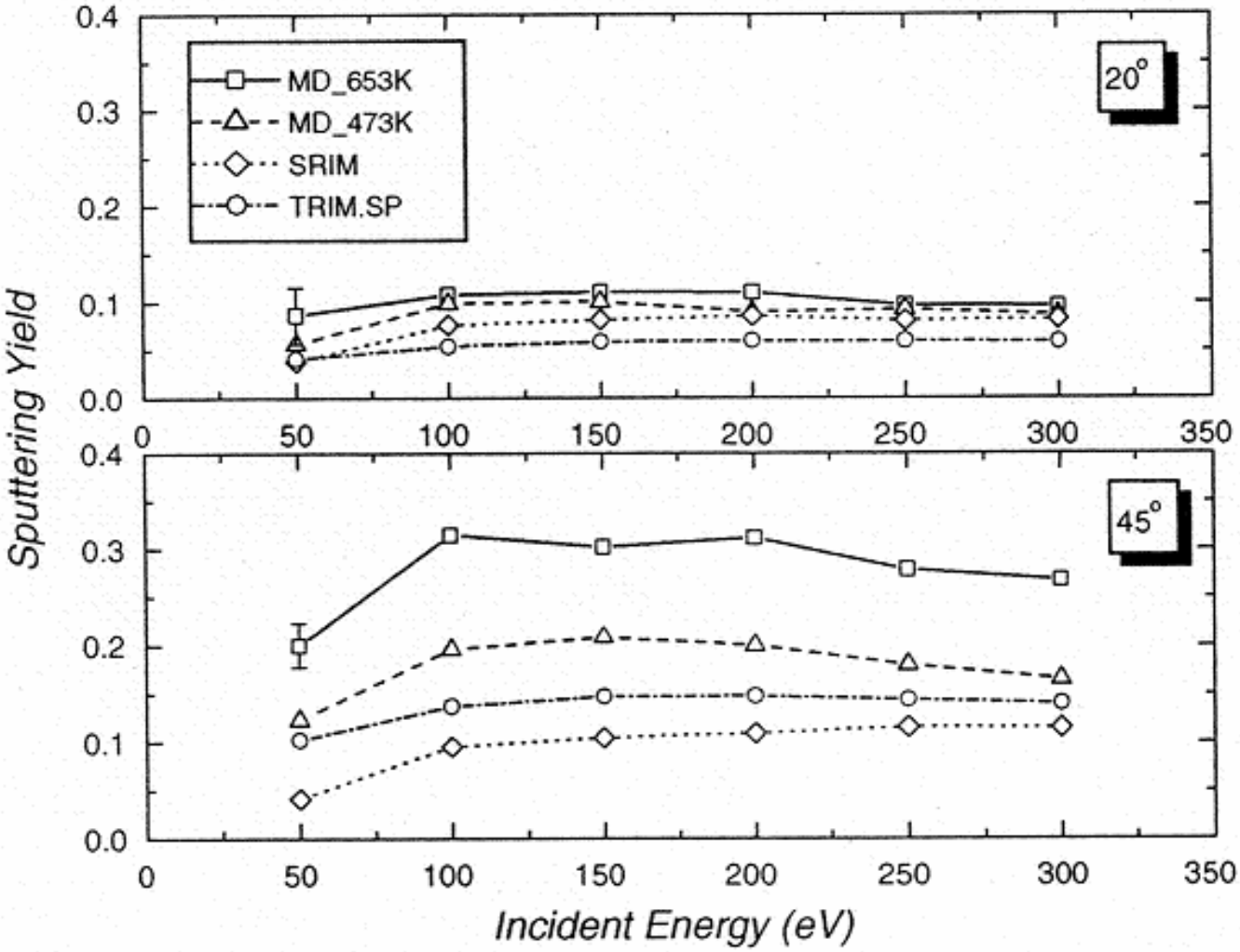

Fig.18. The sputtering yield at the function of incident energy. The error bars shown are representative of the statistical error for every point. (Hua-Tan Qiu, D. N. Ruzic, J. Nucl. Mater. 337-339 (2005) 1029.)

Classical MD with Li-Li pot. by NPA method , singlet ab initio pot.
for D-Li, bcc (42.2 Å x 42.2 Å x 59.8Å), 5040 Li atoms.

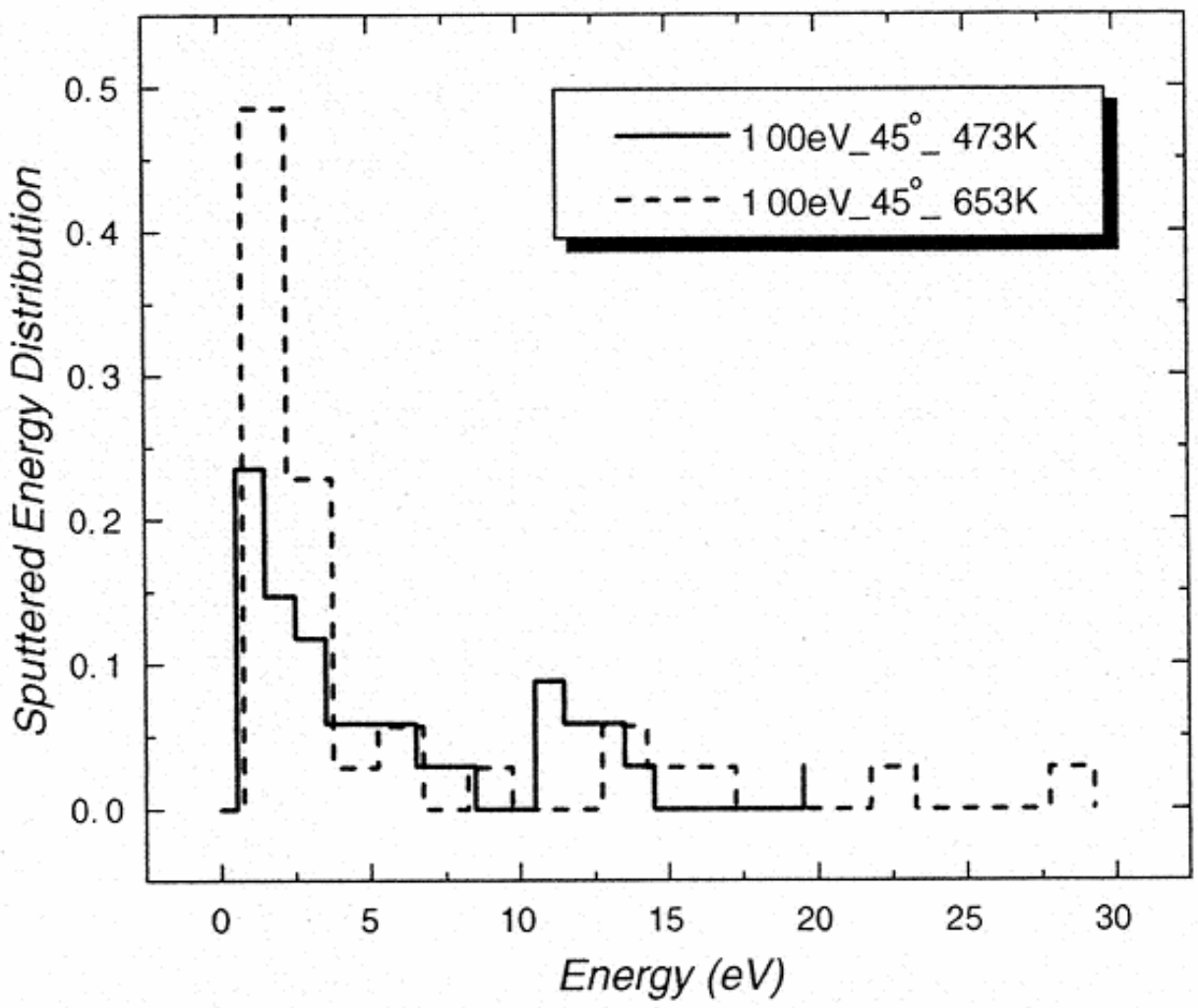

Fig. 19. The energy distribution of the sputtered atoms at different surface temperature. The low energy peak comes from the thermal sputtering due to evaporation flux on the surface. (Hua-Tan Qiu, D. N. Ruzic, J. Nucl. Mater. 337-339 (2005) 1029.)

Classical MD with Li-Li pot.by NPA metod, singlet ab initio pot.
for D-Li, bcc (42.2Å x 42.2Å x 59.8Å), 5040 Li atoms.

Summary & future subjects (1)

(1) BCA codes:

- calculate reliable sputtering yield for incident energy E > ~ 50 eV. (for mono-atomic, multi-component materials)

(2) Fitting formula for sputtering yield of compound materials:

- parameters for projectile-targets are needed.

(3) Fitting formula for sputtered energy due to low-energy ions:

- parameters for any E, projectile-targets are needed.

(4) Dynamic MC codes:

- calculate fluence- & temperature- dependent phenomena in long ranges of time.
- transport coefficients (diffusion coefficient, chemical reaction rate, desorption prob. , de-trapping energy, ...), are necessary, but often diverse or lack in experimental data.

Summary & future subjects (2)

(5) MD codes:

- sputtering yield for low-E, reflection, sticking cross-section, molecular formation/destruction, ...
- atomic states (excited states, charging, ..) of sputtered particles,
- transport coefficients (diffusion coefficient, physical/chemical desorption/adsorption, trap, ...), potential, ...
- simulation time for phenomena is very short ~10^{-9} s in real time

(6) Future subjects:

- MD codes can produce transport coefficients, atomic states of sputtered particles for MC modeling.
- MD codes can calculate potentials for classical MD.
- MD codes can make bubble formation ?