Collisional and structural properties of water ice in planet-forming regions

Supplementary material
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112 Pseudopeaks for $I(Q) \times Q^{3}$ for averaged isothermal scans of ices. . . 114
Additional neutron scattering data for low temperature growth and pore collapse of amorphous solid water

This document contains additional graphs that supplement the data presented in Chapter 9. The graphs are grouped into growth, heating and isothermal measurements and are further divided into results from single and averaged scans. In Section 1, the single neutron scattering patterns for the ice growth are presented, along with the quasi-plateaus used to extract Porod constants (and hence specific surface areas) and the pseudopeaks used to extract periodic spacings. In Section 2, the quasi-plateaus used to extract Porod constants and the pseudopeaks used to extract periodic spacings are presented. The neutron scattering patterns appear in Chapter 9. In Section 3, the single neutron scattering patterns for the ice growth are presented, along with the quasi-plateaus used to extract Porod constants (and hence specific surface areas) and the pseudopeaks used to extract periodic spacings. In Section 4, the single neutron scattering patterns for the ice growth are presented, along with the quasi-plateaus used to extract Porod constants, specific surface areas, the pseudopeaks used to extract periodic spacings, periodic spacings, radii of gyration, s parameters and d parameters. In Section 5, the quasi-plateaus used to extract Porod constants and the pseudopeaks used to extract periodic spacings are presented. The neutron scattering patterns appear in Chapter 9.

The \( I(Q) \times Q^3 \) pseudopeaks are not shown for the growth of the 50 K and 52 K ices as they were not used to extract periodic spacings. The \( I(Q) \times Q^{2.5} \) pseudopeaks are
not shown for the growth, heating or isothermal scans of the 17 K ices for the same reason. Elsewhere, both sets of pseudopeaks are shown, with the one used to extract periodic spacings indicated in the caption. For the single isothermal scans, only the pseudopeaks actually used to extract periodic spacings are shown.
1 Ice growth: single scans

1.1 Neutron scattering patterns

Figure 1: Single neutron scattering patterns for deposition of ices at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second).
1.2 Quasi-plateaus for specific surface area

Figure 2: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for deposition of ices at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second).
1.3 Pseudopeaks for periodic spacings

Figure 3: Pseudopeaks used to extract periodic spacings for deposition of ices at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second).
2 Ice growth: averaged scans

2.1 Quasi-plateaus for specific surface area

Figure 4: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for averaged deposition scans of ices deposited at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second).
2.2 Pseudopeaks for periodic spacings

Figure 5: Pseudopeaks used to extract periodic spacings for averaged deposition scans of ices deposited at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second).
3 Ice heating: single scans

3.1 Neutron scattering patterns

Figure 6: Single neutron scattering patterns for heating of ices deposited at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second).
3.2 Quasi-plateaus for specific surface area

Figure 7: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for heating of ices deposited at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second).
3.3 Pseudopeaks for periodic spacings

Figure 8: Pseudopeaks for \( I(Q) \times Q^{2.5} \) for heating of ices deposited at a. 50 K and b. 52 K. The pseudopeaks shown here were used up to 90 K for the 50 K ice and up to 100 K for the 52 K ice.
Figure 9: Pseudopeaks for $I(Q) \times Q^3$ for heating of ices deposited at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second). The pseudopeaks shown here were used from 90 K for the 50 K ice, from 100 K for the 52 K ice and throughout for the 17 K ices.
4 Ice isothermal: single scans

4.1 Neutron scattering patterns

50 K deposition

![Graphs showing neutron scattering patterns for isothermal scans at 60 K, 70 K, 80 K, and 90 K.](Figure 10)

Figure 10: Single neutron scattering patterns for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 11: Single neutron scattering patterns for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
Figure 12: Single neutron scattering patterns for isothermal scans at a. 140 K, b. 150 K, c. 160 K and d. 170 K. The last isothermal scan for isothermal at 150 K was corrupted and so the result is not shown.
52 K deposition

Figure 13: Single neutron scattering patterns for isothermal scans at a. 70 K, b. 80 K, c. 90 K and d. 100 K.
Figure 14: Single neutron scattering patterns for isothermal scans at a. 110 K, b. 120 K, c. 130 K and d. 140 K.
Figure 15: Single neutron scattering patterns for isothermal scans at a. 150 K, b. 160 K, c. 170 K and d. 180 K.
**1st 17 K deposition**

Figure 16: Single neutron scattering patterns for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K. There is only 30 minutes of data for 40 K because the beam went off during measurements.
Figure 17: Single neutron scattering patterns for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 18: Single neutron scattering patterns for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
Figure 19: Single neutron scattering patterns for isothermal scans at a. 140 K and b. 150 K.
2\textsuperscript{nd} 17 K deposition

Figure 20: Single neutron scattering patterns for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K.
Figure 21: Single neutron scattering patterns for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 22: Single neutron scattering patterns for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
4.1 Neutron scattering patterns

Figure 23: Single neutron scattering patterns for isothermal scans at a. 140 K, b. 150 K, c. 160 K and d. 170 K.
Figure 24: Single neutron scattering patterns for isothermal scans at 180 K.
4.2 Quasi-plateaus for specific surface area

50 K deposition

Figure 25: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 26: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
Figure 27: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 140 K, b. 150 K, c.160 K and d. 170 K. The last isothermal scan for isothermal at 150 K was corrupted and so the result is not shown.
52 K deposition

Figure 28: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at **a. 70 K, b. 80 K, c. 90 K and d. 100 K.**
4.2 Quasi-plateaus for specific surface area

Figure 29: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 110 K, b. 120 K, c. 130 K and d. 140 K.
Figure 30: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 150 K, b. 160 K, c. 170 K and d. 180 K.
4.2 Quasi-plateaus for specific surface area

1st 17 K deposition

![Graphs showing Quasi-plateaus for specific surface area at 20 K, 30 K, 40 K, and 50 K.](image)

Figure 31: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K. There is only 30 minutes of data for 40 K because the beam went off during measurements.
Figure 32: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
4.2 Quasi-plateaus for specific surface area

Figure 33: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
Figure 34: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 140 K and b. 150 K.
2nd 17 K deposition

Figure 35: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K.
Figure 36: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
4.2 Quasi-plateaus for specific surface area

Figure 37: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
Figure 38: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at a. 140 K, b. 150 K, c.160 K and d. 170 K.
4.2 Quasi-plateaus for specific surface area

Figure 39: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for isothermal scans at 180 K.
4.3 Specific surface area

50 K deposition

Figure 40: Specific surface area for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 41: Specific surface area for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
Figure 42: Specific surface area for isothermal scans at a. 140 K, b. 150 K, c. 160 K and d. 170 K. The last isothermal scan for isothermal at 150 K was corrupted and so the result is not shown.
52 K deposition

Figure 43: Specific surface area for isothermal scans at a. 70 K, b. 80 K, c. 90 K and d. 100 K.
Figure 44: Specific surface area for isothermal scans at a. 110 K, b. 120 K, c. 130 K and d. 140 K.
4.3 Specific surface area

Figure 45: Specific surface area for isothermal scans at a. 150 K, b. 160 K, c. 170 K and d. 180 K.
1st 17 K deposition

Figure 46: Specific surface area for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K. There is only 30 minutes of data for 40 K because the beam went off during measurements.
4.3 Specific surface area

Figure 47: Specific surface area for isothermal scans at

a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 48: Specific surface area for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
4.3 Specific surface area

Figure 49: Specific surface area for isothermal scans at a. 140 K and b. 150 K.
2\textsuperscript{nd} 17 K deposition

![Graphs showing specific surface area for isothermal scans at different temperatures.](image)

Figure 50: Specific surface area for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K.
Figure 51: Specific surface area for isothermal scans at **a.** 60 K, **b.** 70 K, **c.** 80 K and **d.** 90 K.
Figure 52: Specific surface area for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
Figure 53: Specific surface area for isothermal scans at a. 140 K, b. 150 K, c.160 K and d. 170 K.
Figure 54: Specific surface area for isothermal scans at 180 K.
4.4 Pseudopeaks for periodic spacings

50 K deposition

Figure 55: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K. $I(Q) \times Q^{2.5}$ was used up to 80 K and $I(Q) \times Q^3$ was used from 90 K onwards.
Figure 56: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K. The pseudopeak disappears after 110 K. $I(Q) \ast Q^{2.5}$ was used up to 80 K and $I(Q) \ast Q^3$ was used from 90 K onwards.
Figure 57: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 140 K, b. 150 K, c. 160 K and d. 170 K. $I(Q) \times Q^{2.5}$ was used up to 80 K and $I(Q) \times Q^{3}$ was used from 90 K onwards. The last isothermal scan for isothermal at 150 K was corrupted and so the result is not shown.
52 K deposition

Figure 58: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 70 K, b. 80 K, c. 90 K and d. 100 K. \( I(Q) \times Q^{2.5} \) was used up to 100 K and \( I(Q) \times Q^3 \) was used from 110 K onwards.
Figure 59: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 110 K, b. 120 K, c. 130 K and d. 140 K. The pseudopeak disappears after 120 K. $I(Q) \times Q^{2.5}$ was used up to 100 K and $I(Q) \times Q^3$ was used from 110 K onwards.
Figure 60: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 150 K, b. 160 K, c. 170 K and d. 180 K. $I(Q) \ast Q^{2.5}$ was used up to 100 K and $I(Q) \ast Q^3$ was used from 110 K onwards.
1st 17 K deposition

Figure 61: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K. There is only 30 minutes of data for 40 K because the beam went off during measurements.
Figure 62: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 63: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
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Figure 65: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K.
Figure 66: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 67: Pseudopeaks used to extract periodic spacings for isothermal scans at a. 100 K, b. 110 K, c. 120 K and d. 130 K.
Figure 68: Pseudopeaks used to extract periodic spacings for isothermal scans at 
a. 140 K, b. 150 K, c. 160 K and d. 170 K.
Figure 69: Pseudopeaks used to extract periodic spacings for isothermal scans at 180 K.
4.5 Periodic spacings

50 K deposition

Figure 70: Periodic spacings for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
4.5 Periodic spacings

Figure 71: Periodic spacings for isothermal scans at a. 100 K, b. 110 K and c. 120 K. After 120 K, the periodic spacings can no longer be extracted.
52 K deposition

Figure 72: Periodic spacings for isothermal scans at **a.** 70 K, **b.** 80 K, **c.** 90 K and **d.** 100 K.
4.5 Periodic spacings

Figure 73: Periodic spacings for isothermal scans at a. 110 K and b. 120 K. After 120 K, the periodic spacings can no longer be extracted.
1st 17 K deposition

Figure 74: Periodic spacings for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K. There is only 30 minutes of data for 40 K because the beam went off during measurements.
Figure 75: Periodic spacings for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 76: Periodic spacings for isothermal scans at a. 100 K, b. 110 K. After 110 K, the periodic spacings can no longer be extracted.
2nd 17 K deposition

Figure 77: Periodic spacings for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K.
Figure 78: Periodic spacings for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 79: Periodic spacings for isothermal scans at a. 100 K and b. 110 K. After 110 K, the periodic spacings can no longer be extracted.
4.6 Radius of gyration

50 K deposition

Figure 80: Radius of gyration for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 81: Radius of gyration for isothermal scans at a. 100 K and b. 110 K. After 110 K, the radius of gyration can no longer be extracted.
52 K deposition

Figure 82: Radius of gyration for isothermal scans at a. 70 K, b. 80 K, c. 90 K and d. 100 K.
Figure 83: Radius of gyration for isothermal scans at a. 110 K and b. 120 K. After 120 K, the radius of gyration can no longer be extracted.
1st 17 K deposition

Figure 84: Radius of gyration for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K. There is only 30 minutes of data for 40 K because the beam went off during measurements.
4.6 Radius of gyration

Figure 85: Radius of gyration for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 86: Radius of gyration for isothermal scans at 100 K. After 100 K, the radius of gyration can no longer be extracted.
2nd 17 K deposition

Figure 87: Radius of gyration for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K.
Figure 88: Radius of gyration for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 89: Radius of gyration for isothermal scans at a. 100 K. After 100 K, the radius of gyration can no longer be extracted.
4.7 \(s\) parameter

50 K deposition

Figure 90: \(s\) parameter for isothermal scans at **a. 60 K**, **b. 70 K**, **c. 80 K** and **d. 90 K**.
Figure 91: $s$ parameter for isothermal scans at a. 100 K and b. 110 K. After 110 K, the $s$ parameter can no longer be extracted.
52 K deposition

Figure 92: $s$ parameter for isothermal scans at a. 70 K, b. 80 K, c. 90 K and d. 100 K.
Figure 93: $s$ parameter for isothermal scans at a. 110 K and b. 120 K. After 120 K, the $s$ parameter can no longer be extracted.
1st 17 K deposition

Figure 94: $s$ parameter for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K. There is only 30 minutes of data for 40 K because the beam went off during measurements.
Figure 95: $s$ parameter for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 96: $s$ parameter for isothermal scans at a. 100 K. After 100 K, the $s$ parameter can no longer be extracted.
Figure 97: $s$ parameter for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K.
Figure 98: $s$ parameter for isothermal scans at **a.** 60 K, **b.** 70 K, **c.** 80 K and **d.** 90 K.
Figure 99: $s$ parameter for isothermal scans at 100 K. After 100 K, the $s$ parameter can no longer be extracted.
4.8  $d$ parameter

50 K deposition

![Graphs a to d showing $d$ parameter over time for different temperatures.](image)

Figure 100: $d$ parameter for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 101: $d$ parameter for isothermal scans at a. 100 K and b. 110 K. After 110 K, the $d$ parameter can no longer be extracted.
52 K deposition

Figure 102: $d$ parameter for isothermal scans at a. 70 K, b. 80 K, c. 90 K and d. 100 K.
Figure 103: $d$ parameter for isothermal scans at a. 110 K and b. 120 K. After 120 K, the $d$ parameter can no longer be extracted.
**1st 17 K deposition**

Figure 104: $d$ parameter for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K. There is only 30 minutes of data for 40 K because the beam went off during measurements.
Figure 105: $d$ parameter for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 106: $d$ parameter for isothermal scans at 100 K. After 100 K, the $d$ parameter can no longer be extracted.
2nd 17 K deposition

Figure 107: $d$ parameter for isothermal scans at a. 20 K, b. 30 K, c. 40 K and d. 50 K.
Figure 108: $d$ parameter for isothermal scans at a. 60 K, b. 70 K, c. 80 K and d. 90 K.
Figure 109: $d$ parameter for isothermal scans at 100 K. After 100 K, the $d$ parameter can no longer be extracted.
5 Ice isothermal: averaged scans

5.1 Quasi-plateaus for specific surface area

Figure 110: Quasi-plateaus used to extract Porod constants (shown by dashed lines) and hence specific surface area for averaged isothermal scans of ices deposited at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second).
5.2 Pseudopeaks for periodic spacings

Figure 111: Pseudopeaks for $I(Q) \times Q^{2.5}$ for averaged isothermal scans of ices deposited at a. 50 K and b. 52 K. The pseudopeaks shown here were used up to 80 K for the 50 K ice and up to 90 K for the 52 K ice.
Figure 112: Pseudopeaks for $I(Q) \cdot Q^3$ for averaged isothermal scans of ices deposited at a. 50 K, b. 52 K, c. 17 K (first) and d. 17 K (second). The pseudopeaks shown here were used from 90 K for the 50 K ice, from 100 K for the 52 K ice and throughout for the 17 K ices.