Molecular Dynamics Simulation of Redeposition Effect on Kinetic Roughening by High Energy Ar Bombardment

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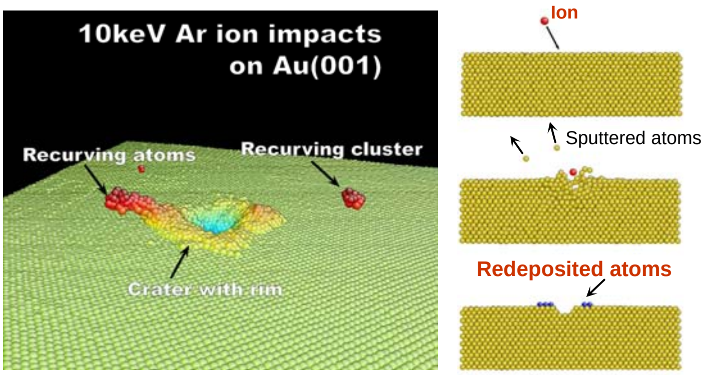
Abstract

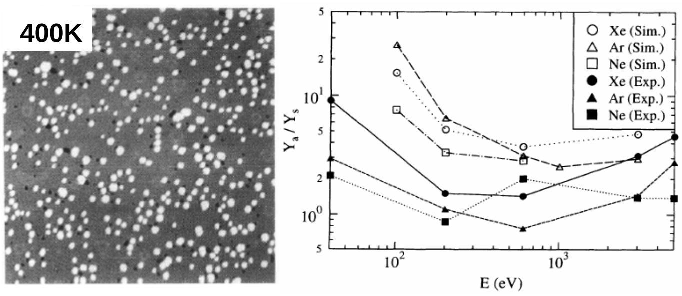
High energy ion bombardment on solid surface has attracted much attention, owing to its capability to fabricate ordered nanoscale structures such as self aligned quantum dots. In the present work, we employed classical molecular dynamics (MD) simulation to investigate the details of the surface structure evolution during the high energy Ar bombardment on Au and Pd (001) surface. Atomic collisions, sputtering yield, redeposition yield, distribution, crater formations and propagations of impact energy could be obtained by MD calculation. When Ar ion bombarded on the metal surface with high incident energy, we could observe that number of redeposited atoms was much larger than that of sputtering and distribution of redeposited atoms show variously with respect to the incident angle and energy. Considering kinetic roughening phenomena, we could confirm that redeposition effect would play an important role in the formation of surface patterns.

Redeposition Effect



- Residues on the surface after ion bombardment → **Redeposition.**
- Redeposition effect could observe by **only Molecular Dynamics.**
- As the scale goes down, **this effect becomes more important.**

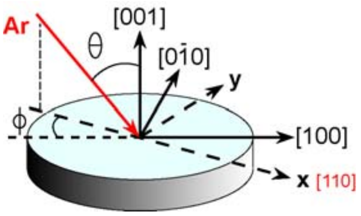
Previous work



5keV Xe on Pd(111) PRB 50, 11156 (1994)

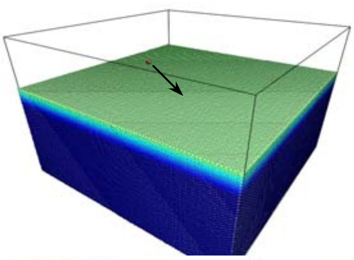
- Yield ratio between adatom & sputtering is more than 1
- Clearly shown the **'Redeposition Effect'**

Calculation Procedure



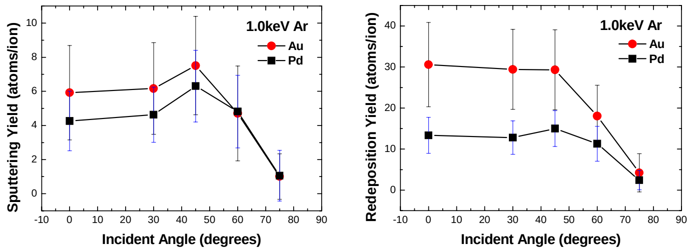
- Ion: Ar
- Substrate: Au & Pd(001)
- Incident Energy: 0.5, 1 keV
- Incident Angle
  → Θ = 0°, 30°, 45°, 60°, 75°
  → Φ = 45° : <110> direction

- Temperature: 300 K
  → damping layer included
- Force field
  → EAM[1] + ZBL[2]
- 1,000 trials for each case



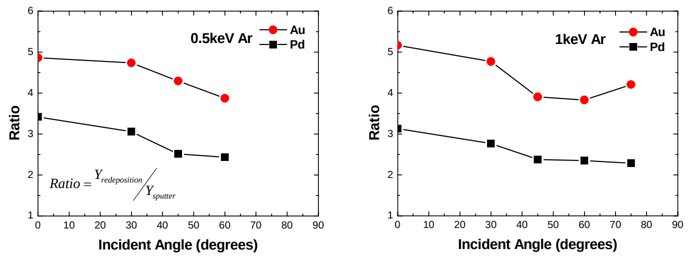
1) S.M. Foiles et al., PRB 33, 7983 (1986).
2) J.F. Ziegler et al., The Stopping and Range of Ions in Matter, Pergamon, New York (1985).

Redeposition Yields



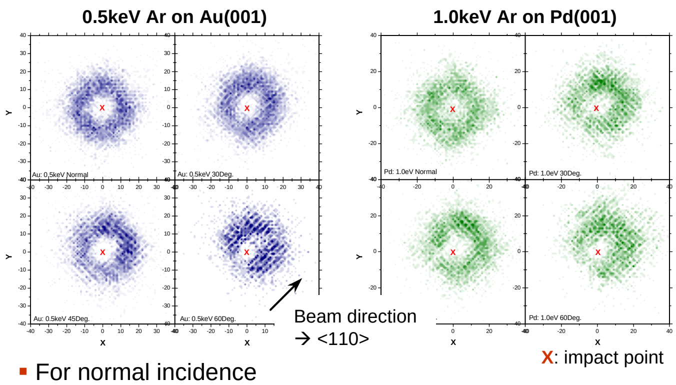
- Number of redeposition atoms was shown much larger than that of sputtered atoms.
- Both yields show variously for the incident angles.

Yield Ratio



- Ratio between redeposition and sputtering is **4~5 for Au, 2.5~3.5 for Pd** *irrespective of incident energy & angle.*
- These values are in good agreement with other results.

Redeposition Distributions



- For normal incidence
  → Au: isotropic distribution, Pd: anisotropic distribution
- For off-normal incidence, redeposition atoms
  → ~45°: accumulate in front of impact point
  → 45°~: accumulate beside impact point

Summary

- The effect of redeposition was clearly shown during ion sputtering.
- Redeposition atoms were significantly larger than sputtering atoms.
- Redeposited atoms were distributed variously with respect to the incident angle.