

Deposition and annealing of interstellar ices: a mixed neutron scattering and molecular dynamics study.

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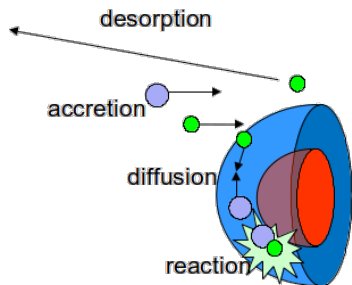
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Interstellar ices

Complex processes occur...



- Molecular layer on grains
- Surfaces are key for gas-solid phase exchanges

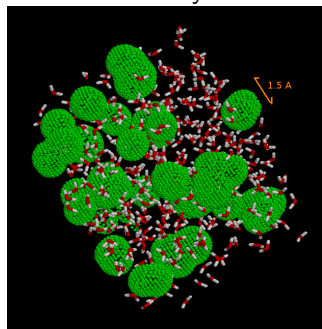
Structure ?

- Amorphous/crystalline ?
- Porosity (open/closed) ?
- Surface area ?

Interstellar ices

A mixed Theory and Experimental approach

Molecular Dynamics



Ghesquière et al, PCCP, 2014

- Deposition

Neutron Scattering experiments

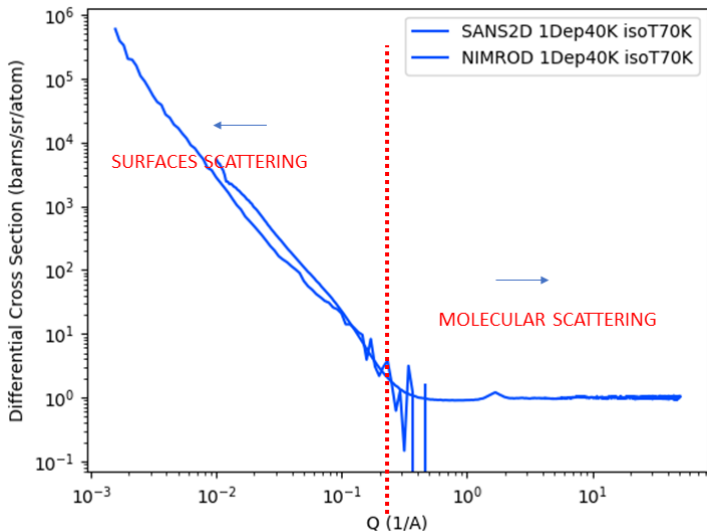


Bowron et al., Rev Sci Inst, 2010

- Heating

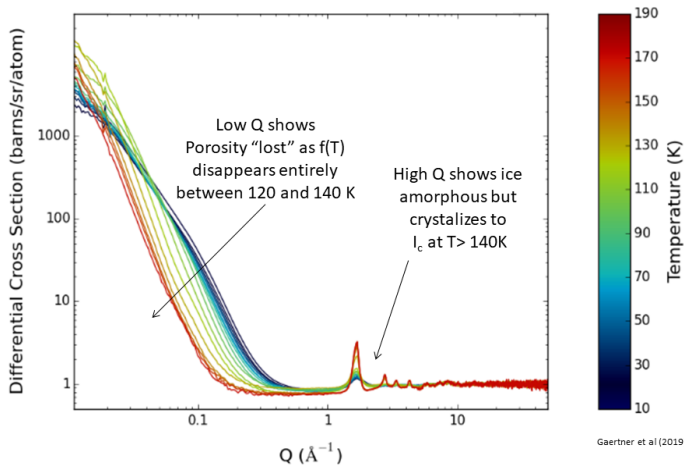
Deposition and Heating of Interstellar ices

What is a neutron scattering spectrum ?



Deposition and Heating of Interstellar ices

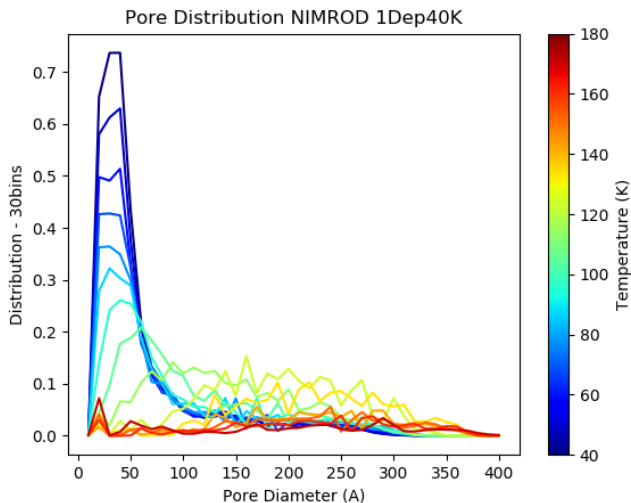
What happens when we warm it up?



Gaertner et al (2019) in prep

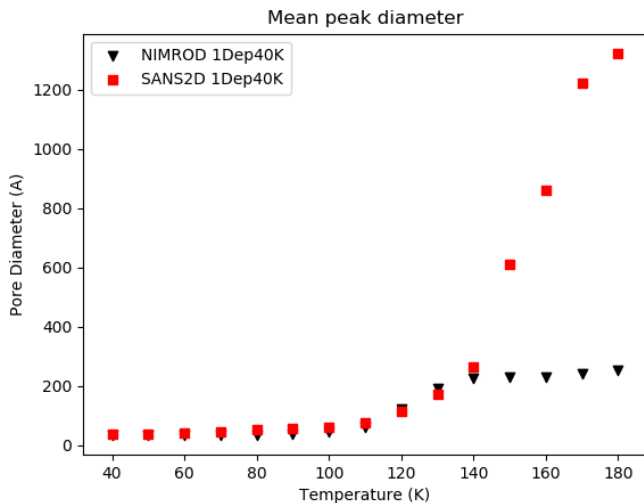
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Thermal evolution of the ice



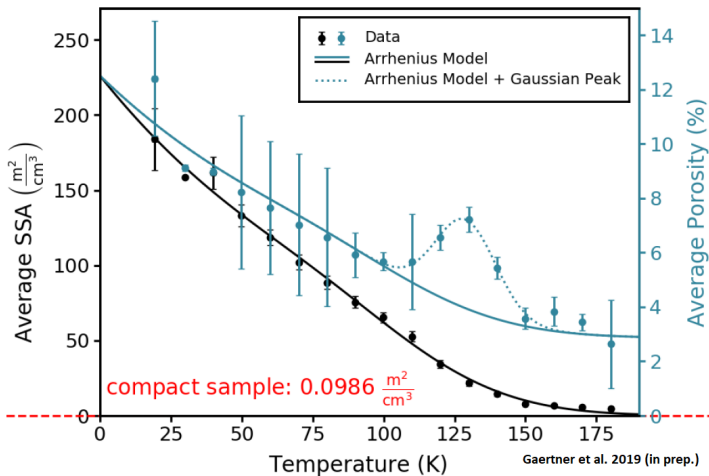
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from the Low-Q Part : Pore-size distribution



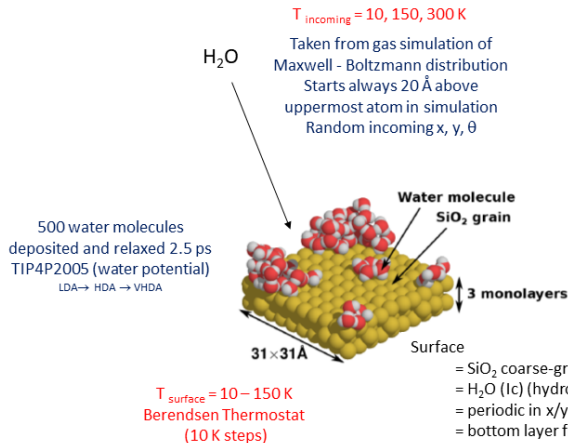
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Surface area and porosity estimation.



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Molecular dynamics insight



DL_POLY 2.20
60 ps/day

Classical molecular dynamics

Lennard-Jones potential

$$E(r) \sim \epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

for $E(\text{O}-\text{O})$ $E(\text{H}-\text{O})$ $E(\text{H}-\text{H})$

Coulomb potential

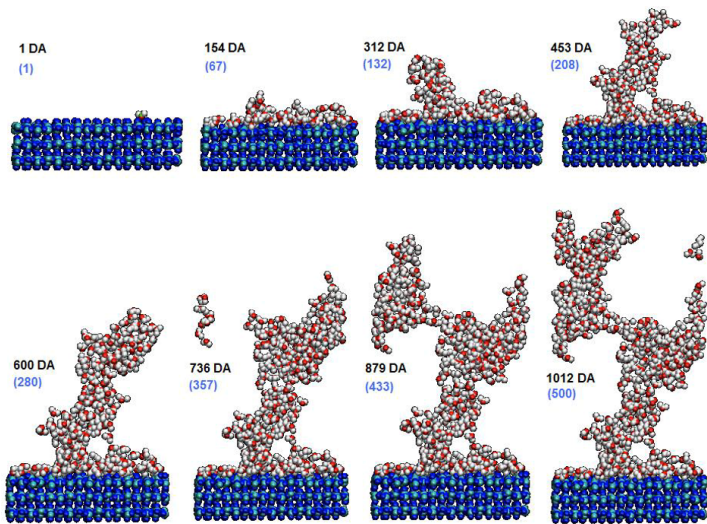
$$E(r) \sim \frac{q_1 q_2}{r}$$

for $E(\text{O}-\text{O})$

Elkind & Fraser JCP (2019) in prep

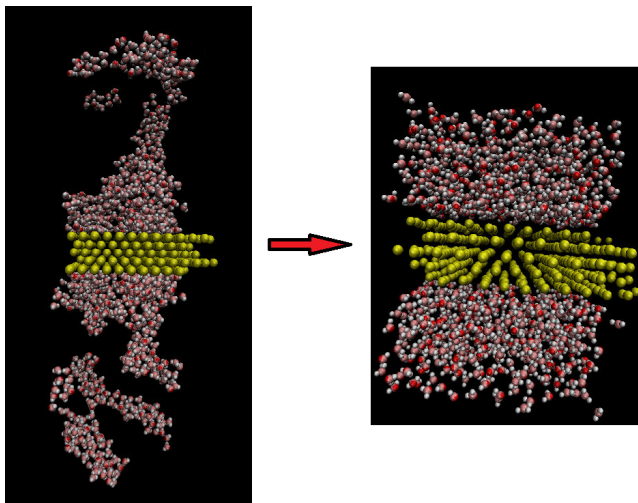
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Simulating the deposition



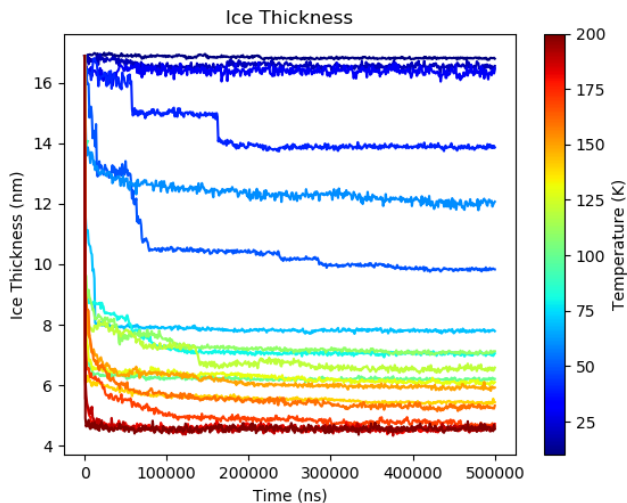
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Annealing them



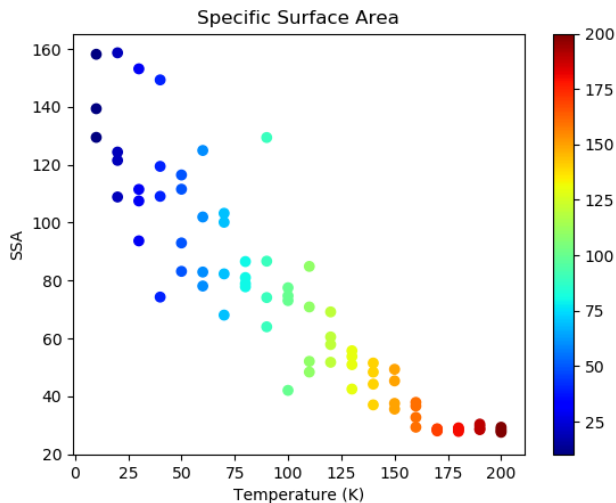
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Annealing them



Deposition and Heating of Interstellar ices

Annealing them



Interstellar ice evolution

Take-Home Messages

- Neutron scattering : a powerful technique to scan large-scale structures in ices
- Molecular dynamics : gives a molecular picture of the ice
- Ice deposits with a "tower-like" structure with typical pore size of around 4nm
- Ice is compacted with temperature
- Pores become larger but specific surface decreases

A big thank you !

H. Fraser, V. Deguin, and S. Gaertner from ISIS



Questions ?

