Equilibrium Shape of Nanometric Holes

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Introduction

- Single nanometric holes (nanopores) drilled in thin membranes are widely used for separation of single molecules and in microelectronics [1].
- Nanopores drilled in conductive and semi-conductive crystalline materials are prone to have improved electrical properties due to surface plasmon enhancement. They can be also used as a geometric confinement in studies of ordering at solid-liquid interfaces.
- The morphology of nanopores have a critical effect both on ordering of the adjacent liquid and on the charge distribution on the nanopore surface.
- Moreover, the stability of nanopores was found to depend on their shape.

Main Goals

- Identification of processes that lead to nanopore formation.
- Evaluation of stable nanopore shape both for amorphous and crystalline materials using Surface Evolver simulations.
- Achievement of control over the nanopore shape and formation of user specified nanopores.

Experimental Methods

- The nanopres were drilled in amorphous Si_3N_4 and in single crystal Si using the FEI Titan 80-300kV FEG S/TEM, operated in STEM mode (converged beam).
- The morphological analysis of the nanopres was conducted using high resolution Cs corrected imaging.
- The shape of nanopores was simulated using Surface Evolver [2].

Results & Discussion

Nanopore Formation Mechanism

Processes that occur under e-beam irradiation are removal of atoms by knock-on, radiolysis and heating [3].

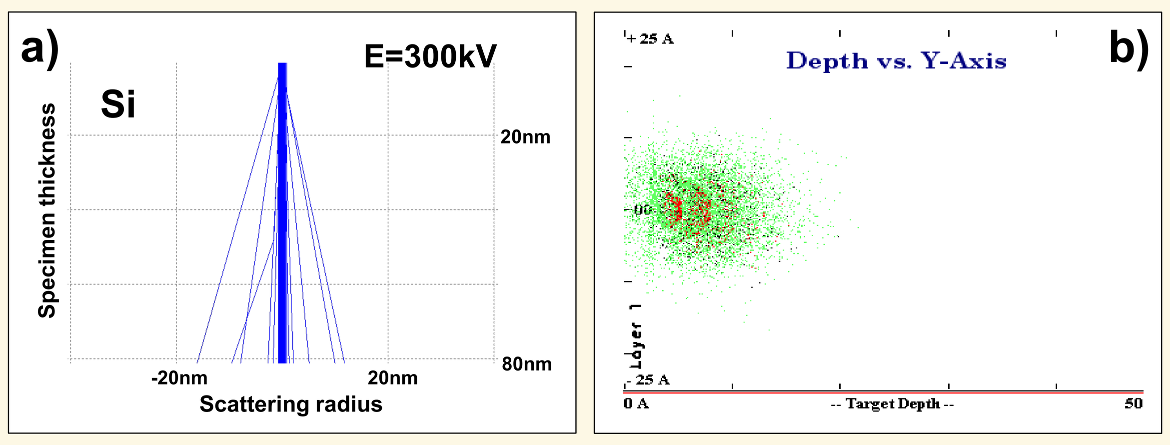

Figure 1. (a) Monte Carlo and (b) Stopping and Range of Ions in Matter (SRIM) simulations of electrons and Si ions respectively, in Si layer.

The increase in scattering radius of electrons (a) is around 2 nm for a 80 nm thick TEM specimen. Only 2% of the ionized Si atoms will sputter in the backward direction (b).

The results for Si_3N_4 are similar to those presented for Si.

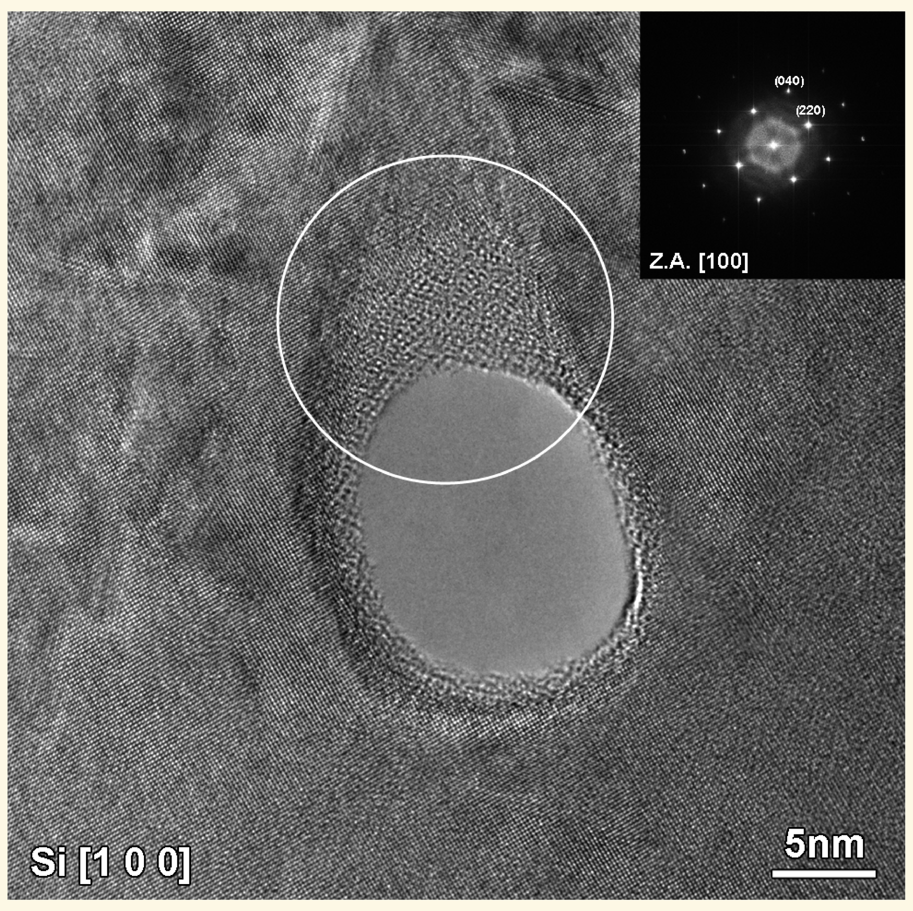

Figure 2. Aberration corrected (Cs=-3.8μm) HRTEM micrograph of a nanopore created in crystalline Si. The amorphous region (indicated with a white circle) was created by a static e-beam after drilling the hole, and shows that radiolysis damage is more rapid than knock-on damage. The FFT (inset) shows the existence of both amorphous and crystalline material.

The Nanopore Shape

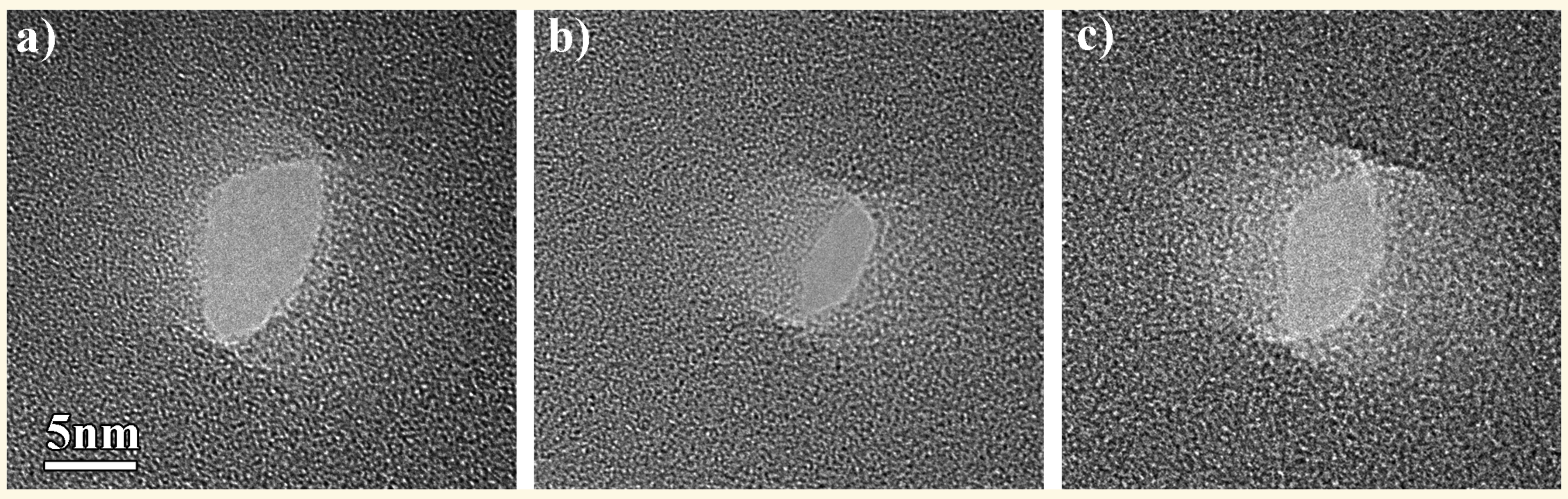

Figure 3. HRTEM micrographs of nanopores drilled in amorphous Si_3N_4 substrates with different diameter to length (D:t) ratios (D:t=0.5, 0.5 and 0.65 for a-c, respectively). The samples were tilted at 30° for image acquisition. The holes drilled in specimens with a slightly lower D:t ratio (a), (b) have an "hour-glass" shape, in contrast to a conical shape for holes drilled in thinner regions of the TEM sample(c).

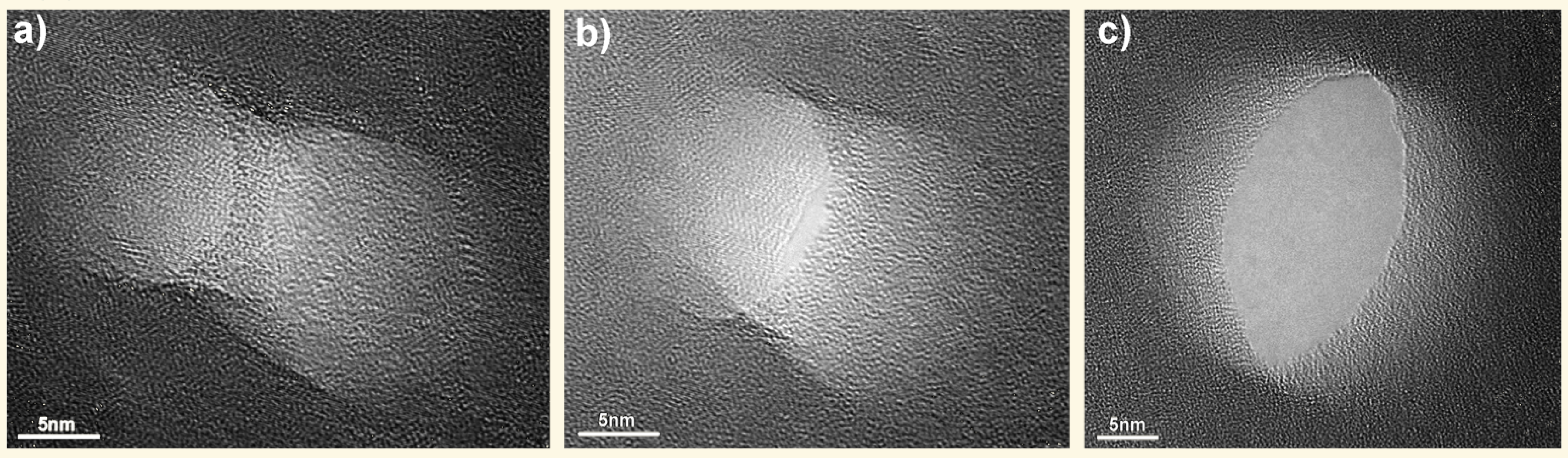

Figure 4. HRTEM micrographs of nanopres drilled in crystalline Si with different D:t ratios (0.2, 0.35 and 0.75 for a-c, respectively) [4]. The samples were tilted at 30° for image acquisition. The nanopores drilled in specimens with a lower D:t ratio (a), (b) have an "hour-glass" shape, in a contrast to a conical shape for holes drilled in thinner regions of the TEM specimen (c).

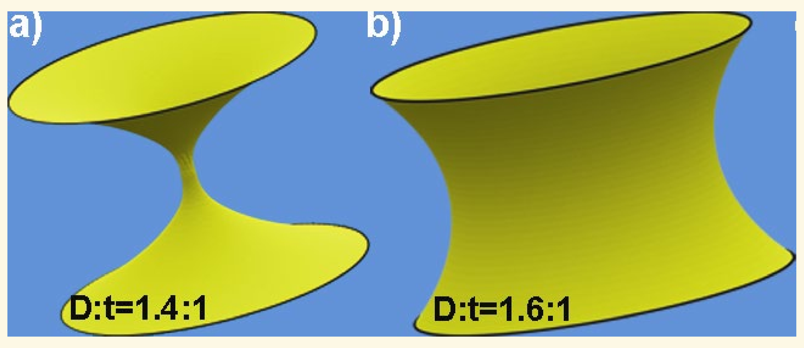

Figure 5. Holes of different D:t ratio equilibrated by Surface Evolver for an amorphous material. (a) partially equilibrated hole with D:t=1.4:1 and (b) fully equilibrated hole with D:t=1.6:1. The hole in (a) is not stable and collapses into a closed pore.

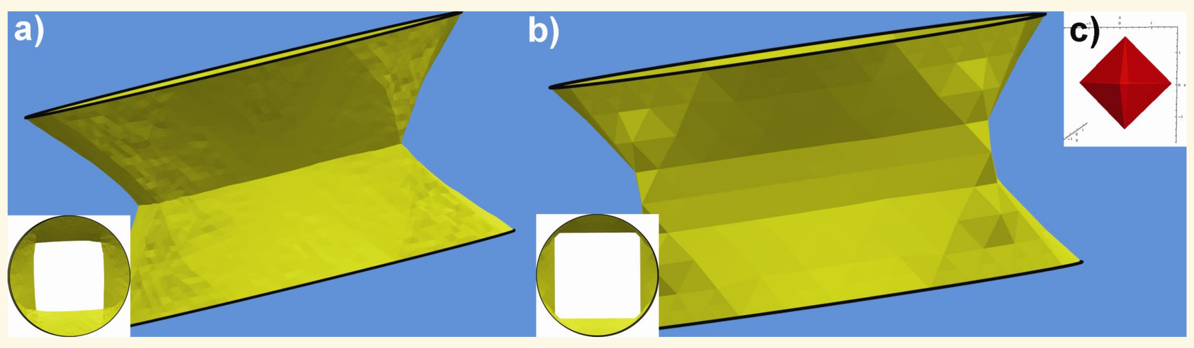

Figure 6. Holes with a D:t=2:1 ratio equilibrated by Surface Evolver and the Wulff shape that contains only {111} surfaces (c). (a) fully equilibrated hole and (b) partially equilibrated hole. The insets are top views of the respective shapes.

Summary & Conclusions

- Nanopores created in amorphous Si_3N_4 and crystalline Si were created and investigated.
- It was found that:
  - Nanopores are formed by radiolysis assisted knock-on.
  - The nanopore shape changes as a function of surface diffusion during nanopore formation, due to thermal energy transferred to the nanopore from the electron beam.
  - The nanopore shape depends on the dimensions of the nanopore and the material in which they are formed.

Future Work

- Analysis of confined solid- liquid interfaces between Si and molten metals.

References

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