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Data Article

# Data on the theoretical X-Ray attenuation and transmissions for lithium-ion battery cathodes

T.M.M. Heenan [a,b,*], C. Tan [a,b], A.J. Wade [a,b], R. Jervis [a,b], D.J.L. Brett [a,b], P.R. Shearing [a,b,*]

[a] *Electrochemical Innovation Lab, Department of Chemical Engineering, UCL, London WC1E 7JE, UK*
[b] *The Faraday Institution, Quad One, Harwell Science and Innovation Campus, Didcot, OX11 0RA, UK*

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A B S T R A C T

This article reports the data required for planning attenuation-based X-ray characterisation e.g. X-ray computed tomography (CT), of lithium-ion (Li-ion) battery cathodes. The data reported here is to accompany a co-submitted manuscript (10.1016/j.matdes.2020.108585 [1]) which compares two well-known X-ray attenuation data sources: Henke et al. and Hubbell et al., and applies methodology reported by Reiter et al. to extend this data towards the practical characterisation of prominent cathode materials. This data may be used to extend beyond the analysis reported in the accompanying manuscript, and may aid in the applications for other materials, not limited to Li-ion batteries.



* Corresponding authors at: Electrochemical Innovation Lab, Department of Chemical Engineering, UCL, London WC1E 7JE, UK.

*E-mail addresses:* t.heenan@ucl.ac.uk (T.M.M. Heenan), p.shearing@ucl.ac.uk (P.R. Shearing).

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Specifications table

| | |
|---|---|
| Subject | Materials Science |
| Specific subject area | X-ray properties of prominent Li-ion battery cathode materials, for optimising X-ray computed tomography characterisation. |
| Type of data | 38 Tables |
| How data were acquired | No experimental data was collected for this work, all data reported is calculated using spreadsheets generated in Excel 2016 software from spectroscopy and modelling data from published sources [2] and [3]. |
| Data format | Computed from analysed from raw reference data. |
| Parameters for data collection | All parameters and equations used for the calculations that generated this data are in Section 2.1. |
| Description for data collection | The methodology for the calculations that were employed in order to obtain this data is outlined within the complimentary article and within Section 2 of this article. |
| Data source location | City: London<br>Country: England<br>GPS: N/A |
| Data accessibility | Within the article |
| Related research article | Heenan, T.M.M.<br>Theoretical transmissions for X-ray computed tomography studies of lithium-ion battery cathodes.<br>Materials & Design<br>10.1016/j.matdes.2020.108585 |

## Value of the Data

- This data allows for the optimisation of X-ray CT imaging for Li-ion cathodes
- These tables will benefit all who investigate structures using attenuation-based X-ray imaging
- This may also be used to calculated X-ray properties for analogous chemistries

## 1. Data description

Table 1 displays literature references for the crystallographic densities and chemical compositions for NMC111, 532, 622 and 811. Tables 2–9 report the first set of data calculated from the information published by Hubbell and Seltzer [2], followed by Tables 10–19 using information published by Henke et al. [3]. It should be noted that, for direct comparison, the same literature references for the crystallographic densities of the various NMC chemistries were used for both sets of calculations [4–7]. Tables 20–35 report the theoretical X-ray transmissions for the various cathode materials for numerous experimental scenarios, e.g. incident beam energies and sample thickness. Using derivations outlined by Reiter et al. [8], the optimal thicknesses for NMC for beam energies from 1 – 100 keV are reported in Tables 36 and 37. And finally, the applicability of these values for operational experiments is considered by examining the influence of lithiaiton upon the aforementioned metrics in Table 38. For a full analysis and discussion see the related research article [1].

## 2. Experimental design, materials and methods

### 2.1. Essential X-ray equations

No raw data was acquired for this work. All data was calculated from the references. The following set of equations describe all calculations within this work.

X-ray mass attenuation coefficient for a material, from its constituent elements (Eq. (1)).

$$\mu_m(E_0) = \sum_i [w_i.\mu_m(i,\ E_0)] \tag{1}$$

Converting X-ray mass attenuation coefficient to the X-ray linear attenuation coefficient (Eq. (2)).

$$\mu(E_0) = \mu_m(E_0).\rho \tag{2}$$

Converting X-ray linear attenuation coefficient to the X-ray attenuation length (Eq. (3)).

$$\lambda(E_0) = \ \mu(E_0)^{-1} \tag{3}$$

Calculating X-ray transmission from the X-ray linear attenuation coefficient or the X-ray attenuation length (Eq. (4)).

$$T = e^{-t.\mu(E_0)} = e^{\frac{-t}{\lambda(E_0)}} \tag{4}$$

Material thickness for optimum image contrast (Eq. (5)).

$$t.\mu(E_o) = 2 \tag{5}$$

| | | |
|---|---|---|
| $T$ | *Transmission* | *%* |
| $I$ | *Transmitted X-ray intensity* | *energy per area per time* |
| $I_0$ | *Incident X-ray intensity* | *energy per area per time* |
| $E_0$ | *Incident X-ray energy* | *energy* |
| $t$ | *Thickness of the sample* | *length* |
| $i$ | *Constituent element* | *no-units* |
| $w_i$ | *Weight fraction of element i* | *%* |
| $\mu_m(E_0)$ | *X-ray mass attenuation coefficient* | *area per weight* |
| $\mu(E_0)$ | X-ray linear attenuation coefficient | *inverse length* |
| $\lambda(E_0)$ | *X-ray attenuation length* | *length* |

**Table 1**
Referenced crystallographic densities, in g cm$^{-3}$ for four NMC chemistries (to 2 d.p) [4–7].

| | NMC111 | NMC532 | NMC622 | NMC811 |
|---|---|---|---|---|
| Chemistry | $LiNi_{0.1}Mn_{0.1}Co_{0.1}O_2$ | $LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ | $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ | $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ |
| $\rho$ | 4.74 | 4.72 | 4.75 | 4.80 |

## 2.2. X-Ray attenuation data calculated from Hubbell

These tables report data produced from work by Hubbell and Seltzer [2].

**Table 2**
X-ray mass attenuation coefficients for the constituent elements within NMC for incident beam energies of 1 – 10 keV, produced from work by Hubbell and Seltzer [2] and presented in cm$^2$ g$^{-1}$ to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| Li | 233.90 | 27.07 | 7.55 | 3.11 | 1.62 | 0.99 | 0.51 | 0.34 |
| Ni | 9855.00 | 2049.00 | 709.40 | 328.20 | 179.30 | 109.00 | 49.52 | 209.00 |
| Mn | 8093.00 | 1421.00 | 485.10 | 222.90 | 121.20 | 73.50 | 273.40 | 151.40 |
| Co | 9796.00 | 1779.00 | 612.90 | 283.00 | 154.30 | 93.70 | 324.80 | 184.10 |
| O | 4590.00 | 694.90 | 217.10 | 93.15 | 47.90 | 27.70 | 11.63 | 5.95 |

**Table 3**
X-ray mass attenuation coefficients for the constituent elements within NMC for incident beam energies of 10 – 100 keV, produced from work by Hubbell and Seltzer [2] and presented in $cm^2\,g^{-1}$ to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| Li | 0.34 | 0.19 | 0.16 | 0.16 | 0.15 | 0.14 | 0.14 | 0.13 |
| Ni | 209.00 | 32.20 | 10.34 | 4.60 | 2.47 | 1.51 | 0.73 | 0.44 |
| Mn | 151.40 | 22.53 | 7.14 | 3.17 | 1.71 | 1.06 | 0.53 | 0.34 |
| Co | 184.10 | 28.03 | 8.96 | 3.98 | 2.14 | 1.31 | 0.64 | 0.39 |
| O | 5.95 | 0.87 | 0.38 | 0.26 | 0.21 | 0.19 | 0.17 | 0.16 |

**Table 4**
X-ray mass attenuation coefficients for various NMC chemistries for incident beam energies of 1 – 10 keV, produced from work by Hubbell and Seltzer [2] and presented in $cm^2\ g^{-1}$ to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| NMC 111 | 7056.50 | 1277.27 | 432.33 | 197.15 | 106.53 | 64.24 | 131.49 | 110.20 |
| NMC 532 | 7110.63 | 1314.75 | 445.73 | 203.44 | 110.01 | 66.37 | 105.26 | 113.84 |
| NMC 622 | 7221.13 | 1353.19 | 459.47 | 209.90 | 113.57 | 68.54 | 92.36 | 117.47 |
| NMC 811 | 7333.73 | 1407.53 | 478.88 | 219.01 | 118.61 | 71.62 | 62.88 | 122.56 |

**Table 5**
X-ray mass attenuation coefficients for various NMC chemistries for incident beam energies of 10 – 100 keV, produced from work by Hubbell et al. [1] and presented in $cm^2\ g^{-1}$ to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| NMC 111 | 110.20 | 16.75 | 5.39 | 2.43 | 1.34 | 0.85 | 0.44 | 0.29 |
| NMC 532 | 113.84 | 17.35 | 5.59 | 2.52 | 1.39 | 0.87 | 0.46 | 0.30 |
| NMC 622 | 117.47 | 17.96 | 5.79 | 2.61 | 1.43 | 0.90 | 0.47 | 0.31 |
| NMC 811 | 122.56 | 18.81 | 6.07 | 2.74 | 1.50 | 0.94 | 0.49 | 0.32 |

**Table 6**
X-ray linear attenuation coefficients for various NMC chemistries for incident beam energies of 1 – 10 keV, produced from work by Hubbell and Seltzer [2] and presented in $cm^{-1}$ to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| NMC 111 | 33,447.82 | 6054.24 | 2049.24 | 934.51 | 504.97 | 304.48 | 623.28 | 522.33 |
| NMC 532 | 33,562.19 | 6205.63 | 2103.86 | 960.26 | 519.26 | 313.25 | 496.83 | 537.32 |
| NMC 622 | 34,300.38 | 6427.66 | 2182.47 | 997.01 | 539.48 | 325.58 | 438.69 | 557.99 |
| NMC 811 | 35,201.91 | 6756.14 | 2298.65 | 1051.24 | 569.31 | 343.78 | 301.83 | 588.31 |

**Table 7**
X-ray linear attenuation coefficients for various NMC chemistries for incident beam energies of 10 – 100 keV, produced from work by Hubbell and Seltzer [2] and presented in $cm^{-1}$ to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| NMC 111 | 522.33 | 79.40 | 25.57 | 11.53 | 6.35 | 4.01 | 2.10 | 1.40 |
| NMC 532 | 537.32 | 81.91 | 26.40 | 11.90 | 6.55 | 4.13 | 2.15 | 1.42 |
| NMC 622 | 557.99 | 85.31 | 27.51 | 12.40 | 6.82 | 4.29 | 2.23 | 1.46 |
| NMC 811 | 588.31 | 90.29 | 29.15 | 13.14 | 7.21 | 4.52 | 2.33 | 1.52 |

**Table 8**
X-ray attenuation length for various NMC chemistries for incident beam energies of 1 – 10 keV, produced from work by Hubbell and Seltzer [2] and presented in µm to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| NMC 111 | 0.30 | 1.65 | 4.88 | 10.70 | 19.80 | 32.84 | 16.04 | 19.15 |
| NMC 532 | 0.30 | 1.61 | 4.75 | 10.41 | 19.26 | 31.92 | 20.13 | 18.61 |
| NMC 622 | 0.29 | 1.56 | 4.58 | 10.03 | 18.54 | 30.71 | 22.80 | 17.92 |
| NMC 811 | 0.28 | 1.48 | 4.35 | 9.51 | 17.56 | 29.09 | 33.13 | 17.00 |

**Table 9**
X-ray attenuation length for various NMC chemistries for incident beam energies of 10 – 100 keV, produced from work by Hubbell and Seltzer [2] and presented in µm to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| NMC 111 | 19.15 | 125.94 | 391.07 | 867.00 | 1573.69 | 2492.53 | 4753.60 | 7162.80 |
| NMC 532 | 18.61 | 122.08 | 378.81 | 840.11 | 1526.83 | 2422.85 | 4643.21 | 7031.71 |
| NMC 622 | 17.92 | 117.22 | 363.44 | 806.29 | 1467.19 | 2332.62 | 4491.83 | 6836.76 |
| NMC 811 | 17.00 | 110.75 | 343.04 | 761.30 | 1387.44 | 2211.00 | 4283.76 | 6562.53 |

## *2.3. X-Ray attenuation data calculated from Henke*

These tables report data produced from work by Henke et al. [3].

**Table 10**
X-ray attenuation lengths for the light elements within NMC for incident beam energies of 1 – 8 keV, produced from work by Henke et al. [3] and presented in cm to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV |
|---|---|---|---|---|---|---|---|
| Li | 0.01 | 0.07 | 0.28 | 0.71 | 1.44 | 2.47 | 5.03 |
| O | 0.15 | 1.00 | 3.20 | 7.44 | 14.67 | 25.72 | 62.10 |

**Table 11**
X-ray attenuation lengths for the light elements within NMC for incident beam energies of 10 – 30 keV, produced from work by Henke et al. [3] and presented in cm to 2 d.p.

| | 10 keV | 20 keV | 30 keV |
|---|---|---|---|
| Li | 7.50 | 11.74 | 12.32 |
| O | 124.57 | 949.88 | 2188.29 |

**Table 12**
X-ray attenuation lengths for the heavy elements within NMC for incident beam energies of 1 – 8 keV, produced from work by Henke et al. [3] and presented in µm to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV |
|---|---|---|---|---|---|---|---|
| Ni | 0.11 | 0.56 | 1.64 | 3.52 | 6.45 | 10.66 | 23.76 |
| Mn | 0.17 | 0.98 | 2.94 | 6.45 | 11.91 | 19.53 | 5.03 |
| Co | 0.12 | 0.64 | 1.91 | 4.18 | 7.76 | 12.85 | 3.52 |

**Table 13**
X-ray attenuation lengths for the heavy elements within NMC for incident beam energies of 10 – 30 keV, produced from work by Henke et al. [3] and presented in µm to 2 d.p.

| | 10 keV | 20 keV | 30 keV |
|---|---|---|---|
| Ni | 5.43 | 36.04 | 113.42 |
| Mn | 9.10 | 63.52 | 202.47 |
| Co | 6.25 | 42.24 | 133.55 |

**Table 14**
X-ray linear attenuation coefficients for the constituent elements within NMC for incident beam energies of 1 – 8 keV, produced from work by Henke et al. [3] and presented in $cm^{-1}$ to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV |
|---|---|---|---|---|---|---|---|
| Li | 118.99 | 13.42 | 3.59 | 1.40 | 0.69 | 0.41 | 0.20 |
| Ni | 92,912.63 | 17,818.17 | 6093.96 | 2842.15 | 1550.51 | 938.30 | 420.95 |
| Mn | 58,254.01 | 10,241.16 | 3398.57 | 1550.98 | 839.83 | 512.05 | 1988.30 |
| Co | 86,464.80 | 15,618.92 | 5236.07 | 2391.96 | 1288.96 | 778.43 | 2840.83 |
| O | 6.60 | 1.00 | 0.31 | 0.13 | 0.07 | 0.04 | 0.02 |

**Table 15**
X-ray linear attenuation coefficients for the constituent elements within NMC for incident beam energies of 10 – 30 keV, produced from work by Henke et al. [3] and presented in $cm^{-1}$ to 2 d.p.

| | 10 keV | 20 keV | 30 keV |
|---|---|---|---|
| Li | 0.13 | 0.09 | 0.08 |
| Ni | 1842.54 | 277.50 | 88.17 |
| Mn | 1098.94 | 157.43 | 49.39 |
| Co | 1601.10 | 236.72 | 74.88 |
| O | 0.01 | 0.00 | 0.00 |

**Table 16**
X-ray mass attenuation coefficients for the constituent elements within NMC for incident beam energies of 1 – 8 keV, produced from work by Henke et al. [3] and presented in $cm^{-2}$ $g^{-1}$ to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV |
|---|---|---|---|---|---|---|---|
| Li | 222.80 | 25.10 | 6.70 | 2.60 | 1.30 | 0.80 | 0.40 |
| Ni | 10,437.30 | 2001.60 | 684.60 | 319.30 | 174.20 | 105.40 | 47.30 |
| Mn | 7980.00 | 1402.90 | 465.60 | 212.50 | 115.00 | 70.10 | 272.40 |
| Co | 9715.10 | 1754.90 | 588.30 | 268.80 | 144.80 | 87.50 | 319.20 |
| O | 4615.50 | 699.20 | 218.40 | 94.10 | 47.70 | 27.20 | 11.30 |

**Table 17**
X-ray mass attenuation coefficients for the constituent elements within NMC for incident beam energies of 10 – 30 keV, produced from work by Henke et al. [3] and presented in $cm^{-2}$ $g^{-1}$ to 2 d.p.

| | 10 keV | 20 keV | 30 keV |
|---|---|---|---|
| Li | 0.20 | 0.20 | 0.20 |
| Ni | 207.00 | 31.20 | 9.90 |
| Mn | 150.50 | 21.60 | 6.80 |
| Co | 179.90 | 26.60 | 8.40 |
| O | 5.60 | 0.70 | 0.30 |

**Table 18**
X-ray mass attenuation coefficients for the various NMC chemistries for incident beam energies of 1 – 8 keV, produced from work by Henke et al. [3] and presented in $cm^{-2}$ $g^{-1}$ to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV |
|---|---|---|---|---|---|---|---|
| NMC 111 | 7144.06 | 1260.68 | 419.02 | 190.76 | 102.32 | 61.43 | 129.58 |
| NMC 532 | 7266.10 | 1295.60 | 432.23 | 197.48 | 106.16 | 63.76 | 103.59 |
| NMC 622 | 7417.66 | 1332.26 | 445.63 | 204.01 | 109.77 | 65.92 | 90.62 |
| NMC 811 | 7611.09 | 1383.44 | 464.69 | 213.52 | 115.12 | 69.14 | 61.28 |

**Table 19**
X-ray mass attenuation coefficients for the various NMC chemistries for incident beam energies of 10 – 30 keV, produced from work by Henke et al. [3] and presented in $cm^{-2}$ $g^{-1}$ to 2 d.p.

| | 10 keV | 20 keV | 30 keV |
|---|---|---|---|
| NMC 111 | 108.65 | 16.03 | 5.10 |
| NMC 532 | 112.45 | 16.66 | 5.31 |
| NMC 622 | 116.01 | 17.26 | 5.50 |
| NMC 811 | 121.17 | 18.13 | 5.79 |

The same literature references for the crystallographic densities of the various NMC chemistries were used for both the attenuation calculations based upon Hubbell and Henke [4–7].

### 2.4. X-Ray transmissions for NMC111

Firstly transmission values for small samples.

**Table 20**
Theoretical X-ray transmission for NMC 111 for thicknesses of 1 – 10 µm and incident beam energies of 1 – 10 keV, presented as a percentage to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| 1 µm | 3.53% | 54.58% | 81.47% | 91.08% | 95.08% | 97.00% | 93.96% | 94.91% |
| 2 µm | 0.12% | 29.79% | 66.38% | 82.95% | 90.39% | 94.09% | 88.28% | 90.08% |
| 3 µm | 0.00% | 16.26% | 54.08% | 75.55% | 85.94% | 91.27% | 82.95% | 85.50% |
| 4 µm | 0.00% | 8.88% | 44.06% | 68.81% | 81.71% | 88.53% | 77.93% | 81.15% |
| 5 µm | 0.00% | 4.85% | 35.89% | 62.67% | 77.69% | 85.88% | 73.22% | 77.02% |
| 6 µm | 0.00% | 2.64% | 29.24% | 57.08% | 73.86% | 83.30% | 68.80% | 73.10% |
| 7 µm | 0.00% | 1.44% | 23.82% | 51.99% | 70.22% | 80.80% | 64.64% | 69.38% |
| 8 µm | 0.00% | 0.79% | 19.41% | 47.35% | 66.77% | 78.38% | 60.74% | 65.85% |
| 9 µm | 0.00% | 0.43% | 15.81% | 43.13% | 63.48% | 76.03% | 57.07% | 62.49% |
| 10 µm | 0.00% | 0.23% | 12.88% | 39.28% | 60.35% | 73.75% | 53.62% | 59.31% |

**Table 21**
Theoretical X-ray transmission for NMC 111 for thicknesses of 1 – 10 µm and incident beam energies of 10 – 100 keV, presented as a percentage to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| 1 µm | 94.91% | 99.21% | 99.74% | 99.88% | 99.94% | 99.96% | 99.98% | 99.99% |
| 2 µm | 90.08% | 98.42% | 99.49% | 99.77% | 99.87% | 99.92% | 99.96% | 99.97% |
| 3 µm | 85.50% | 97.65% | 99.24% | 99.65% | 99.81% | 99.88% | 99.94% | 99.96% |
| 4 µm | 81.15% | 96.87% | 98.98% | 99.54% | 99.75% | 99.84% | 99.92% | 99.94% |
| 5 µm | 77.02% | 96.11% | 98.73% | 99.42% | 99.68% | 99.80% | 99.89% | 99.93% |
| 6 µm | 73.10% | 95.35% | 98.48% | 99.31% | 99.62% | 99.76% | 99.87% | 99.92% |
| 7 µm | 69.38% | 94.59% | 98.23% | 99.20% | 99.56% | 99.72% | 99.85% | 99.90% |
| 8 µm | 65.85% | 93.85% | 97.98% | 99.08% | 99.49% | 99.68% | 99.83% | 99.89% |
| 9 µm | 62.49% | 93.10% | 97.72% | 98.97% | 99.43% | 99.64% | 99.81% | 99.87% |
| 10 µm | 59.31% | 92.37% | 97.48% | 98.85% | 99.37% | 99.60% | 99.79% | 99.86% |

Secondly transmission values for large samples.

**Table 22**
Theoretical X-ray transmission for NMC 111 for thicknesses of 10 – 100 μm and incident beam energies of 1 – 10 keV, presented as a percentage to 2 dp.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| 10 μm | 0.00% | 0.23% | 12.88% | 39.28% | 60.35% | 73.75% | 53.62% | 59.31% |
| 20 μm | 0.00% | 0.00% | 1.66% | 15.43% | 36.42% | 54.39% | 28.75% | 35.18% |
| 30 μm | 0.00% | 0.00% | 0.21% | 6.06% | 21.98% | 40.11% | 15.42% | 20.87% |
| 40 μm | 0.00% | 0.00% | 0.03% | 2.38% | 13.27% | 29.58% | 8.27% | 12.38% |
| 50 μm | 0.00% | 0.00% | 0.00% | 0.93% | 8.01% | 21.82% | 4.43% | 7.34% |
| 60 μm | 0.00% | 0.00% | 0.00% | 0.37% | 4.83% | 16.09% | 2.38% | 4.35% |
| 70 μm | 0.00% | 0.00% | 0.00% | 0.14% | 2.92% | 11.87% | 1.27% | 2.58% |
| 80 μm | 0.00% | 0.00% | 0.00% | 0.06% | 1.76% | 8.75% | 0.68% | 1.53% |
| 90 μm | 0.00% | 0.00% | 0.00% | 0.02% | 1.06% | 6.46% | 0.37% | 0.91% |
| 100 μm | 0.00% | 0.00% | 0.00% | 0.01% | 0.64% | 4.76% | 0.20% | 0.54% |

**Table 23**
Theoretical X-ray transmission for NMC 111 for thicknesses of 10 – 100 μm and incident beam energies of 10 – 100 keV, presented as a percentage to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| 10 μm | 59.31% | 92.37% | 97.48% | 98.85% | 99.37% | 99.60% | 99.79% | 99.86% |
| 20 μm | 35.18% | 85.32% | 95.01% | 97.72% | 98.74% | 99.20% | 99.58% | 99.72% |
| 30 μm | 20.87% | 78.80% | 92.62% | 96.60% | 98.11% | 98.80% | 99.37% | 99.58% |
| 40 μm | 12.38% | 72.79% | 90.28% | 95.49% | 97.49% | 98.41% | 99.16% | 99.44% |
| 50 μm | 7.34% | 67.23% | 88.00% | 94.40% | 96.87% | 98.01% | 98.95% | 99.30% |
| 60 μm | 4.35% | 62.10% | 85.78% | 93.31% | 96.26% | 97.62% | 98.75% | 99.17% |
| 70 μm | 2.58% | 57.36% | 83.61% | 92.24% | 95.65% | 97.23% | 98.54% | 99.03% |
| 80 μm | 1.53% | 52.98% | 81.50% | 91.19% | 95.04% | 96.84% | 98.33% | 98.89% |
| 90 μm | 0.91% | 48.94% | 79.44% | 90.14% | 94.44% | 96.45% | 98.12% | 98.75% |
| 100 μm | 0.54% | 45.20% | 77.44% | 89.11% | 93.84% | 96.07% | 97.92% | 98.61% |

## *2.5. X-Ray transmissions for NMC532*

Firstly transmission values for small samples.

**Table 24**
Theoretical X-ray transmission for NMC 532 for thicknesses of 1 – 10 μm and incident beam energies of 1 – 10 keV, presented as a percentage to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| 1 μm | 3.49% | 53.76% | 81.03% | 90.84% | 94.94% | 96.92% | 95.15% | 94.77% |
| 2 μm | 0.12% | 28.91% | 65.65% | 82.53% | 90.14% | 93.93% | 90.54% | 89.81% |
| 3 μm | 0.00% | 15.54% | 53.20% | 74.97% | 85.57% | 91.03% | 86.15% | 85.11% |
| 4 μm | 0.00% | 8.36% | 43.10% | 68.11% | 81.24% | 88.22% | 81.98% | 80.66% |
| 5 μm | 0.00% | 4.49% | 34.93% | 61.87% | 77.13% | 85.50% | 78.00% | 76.44% |
| 6 μm | 0.00% | 2.42% | 28.30% | 56.21% | 73.23% | 82.87% | 74.22% | 72.44% |
| 7 μm | 0.00% | 1.30% | 22.93% | 51.06% | 69.53% | 80.31% | 70.63% | 68.65% |
| 8 μm | 0.00% | 0.70% | 18.58% | 46.38% | 66.01% | 77.83% | 67.20% | 65.06% |
| 9 μm | 0.00% | 0.38% | 15.05% | 42.14% | 62.67% | 75.43% | 63.94% | 61.66% |
| 10 μm | 0.00% | 0.20% | 12.20% | 38.28% | 59.50% | 73.11% | 60.85% | 58.43% |

**Table 25**
Theoretical X-ray transmission for NMC 532 for thicknesses of 1 – 10 µm and incident beam energies of 10 – 100 keV, presented as a percentage to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| 1 µm | 94.77% | 99.18% | 99.74% | 99.88% | 99.93% | 99.96% | 99.98% | 99.99% |
| 2 µm | 89.81% | 98.38% | 99.47% | 99.76% | 99.87% | 99.92% | 99.96% | 99.97% |
| 3 µm | 85.11% | 97.57% | 99.21% | 99.64% | 99.80% | 99.88% | 99.94% | 99.96% |
| 4 µm | 80.66% | 96.78% | 98.95% | 99.53% | 99.74% | 99.84% | 99.91% | 99.94% |
| 5 µm | 76.44% | 95.99% | 98.69% | 99.41% | 99.67% | 99.79% | 99.89% | 99.93% |
| 6 µm | 72.44% | 95.20% | 98.43% | 99.29% | 99.61% | 99.75% | 99.87% | 99.91% |
| 7 µm | 68.65% | 94.43% | 98.17% | 99.17% | 99.54% | 99.71% | 99.85% | 99.90% |
| 8 µm | 65.06% | 93.66% | 97.91% | 99.05% | 99.48% | 99.67% | 99.83% | 99.89% |
| 9 µm | 61.66% | 92.89% | 97.65% | 98.93% | 99.41% | 99.63% | 99.81% | 99.87% |
| 10 µm | 58.43% | 92.14% | 97.39% | 98.82% | 99.35% | 99.59% | 99.78% | 99.86% |

Secondly transmission values for large samples.

**Table 26**
Theoretical X-ray transmission for NMC 532 for thicknesses of 10 – 100 µm and incident beam energies of 1 – 10 keV, presented as a percentage to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| 10 µm | 0.00% | 0.20% | 12.20% | 38.28% | 59.50% | 73.11% | 60.85% | 58.43% |
| 20 µm | 0.00% | 0.00% | 1.49% | 14.65% | 35.40% | 53.45% | 37.02% | 34.14% |
| 30 µm | 0.00% | 0.00% | 0.18% | 5.61% | 21.06% | 39.07% | 22.53% | 19.95% |
| 40 µm | 0.00% | 0.00% | 0.02% | 2.15% | 12.53% | 28.57% | 13.71% | 11.66% |
| 50 µm | 0.00% | 0.00% | 0.00% | 0.82% | 7.45% | 20.88% | 8.34% | 6.81% |
| 60 µm | 0.00% | 0.00% | 0.00% | 0.31% | 4.44% | 15.27% | 5.07% | 3.98% |
| 70 µm | 0.00% | 0.00% | 0.00% | 0.12% | 2.64% | 11.16% | 3.09% | 2.33% |
| 80 µm | 0.00% | 0.00% | 0.00% | 0.05% | 1.57% | 8.16% | 1.88% | 1.36% |
| 90 µm | 0.00% | 0.00% | 0.00% | 0.02% | 0.93% | 5.97% | 1.14% | 0.79% |
| 100 µm | 0.00% | 0.00% | 0.00% | 0.01% | 0.56% | 4.36% | 0.70% | 0.46% |

**Table 27**
Theoretical X-ray transmission for NMC 532 for thicknesses of 10 – 100 µm and incident beam energies of 10 – 100 keV, presented as a percentage to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| 10 µm | 58.43% | 92.14% | 97.39% | 98.82% | 99.35% | 99.59% | 99.78% | 99.86% |
| 20 µm | 34.14% | 84.89% | 94.86% | 97.65% | 98.70% | 99.18% | 99.57% | 99.72% |
| 30 µm | 19.95% | 78.21% | 92.39% | 96.49% | 98.05% | 98.77% | 99.36% | 99.57% |
| 40 µm | 11.66% | 72.06% | 89.98% | 95.35% | 97.41% | 98.36% | 99.14% | 99.43% |
| 50 µm | 6.81% | 66.39% | 87.63% | 94.22% | 96.78% | 97.96% | 98.93% | 99.29% |
| 60 µm | 3.98% | 61.17% | 85.35% | 93.11% | 96.15% | 97.55% | 98.72% | 99.15% |
| 70 µm | 2.33% | 56.36% | 83.13% | 92.01% | 95.52% | 97.15% | 98.50% | 99.01% |
| 80 µm | 1.36% | 51.93% | 80.96% | 90.92% | 94.90% | 96.75% | 98.29% | 98.87% |
| 90 µm | 0.79% | 47.84% | 78.85% | 89.84% | 94.28% | 96.35% | 98.08% | 98.73% |
| 100 µm | 0.46% | 44.08% | 76.80% | 88.78% | 93.66% | 95.96% | 97.87% | 98.59% |

### 2.6. X-Ray transmissions for NMC622

Firstly transmission values for small samples.

**Table 28**
Theoretical X-ray transmission for NMC 622 for thicknesses of 1 – 10 μm and incident beam energies of 1 – 10 keV, presented as a percentage to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| 1 μm | 3.24% | 52.58% | 80.39% | 90.51% | 94.75% | 96.80% | 95.71% | 94.57% |
| 2 μm | 0.10% | 27.65% | 64.63% | 81.92% | 89.77% | 93.70% | 91.60% | 89.44% |
| 3 μm | 0.00% | 14.54% | 51.96% | 74.15% | 85.06% | 90.69% | 87.67% | 84.59% |
| 4 μm | 0.00% | 7.65% | 41.77% | 67.11% | 80.59% | 87.79% | 83.91% | 80.00% |
| 5 μm | 0.00% | 4.02% | 33.58% | 60.74% | 76.36% | 84.98% | 80.30% | 75.65% |
| 6 μm | 0.00% | 2.11% | 27.00% | 54.98% | 72.35% | 82.25% | 76.86% | 71.55% |
| 7 μm | 0.00% | 1.11% | 21.70% | 49.76% | 68.55% | 79.62% | 73.56% | 67.67% |
| 8 μm | 0.00% | 0.58% | 17.45% | 45.04% | 64.95% | 77.07% | 70.40% | 63.99% |
| 9 μm | 0.00% | 0.31% | 14.03% | 40.77% | 61.54% | 74.60% | 67.38% | 60.52% |
| 10 μm | 0.00% | 0.16% | 11.28% | 36.90% | 58.31% | 72.21% | 64.49% | 57.24% |

**Table 29**
Theoretical X-ray transmission for NMC 622 for thicknesses of 1 – 10 μm and incident beam energies of 10 – 100 keV, presented as a percentage to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| 1 μm | 94.57% | 99.15% | 99.73% | 99.88% | 99.93% | 99.96% | 99.98% | 99.99% |
| 2 μm | 89.44% | 98.31% | 99.45% | 99.75% | 99.86% | 99.91% | 99.96% | 99.97% |
| 3 μm | 84.59% | 97.47% | 99.18% | 99.63% | 99.80% | 99.87% | 99.93% | 99.96% |
| 4 μm | 80.00% | 96.65% | 98.91% | 99.51% | 99.73% | 99.83% | 99.91% | 99.94% |
| 5 μm | 75.65% | 95.82% | 98.63% | 99.38% | 99.66% | 99.79% | 99.89% | 99.93% |
| 6 μm | 71.55% | 95.01% | 98.36% | 99.26% | 99.59% | 99.74% | 99.87% | 99.91% |
| 7 μm | 67.67% | 94.20% | 98.09% | 99.14% | 99.52% | 99.70% | 99.84% | 99.90% |
| 8 μm | 63.99% | 93.40% | 97.82% | 99.01% | 99.46% | 99.66% | 99.82% | 99.88% |
| 9 μm | 60.52% | 92.61% | 97.55% | 98.89% | 99.39% | 99.61% | 99.80% | 99.87% |
| 10 μm | 57.24% | 91.82% | 97.29% | 98.77% | 99.32% | 99.57% | 99.78% | 99.85% |

Secondly transmission values for large samples.

**Table 30**
Theoretical X-ray transmission for NMC 622 for thicknesses of 10 – 100 μm and incident beam energies of 1 – 10 keV, presented as a percentage to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| 10 μm | 0.00% | 0.16% | 11.28% | 36.90% | 58.31% | 72.21% | 64.49% | 57.24% |
| 20 μm | 0.00% | 0.00% | 1.27% | 13.61% | 34.00% | 52.14% | 41.59% | 32.76% |
| 30 μm | 0.00% | 0.00% | 0.14% | 5.02% | 19.82% | 37.65% | 26.82% | 18.75% |
| 40 μm | 0.00% | 0.00% | 0.02% | 1.85% | 11.56% | 27.19% | 17.29% | 10.73% |
| 50 μm | 0.00% | 0.00% | 0.00% | 0.68% | 6.74% | 19.63% | 11.15% | 6.14% |
| 60 μm | 0.00% | 0.00% | 0.00% | 0.25% | 3.93% | 14.18% | 7.19% | 3.52% |
| 70 μm | 0.00% | 0.00% | 0.00% | 0.09% | 2.29% | 10.24% | 4.64% | 2.01% |
| 80 μm | 0.00% | 0.00% | 0.00% | 0.03% | 1.34% | 7.39% | 2.99% | 1.15% |
| 90 μm | 0.00% | 0.00% | 0.00% | 0.01% | 0.78% | 5.34% | 1.93% | 0.66% |
| 100 μm | 0.00% | 0.00% | 0.00% | 0.00% | 0.45% | 3.86% | 1.24% | 0.38% |

**Table 31**
Theoretical X-ray transmission for NMC 622 for thicknesses of 10 – 100 µm and incident beam energies of 10 – 100 keV, presented as a percentage to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| 10 µm | 57.24% | 91.82% | 97.29% | 98.77% | 99.32% | 99.57% | 99.78% | 99.85% |
| 20 µm | 32.76% | 84.31% | 94.65% | 97.55% | 98.65% | 99.15% | 99.56% | 99.71% |
| 30 µm | 18.75% | 77.42% | 92.08% | 96.35% | 97.98% | 98.72% | 99.33% | 99.56% |
| 40 µm | 10.73% | 71.09% | 89.58% | 95.16% | 97.31% | 98.30% | 99.11% | 99.42% |
| 50 µm | 6.14% | 65.28% | 87.15% | 93.99% | 96.65% | 97.88% | 98.89% | 99.27% |
| 60 µm | 3.52% | 59.94% | 84.78% | 92.83% | 95.99% | 97.46% | 98.67% | 99.13% |
| 70 µm | 2.01% | 55.04% | 82.48% | 91.68% | 95.34% | 97.04% | 98.45% | 98.98% |
| 80 µm | 1.15% | 50.54% | 80.24% | 90.55% | 94.69% | 96.63% | 98.23% | 98.84% |
| 90 µm | 0.66% | 46.40% | 78.06% | 89.44% | 94.05% | 96.22% | 98.02% | 98.69% |
| 100 µm | 0.38% | 42.61% | 75.95% | 88.34% | 93.41% | 95.80% | 97.80% | 98.55% |

## *2.7. X-Ray transmissions for NMC811*

Firstly transmission values for small samples.

**Table 32**
Theoretical X-ray transmission for NMC 811 for thicknesses of 1 – 10 µm and incident beam energies of 1 – 10 keV, presented as a percentage to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| 1 µm | 2.96% | 50.88% | 79.46% | 90.02% | 94.47% | 96.62% | 97.03% | 94.29% |
| 2 µm | 0.09% | 25.89% | 63.15% | 81.04% | 89.24% | 93.36% | 94.14% | 88.90% |
| 3 µm | 0.00% | 13.18% | 50.18% | 72.95% | 84.30% | 90.20% | 91.34% | 83.82% |
| 4 µm | 0.00% | 6.70% | 39.87% | 65.67% | 79.63% | 87.15% | 88.63% | 79.03% |
| 5 µm | 0.00% | 3.41% | 31.69% | 59.12% | 75.23% | 84.21% | 85.99% | 74.52% |
| 6 µm | 0.00% | 1.74% | 25.18% | 53.22% | 71.06% | 81.36% | 83.44% | 70.26% |
| 7 µm | 0.00% | 0.88% | 20.01% | 47.91% | 67.13% | 78.61% | 80.95% | 66.24% |
| 8 µm | 0.00% | 0.45% | 15.90% | 43.13% | 63.42% | 75.96% | 78.55% | 62.46% |
| 9 µm | 0.00% | 0.23% | 12.63% | 38.82% | 59.91% | 73.39% | 76.21% | 58.89% |
| 10 µm | 0.00% | 0.12% | 10.04% | 34.95% | 56.59% | 70.91% | 73.95% | 55.53% |

**Table 33**
Theoretical X-ray transmission for NMC 811 for thicknesses of 1 – 10 µm and incident beam energies of 10 – 100 keV, presented as a percentage to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| 1 µm | 94.29% | 99.10% | 99.71% | 99.87% | 99.93% | 99.95% | 99.98% | 99.98% |
| 2 µm | 88.90% | 98.21% | 99.42% | 99.74% | 99.86% | 99.91% | 99.95% | 99.97% |
| 3 µm | 83.82% | 97.33% | 99.13% | 99.61% | 99.78% | 99.86% | 99.93% | 99.95% |
| 4 µm | 79.03% | 96.45% | 98.84% | 99.48% | 99.71% | 99.82% | 99.91% | 99.94% |
| 5 µm | 74.52% | 95.59% | 98.55% | 99.35% | 99.64% | 99.77% | 99.88% | 99.92% |
| 6 µm | 70.26% | 94.73% | 98.27% | 99.21% | 99.57% | 99.73% | 99.86% | 99.91% |
| 7 µm | 66.24% | 93.88% | 97.98% | 99.08% | 99.50% | 99.68% | 99.84% | 99.89% |
| 8 µm | 62.46% | 93.03% | 97.69% | 98.95% | 99.43% | 99.64% | 99.81% | 99.88% |
| 9 µm | 58.89% | 92.20% | 97.41% | 98.82% | 99.35% | 99.59% | 99.79% | 99.86% |
| 10 µm | 55.53% | 91.37% | 97.13% | 98.70% | 99.28% | 99.55% | 99.77% | 99.85% |

Secondly transmission values for large samples.

**Table 34**
Theoretical X-ray transmission for NMC 811 for thicknesses of 10 – 100 µm and incident beam energies of 1 – 10 keV, presented as a percentage to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| 10 µm | 0.00% | 0.12% | 10.04% | 34.95% | 56.59% | 70.91% | 73.95% | 55.53% |
| 20 µm | 0.00% | 0.00% | 1.01% | 12.22% | 32.03% | 50.28% | 54.68% | 30.83% |
| 30 µm | 0.00% | 0.00% | 0.10% | 4.27% | 18.12% | 35.65% | 40.43% | 17.12% |
| 40 µm | 0.00% | 0.00% | 0.01% | 1.49% | 10.26% | 25.28% | 29.90% | 9.51% |
| 50 µm | 0.00% | 0.00% | 0.00% | 0.52% | 5.80% | 17.93% | 22.11% | 5.28% |
| 60 µm | 0.00% | 0.00% | 0.00% | 0.18% | 3.28% | 12.71% | 16.35% | 2.93% |
| 70 µm | 0.00% | 0.00% | 0.00% | 0.06% | 1.86% | 9.01% | 12.09% | 1.63% |
| 80 µm | 0.00% | 0.00% | 0.00% | 0.02% | 1.05% | 6.39% | 8.94% | 0.90% |
| 90 µm | 0.00% | 0.00% | 0.00% | 0.01% | 0.60% | 4.53% | 6.61% | 0.50% |
| 100 µm | 0.00% | 0.00% | 0.00% | 0.00% | 0.34% | 3.21% | 4.89% | 0.28% |

**Table 35**
Theoretical X-ray transmission for NMC 811 for thicknesses of 10 – 100 µm and incident beam energies of 10 – 100 keV, presented as a percentage to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| 10 µm | 55.53% | 91.37% | 97.13% | 98.70% | 99.28% | 99.55% | 99.77% | 99.85% |
| 20 µm | 30.83% | 83.48% | 94.34% | 97.41% | 98.57% | 99.10% | 99.53% | 99.70% |
| 30 µm | 17.12% | 76.27% | 91.63% | 96.14% | 97.86% | 98.65% | 99.30% | 99.54% |
| 40 µm | 9.51% | 69.69% | 88.99% | 94.88% | 97.16% | 98.21% | 99.07% | 99.39% |
| 50 µm | 5.28% | 63.67% | 86.44% | 93.64% | 96.46% | 97.76% | 98.84% | 99.24% |
| 60 µm | 2.93% | 58.17% | 83.95% | 92.42% | 95.77% | 97.32% | 98.61% | 99.09% |
| 70 µm | 1.63% | 53.15% | 81.54% | 91.22% | 95.08% | 96.88% | 98.38% | 98.94% |
| 80 µm | 0.90% | 48.56% | 79.20% | 90.02% | 94.40% | 96.45% | 98.15% | 98.79% |
| 90 µm | 0.50% | 44.37% | 76.92% | 88.85% | 93.72% | 96.01% | 97.92% | 98.64% |
| 100 µm | 0.28% | 40.54% | 74.71% | 87.69% | 93.05% | 95.58% | 97.69% | 98.49% |

## *2.8. Theoretical NMC thickness for optimum image contrast*

Using derivations outlined by Reiter et al. [8], the theoretical thickness for optimum image contrast can be calculated using Eq. (5): firstly, for low energies (Table 36), and secondly, for high energies (Table 37).

**Table 36**
Theoretical thicknesses for optimal contrast-to-noise ratio for various NMC chemistries and incident beam energies of 1 – 10 keV, presented in µm to 2 d.p.

| | 1 keV | 2 keV | 3 keV | 4 keV | 5 keV | 6 keV | 8 keV | 10 keV |
|---|---|---|---|---|---|---|---|---|
| NMC 111 | 0.60 | 3.30 | 9.76 | 21.40 | 39.60 | 65.68 | 32.08 | 38.30 |
| NMC 532 | 0.60 | 3.22 | 9.50 | 20.82 | 38.52 | 63.84 | 40.26 | 37.22 |
| NMC 622 | 0.58 | 3.12 | 9.16 | 20.06 | 37.08 | 61.42 | 45.60 | 35.84 |
| NMC 811 | 0.56 | 2.96 | 8.70 | 19.02 | 35.12 | 58.18 | 66.26 | 34.00 |

**Table 37**
Theoretical thicknesses for optimal contrast-to-noise ratio for various NMC chemistries and incident beam energies of 10 – 100 keV, presented in µm to 2 d.p.

| | 10 keV | 20 keV | 30 keV | 40 keV | 50 keV | 60 keV | 80 keV | 100 keV |
|---|---|---|---|---|---|---|---|---|
| NMC 111 | 38.30 | 251.88 | 782.14 | 1734.00 | 3147.38 | 4985.06 | 9507.20 | 14,325.60 |
| NMC 532 | 37.22 | 244.16 | 757.62 | 1680.22 | 3053.66 | 4845.70 | 9286.42 | 14,063.42 |
| NMC 622 | 35.84 | 234.44 | 726.88 | 1612.58 | 2934.38 | 4665.24 | 8983.66 | 13,673.52 |
| NMC 811 | 34.00 | 221.50 | 686.08 | 1522.60 | 2774.88 | 4422.00 | 8567.52 | 13,125.06 |

### 2.9. Theoretical influence of electrode lithiation

All calculations thus far have reported results based upon fully lithiated material, because the influence of lithiation is assumed negligible with comparison to variations in the incident beam energy or chemical composition. In order to demonstrate the validity of this assumption, Table 38 reports the theoretical variation in X-ray mass attenuation coefficient with state of charge (quantified by the value of x within $Li_{1-x}Ni_{0.8}Mn_{0.1}Co_{0.1}O_2$) for three incident beam energies: 1, 10, 100 keV.

**Table 38**
The influence of lithiation state upon the X-ray attenuation properties of NMC811 for three incident beam energies: 1, 10 and 100 keV, presented are X-ray mass attenuation coefficients in $cm^2\ g^{-1}$ (to 2 d.p.).

| Lithiation state, x | State of Charge (SoC) | Incident Beam Energy | | |
|---|---|---|---|---|
| | | 1 keV | 10 keV | 100 keV |
| 0.0 | $Li_{1.0}Ni_{0.8}Mn_{0.1}Co_{0.1}O_2$ | 7333.73 | 122.56 | 0.32 |
| 0.2 | $Li_{0.8}Ni_{0.8}Mn_{0.1}Co_{0.1}O_2$ | 7436.50 | 124.33 | 0.32 |
| 0.4 | $Li_{0.6}Ni_{0.8}Mn_{0.1}Co_{0.1}O_2$ | 7542.29 | 126.15 | 0.32 |
| 0.6 | $Li_{0.4}Ni_{0.8}Mn_{0.1}Co_{0.1}O_2$ | 7651.23 | 128.03 | 0.33 |
| 0.8 | $Li_{0.2}Ni_{0.8}Mn_{0.1}Co_{0.1}O_2$ | 7763.46 | 129.96 | 0.33 |
| 1.0 | $Li_{0.0}Ni_{0.8}Mn_{0.1}Co_{0.1}O_2$ | 7879.15 | 131.95 | 0.33 |

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## Conflict of Interest

The authors declare that they have no known conflicts of interest to declare.

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