IRRADIATION OF NANOPOROUS STRUCTURES WITH LIGHT AND HEAVY LOW-ENERGY IONS

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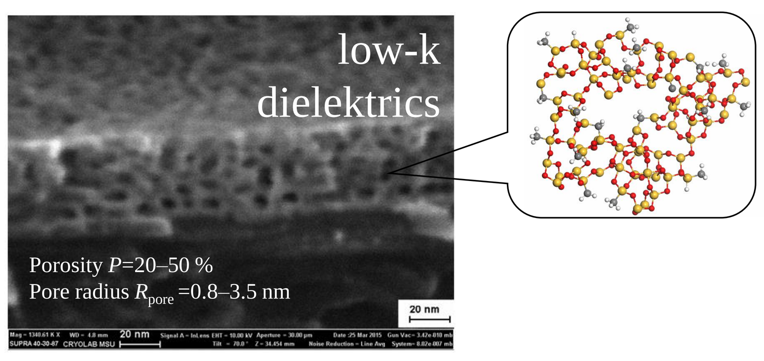
Introduction

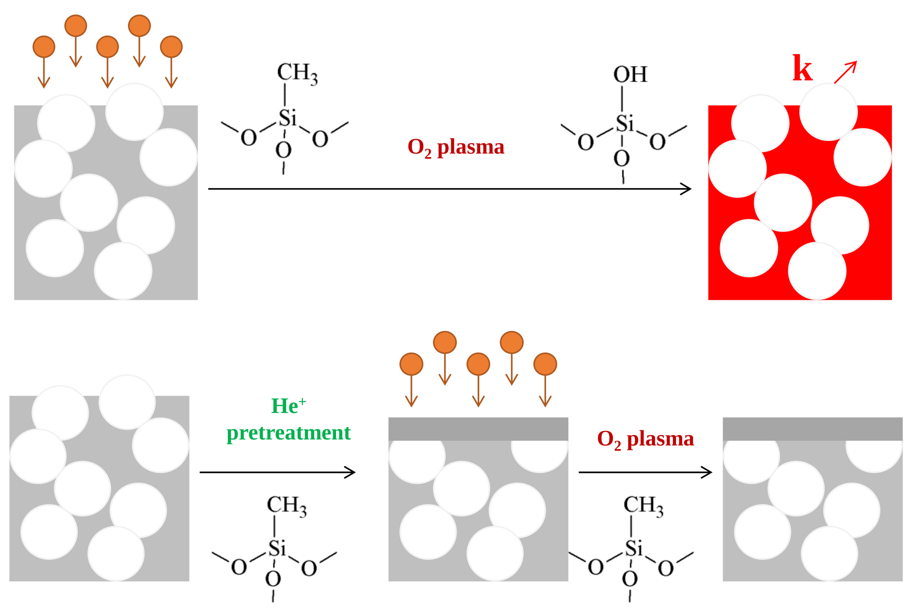
Due to complex morphology, ion irradiation of nanoporous structures could result in very specific physical phenomena, comprising dramatic structural changes. But in certain cases, such an influence can also have beneficial effects on nanoporous materials. It was demonstrated that low-energy ion pretreatment of nanoporous organosilicate glass films with low dielectric constant (low-*k*) results in the decrease of their degradation during further plasma processing.

Low-*k* films are used as interlayer isolators in advanced elements of nanoelectronics. In order to reduce the value of the dielectric constant, these films have a large number of interconnecting nanosized pores covered with methyl groups.

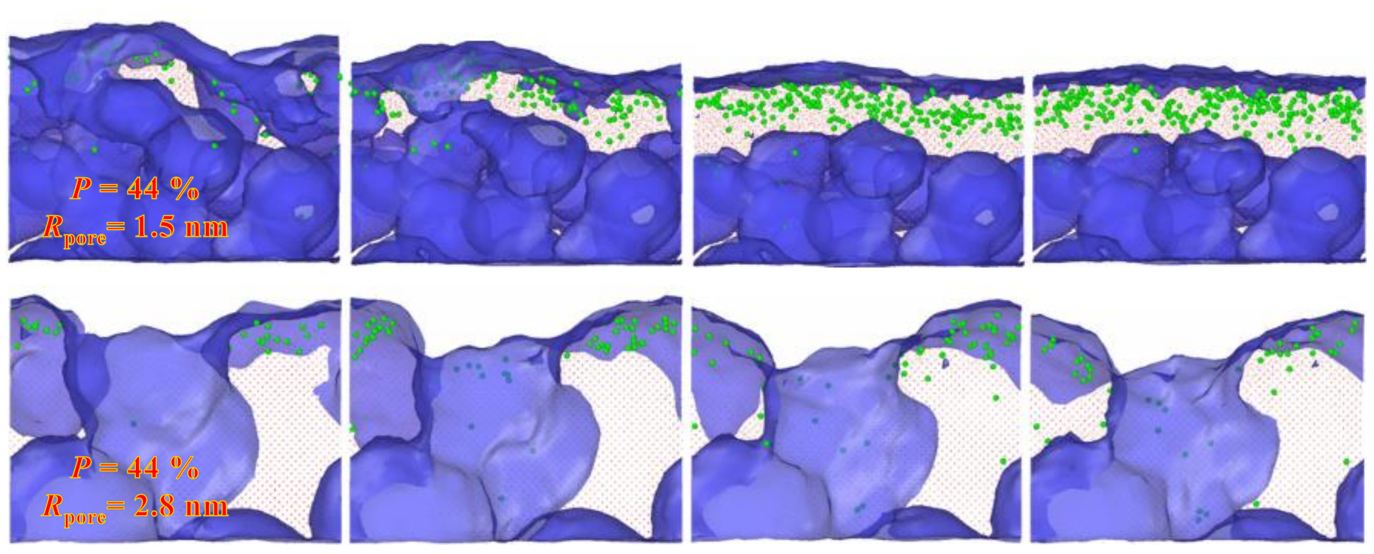


Active plasma species can easily penetrate into deeper layers of these films, damage material structure. This results in decrease of dielectric constant.

It was shown experimentally that for some samples preliminary irradiated with helium ions the damage is reduced significantly. The decrease in damage occurs due to ion-induced densification of the near-surface layers up to pore sealing.



Ar 200 eV



Molecular dynamics simulation of Ar ion irradiation showed that ion impacts initiate near-surface solid layer formation that prevents the material from penetration of active plasma species. The appearance of this layer is the most probable for the film with low porosity and pore radius.

This work aims to reveal how ion mass and energy affect the process of layer formation.

Methodology

Method: Molecular Dynamics

Models:
- Si and SiO_2 nanoporous models
- Stillinger-Weber potential for pure Si
- Tersoff potential for SiO_2
- Firsov-Moliere for ion-surface interactions

Relaxation:
- Time: 20 ps
- Temperature: 300 K
- Nosé-Hoover thermostat

Boundary conditions:

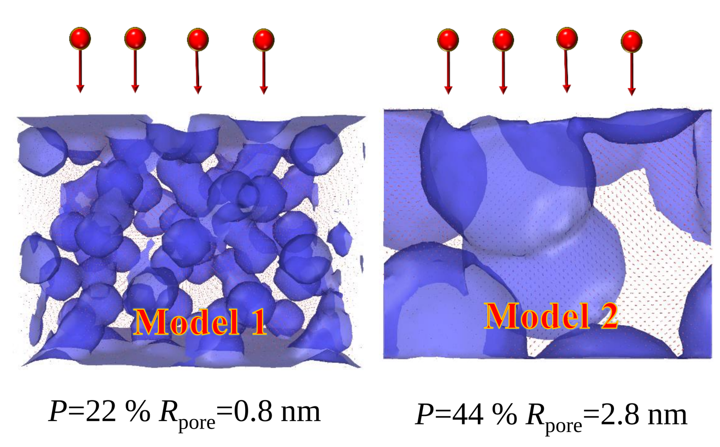
periodic boundary conditions in (100) and (010) directions;
- direction non-periodic
- after passing the upper boundary atoms are deleted from simulated ensemble

Temperature control:

during the simulation of single ion impact Si-cascade had been developing naturally during the first half of time between impacts (3.5 ps). Then the overall temperature was kept at 300 K by using Berendesen damped velocity scaling with a time constant of 18 fs

Timestep: 0.1 fs

He Ne Ar Xe 50–200 eV

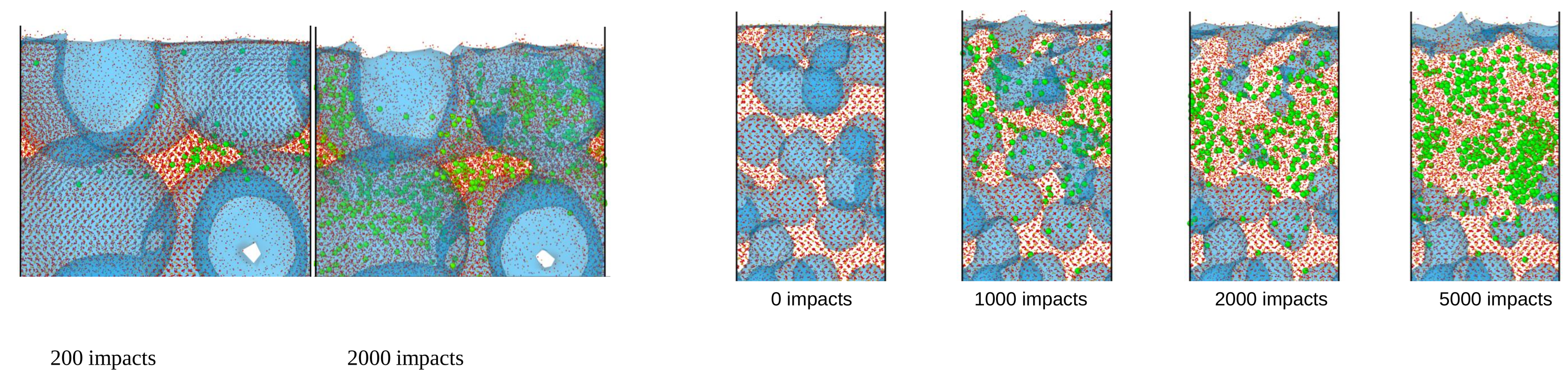


P=22 % R_{pore}=0.8 nm   *P*=44 % R_{pore}=2.8 nm

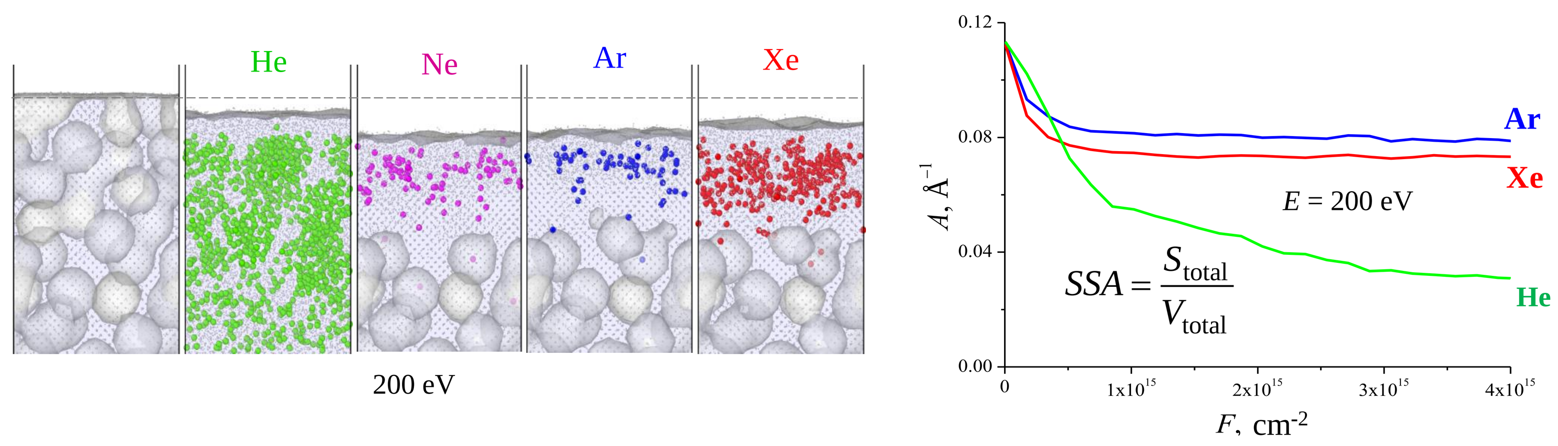
Results

For energies up to 200 eV Model 2 with large pores shows sufficiently high resistance to ion bombardment. In case of Model 1 for all ions the rapid pore collapse and solid layer formation are observed.

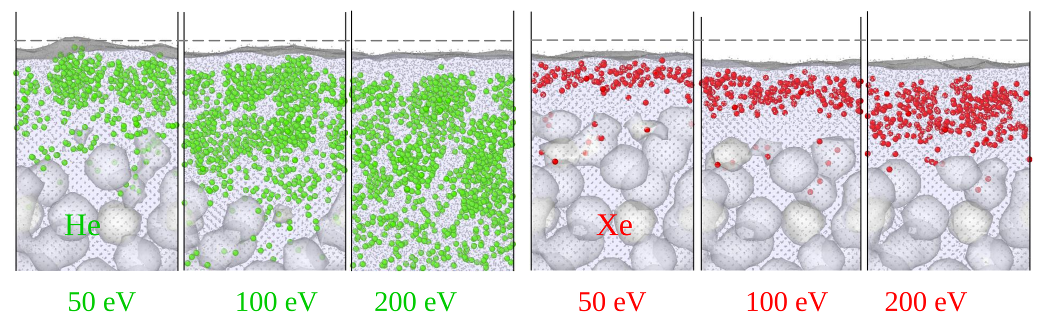
He 100 eV



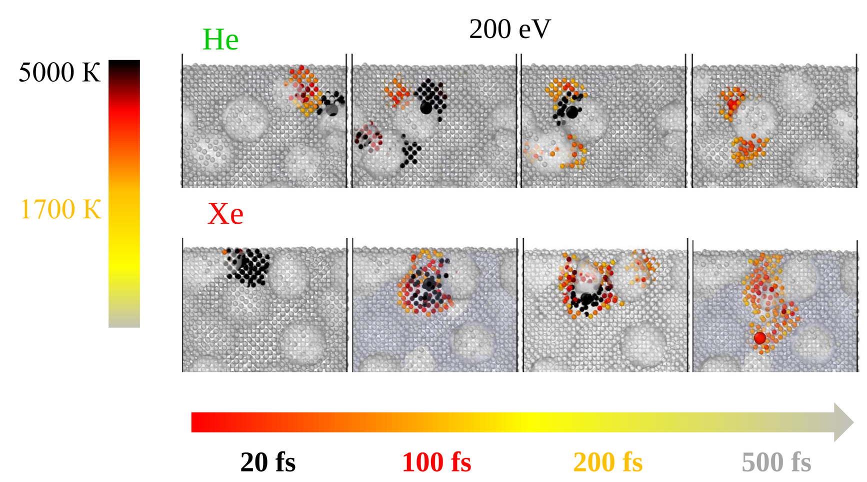
The intensity and rate of pore collapse depend strongly on the ion type and energy.



The depth of the solid layer at the steady state also depends strongly on the sort of ions and their energy. This value is **almost linearly proportional to the ion energy at low energies.**



During the first 100 fs the incident **He ion** manages to move a large distance across the target and create a few small regions of local overheating, but after 500 fs the ion loses almost completely its energy in collisions with atoms. **So high penetrating ability of He ions due to their small size leads to the infiltration of implanted atoms into deeper layers of the material, causing slow collapse of pores that continues even after the formation of an solid layer.**



The impact of the **Xe ion** of the same initial energy leads to the formation of a much more extended overheated region, which exists longer. **So the pore collapse happens most rapidly. However, at certain fluence this process stops due to the formation of a sufficiently extended continuous layer, which prevents incident ions from reaching underlying pores.**

Conclusions

- Results of performed MD simulations explain the effects of densification and pore sealing in low-k films observed experimentally:

  For model with smaller pores (with radius of 0.8 nm in our study) the pore collapse and appearance of a solid layer on the surface are observed occur under ion irradiation.

  For the models with large pores (with radius of 2.8 nm) no significant structural changes under the same irradiation conditions.
- **The pore collapse in the models with small pores happens most rapidly under the heavy Ar and Xe ion irradiation. However, at certain fluence this process stops due to the formation of a sufficiently extended continuous layer, which prevents incident ions from reaching underlying pores.**
- **For light He ions, the collapse of pores occurs more slowly, but due to their high penetrating ability, these ions are able to affect pores located in deeper layers, even after the formation of an solid layer. Moreover, in this case an intensive ion accumulation in the forming layer is observed.**
- The formed solid layer is quite thin (several nanometers) and, therefore, does not influence k-value of OSG films. Thus, the low-energy ion bombardment (preferably by He^+ ions) can be used for pretreatment of low-k films with small pore size in order to reduce their damage under radical exposure in downstream plasma conditions.