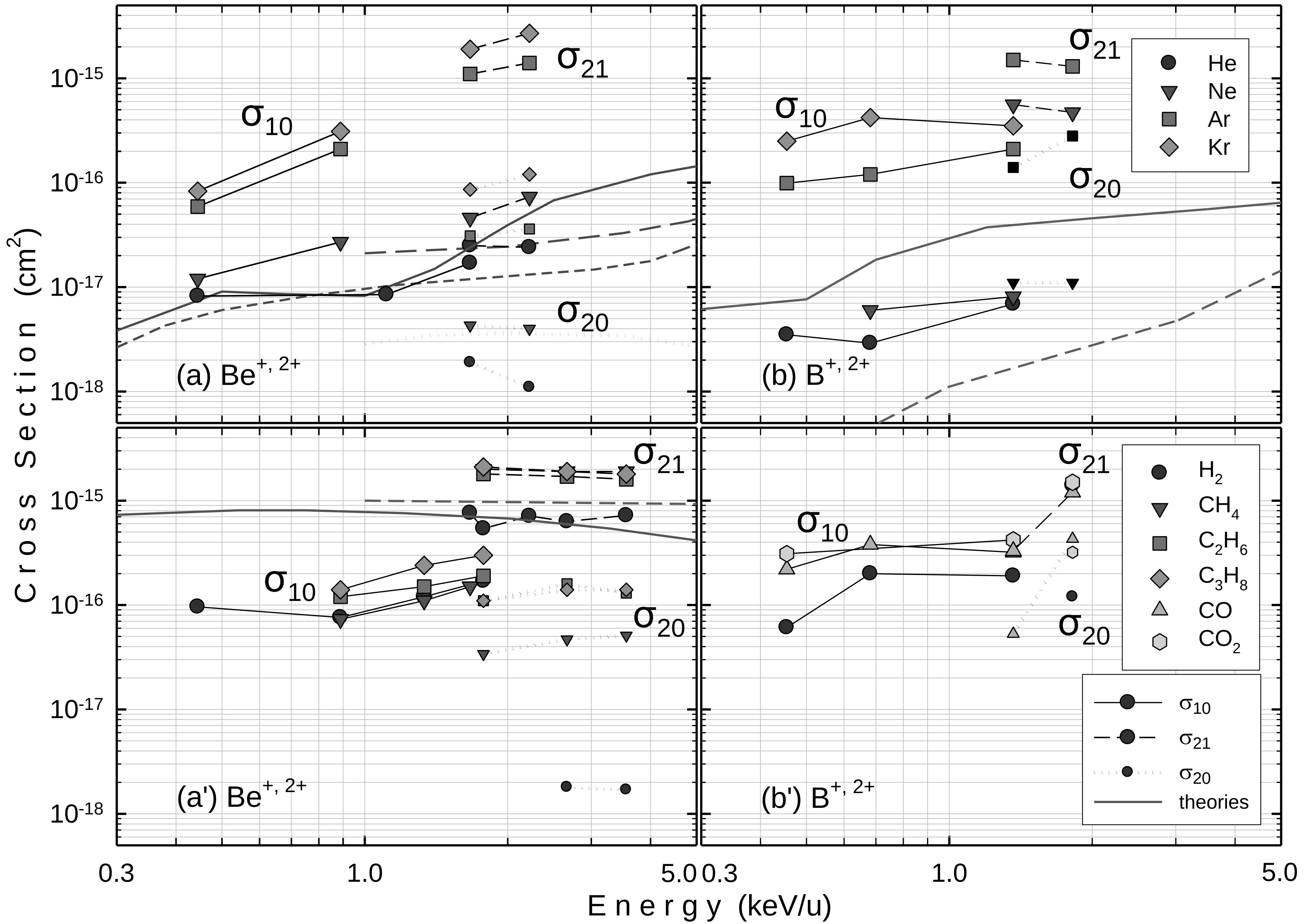
First Step Benchmark of Inelastic Collision Cross Sections for Heavy Ions using Charge State Evolutions via Target Penetration

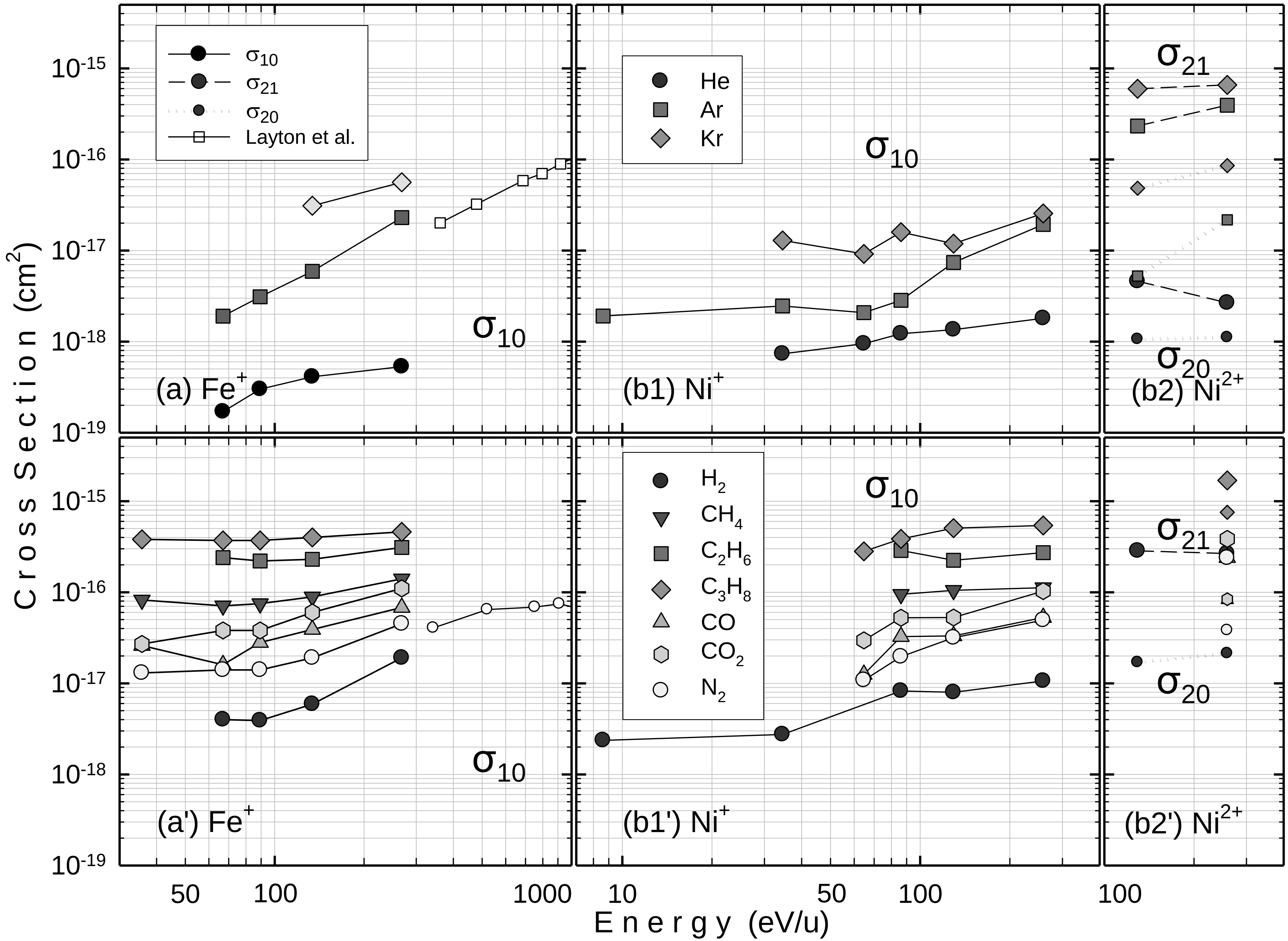
Alex M Imai, Viatcheslav P Shevelko

Department of Nuclear Engineering, Kyoto University
P. N. Lebedev Physical Institute of Russian Academy of Sciences

Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications, 19-21 Dec. 2016, IAEA, Vienna.

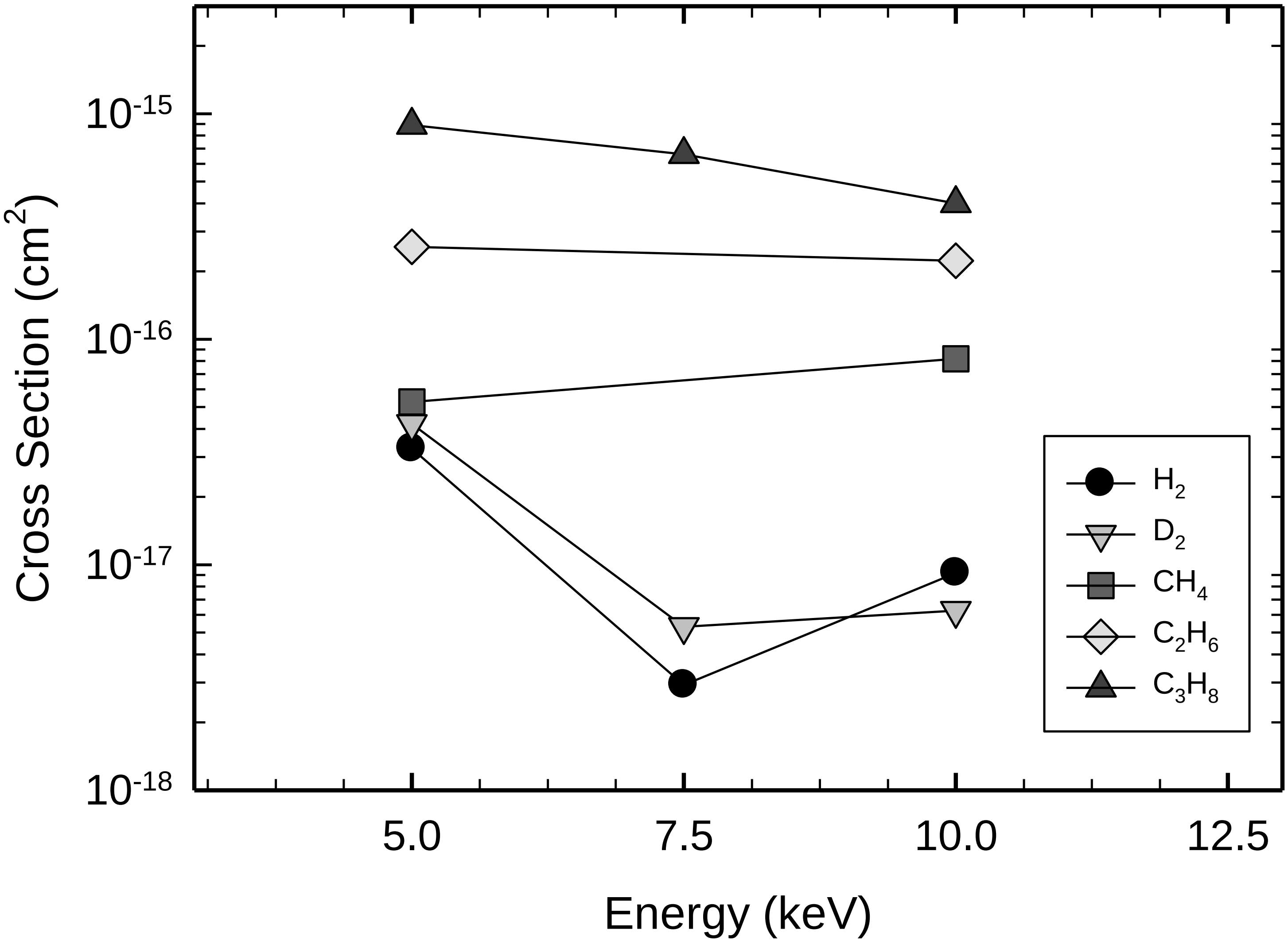


M. Imai *et al*., J. Plasma Fusion Res. SERIES Vol.7, pp.323-326 (2006).



M. Imai *et al.*, J. Plasma Fusion Res. SERIES Vol.7, pp.323-326 (2006).

Single-electron capture cross sections for W+ ions



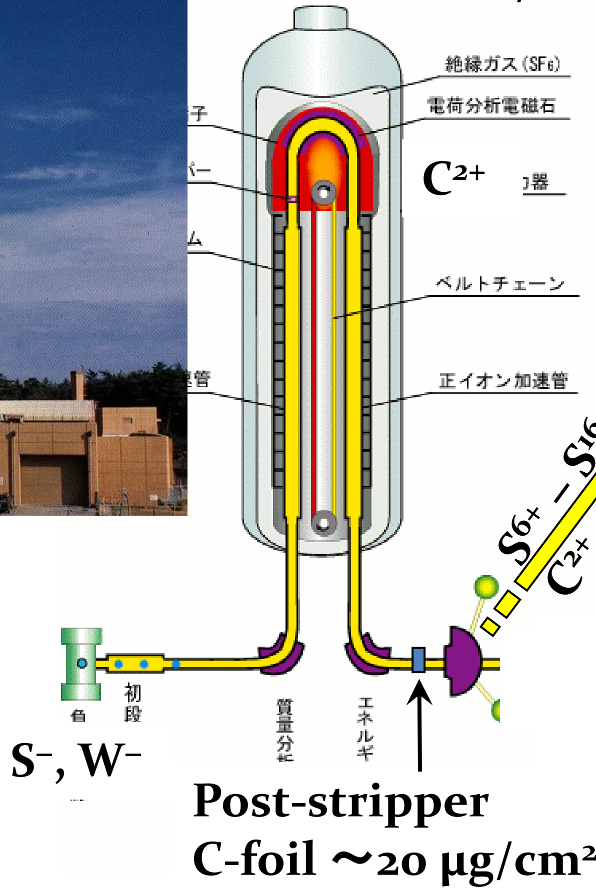
M. Imai *et al*., Fusion Science Tech. 63, pp. 392-399 (2013).

Background

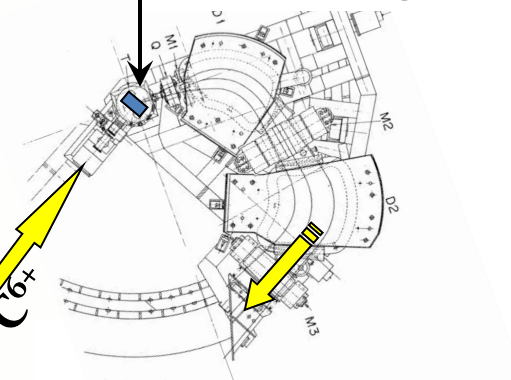
- You require not just accuracy of calculated cross sections but also their completeness.
- Experimentalists would like the evaluation of theoretical data to be done with experiments, but in many cases, there exist few experiments directly comparable to theories.
- Experimentalists are able to provide very accurate experimental results in some cases.

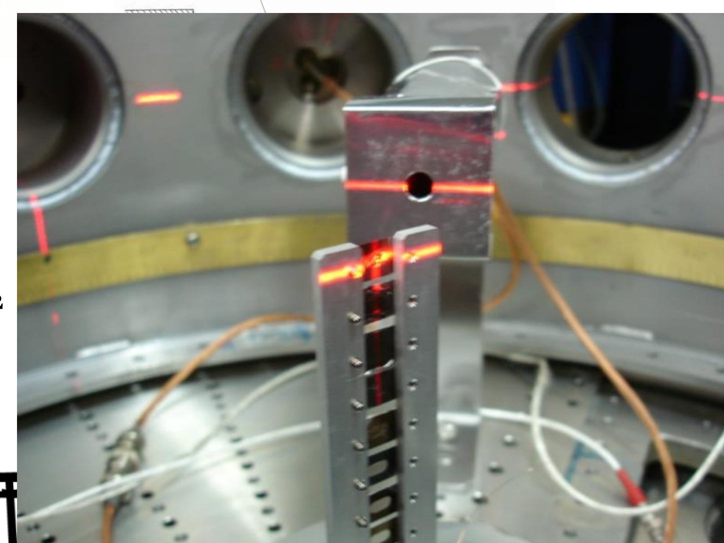
Experimental apparatus in Japan Atomic Energy Agency

2.0 MeV/u C^{q+} (q=2-6), S^{q+} (q=6-16),
1.0 MeV/u W^{q+} (q=13,15,28,29,30,38)

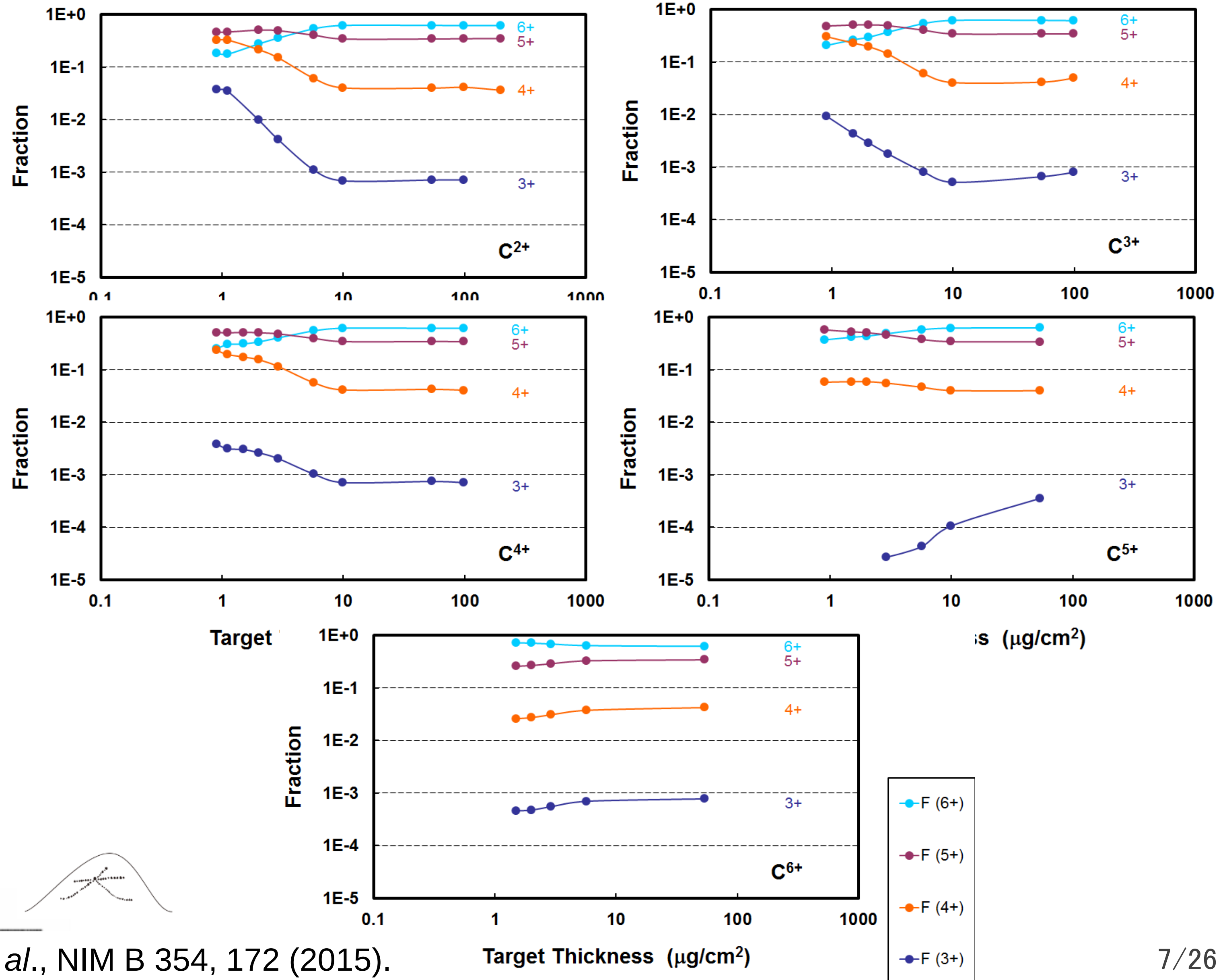


Target C-foil
0.9~200 μg/cm²





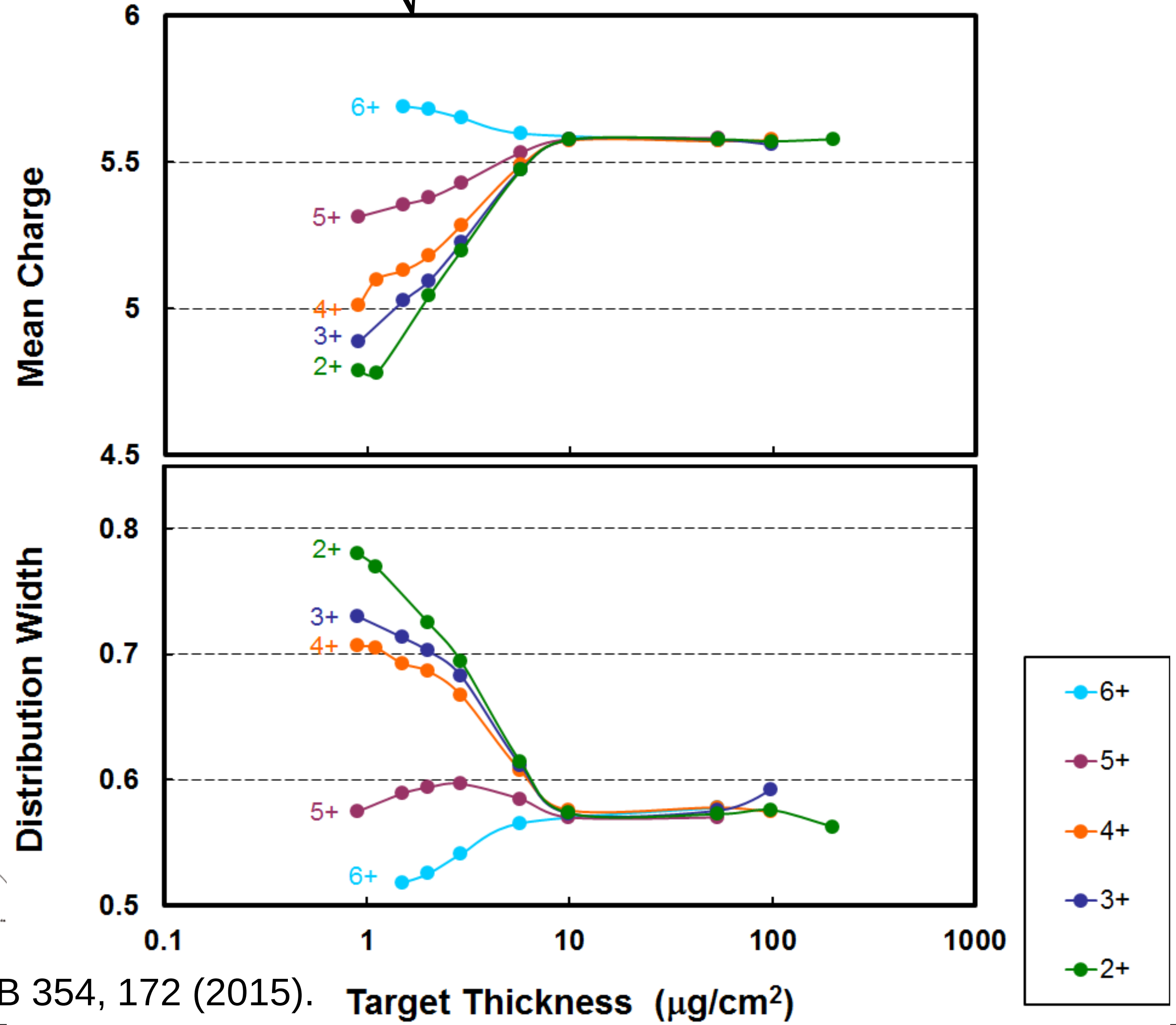
Equilibrium and pre-equilibrium charge-state distributions of 2.0 MeV/u C ions after C-foils



M.Imai *et al*., NIM B 354, 172 (2015).

Equilibrium and pre-equilibrium charge-state distributions of 2.0 MeV/u C ions after C-foils

$$\bar{q} = \sum_q q y_q\,, \qquad d = \sqrt{\sum_q (q-\bar{q})^2 y_q}\,, \qquad s = \frac{\sum_q (q-\bar{q})^3 y_q}{d^3}$$



M.Imai *et al*., NIM B 354, 172 (2015).

Computer codes for charge-state evolutions

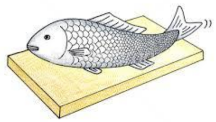
ETACHA:
a program for calculating charge states at GANIL energies, (10 – 80 MeV/u)
J.-P. Rozet, C. Stéphan, D. Vernhet, NIM B 107, 67 (1996).

Matrix Method:
Charge evolution of swift-heavy-ion beams explored by matrix method,
O. Osmani, P. Sigmund, NIM B 269, 813 (2011).

ETACHA3, **ETACHA4**: Extention of charge state distribution calculations for ion-solid collisions towards low velocities and many-electron ions,
E. Lamour, P. D. Fainstein, M. Galassi, C. Prigent, C. A. Ramirez, R. D. Rivarola, J.-P. Rozet, M. Trassinelli, D. Vernhet, PRA 92, 042703 (2015).

BEAR (Balance Equations for Atomic Reactions)
V. P. Shevelko, N. Winckler, I. Yu. Tolstikhina,
NIM B 377, 77 (2016).

Set of cross sections on the cutting-board

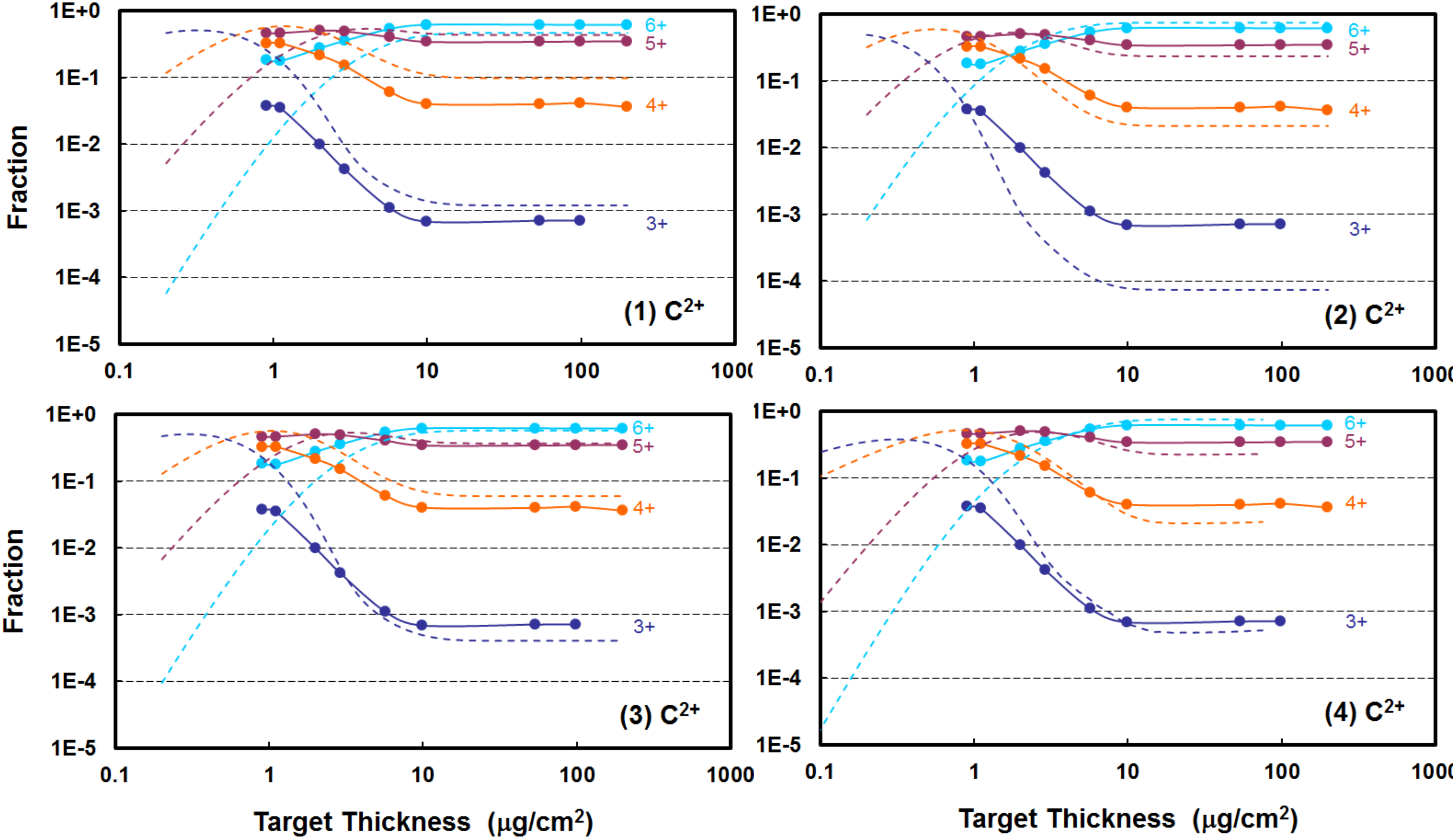


Case	Cross Sections		References	Accuracy
(1)-(3)	e-cap. e-loss ex.	OBK relativistic Born relativistic Born	JPB37,201(2004) JETP119,1(2014) NIMB184,295(2001)	50% 30-50% 30-50%
(4) ETACHA	REC	Bethe-Salpeter	(1957)	Scaling used partly

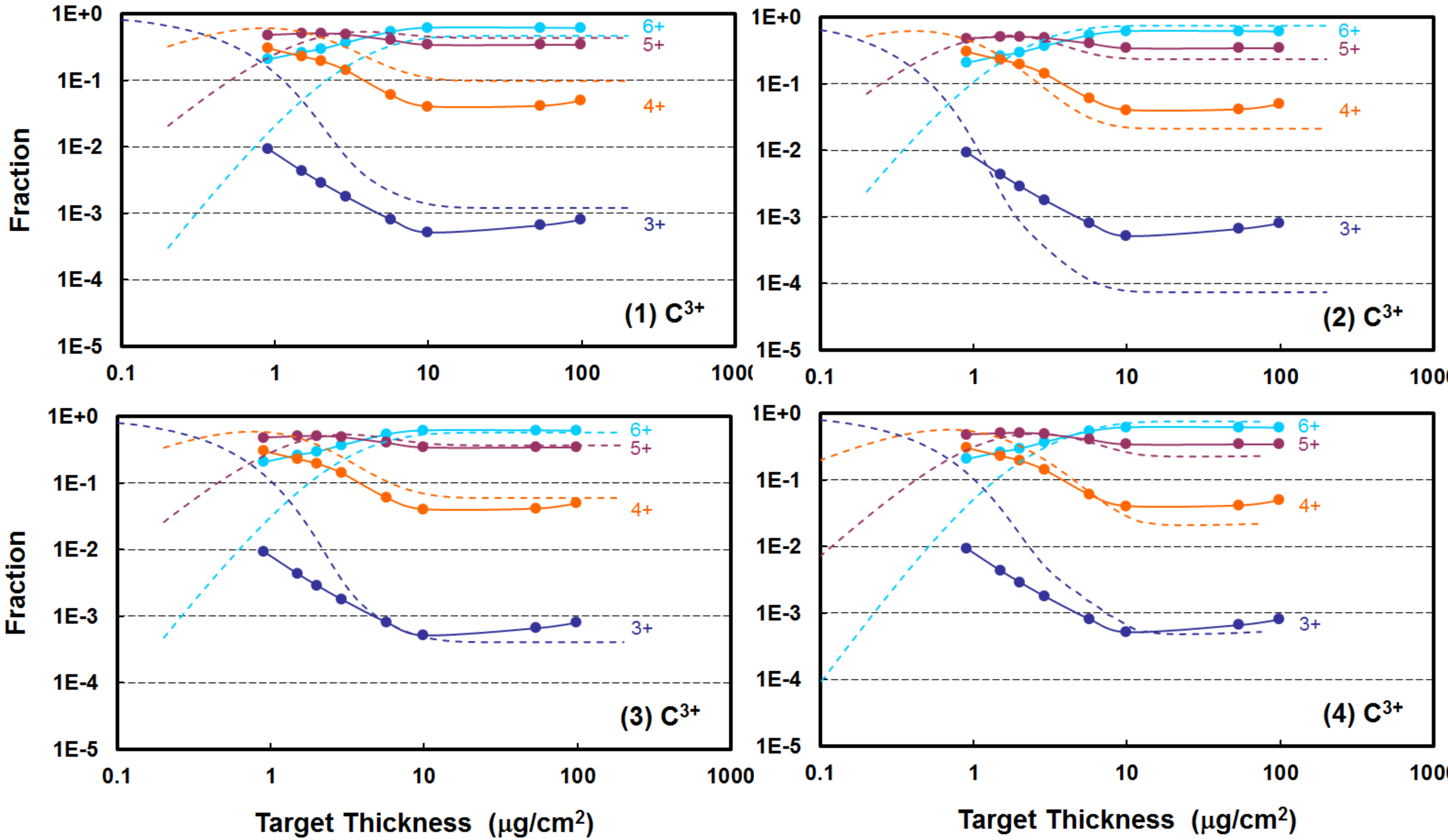
$$\frac{\mathrm{d}y_i}{\mathrm{d}x} = \sum_{i \neq j} y_j(x)\sigma_{ji} - \sum_{i \neq j} y_i(x)\sigma_{ij} \qquad \sum_i y_j = 1$$

Case	Calculation	Yields Y_i	Density Effect
(1)	Present	Charge-State 7(C^0 – C^{6+})	Not involved.
(2)	Present	Charge-State 7(C^0 – C^{6+})	High *n* states are ionized. JPB38,2675(2005)
(3)	Present	CS + *n* =1,2-state 18(C^0 – C^{6+})	High *n* states are ionized.
(4)	ETACHA4 PRA92,042703(2015)	CS + *nl* -substate many(C^0 – C^{6+})	Shorter collision intervals are involved in the RE.

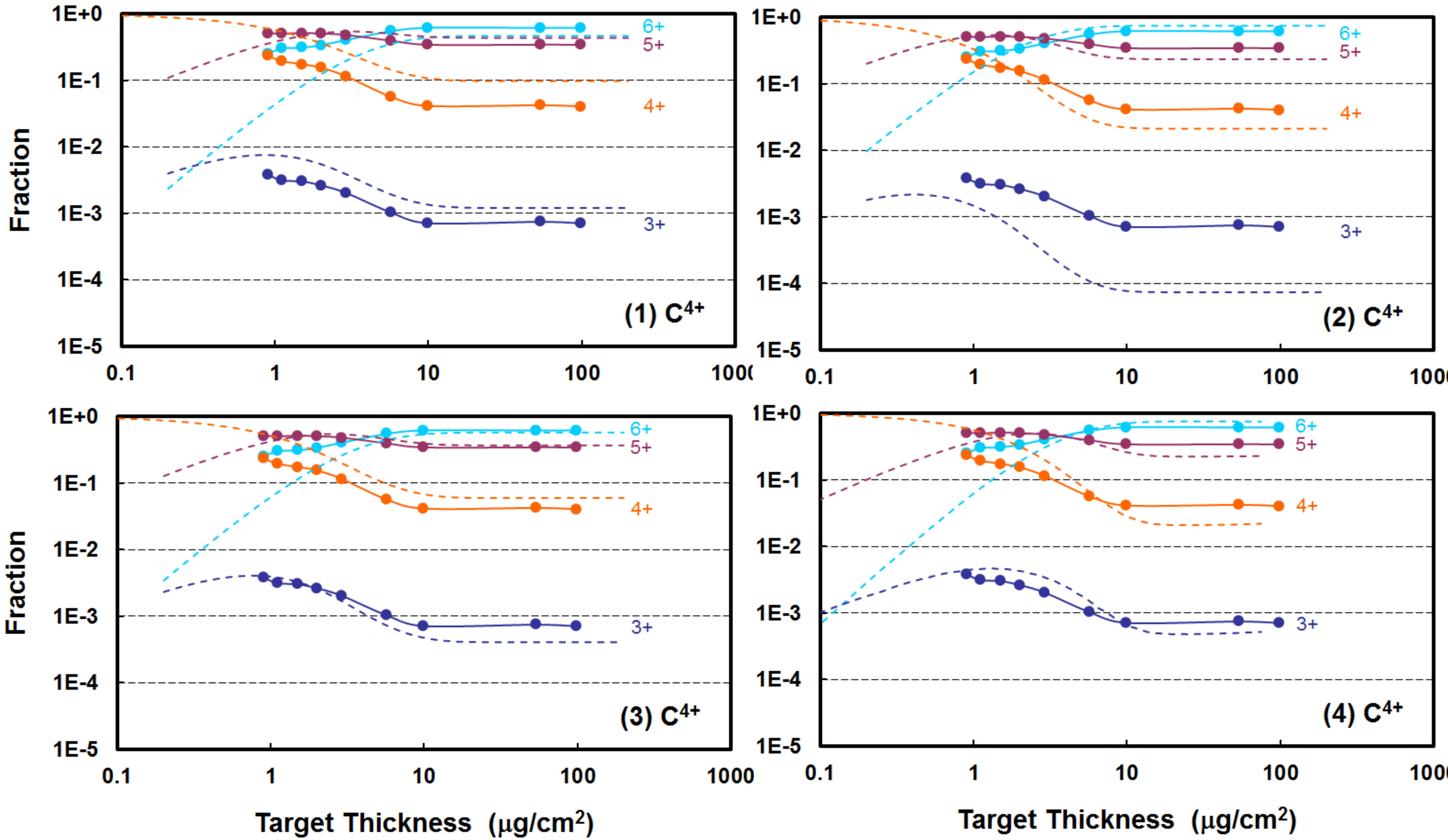
Model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



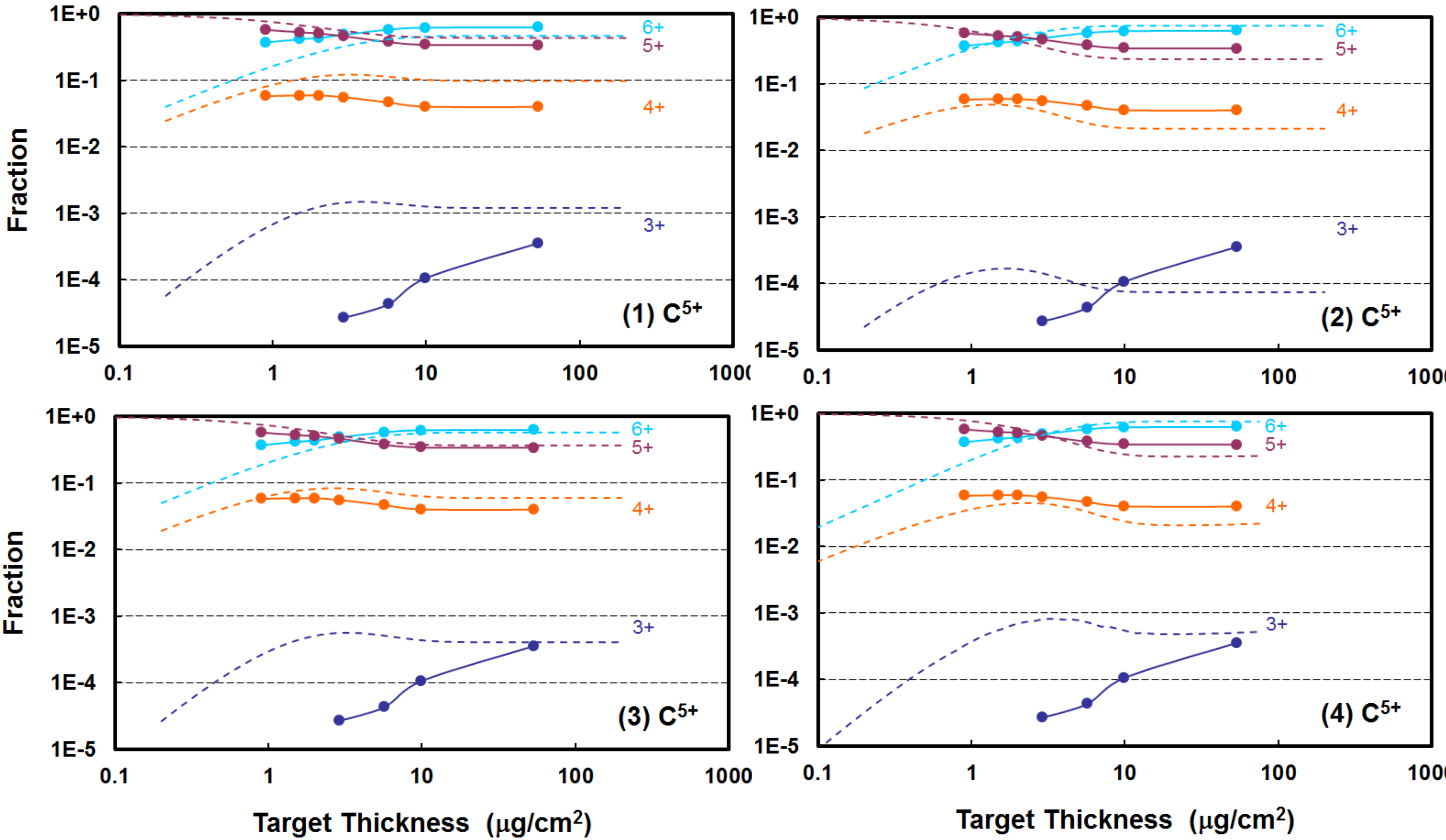
Model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



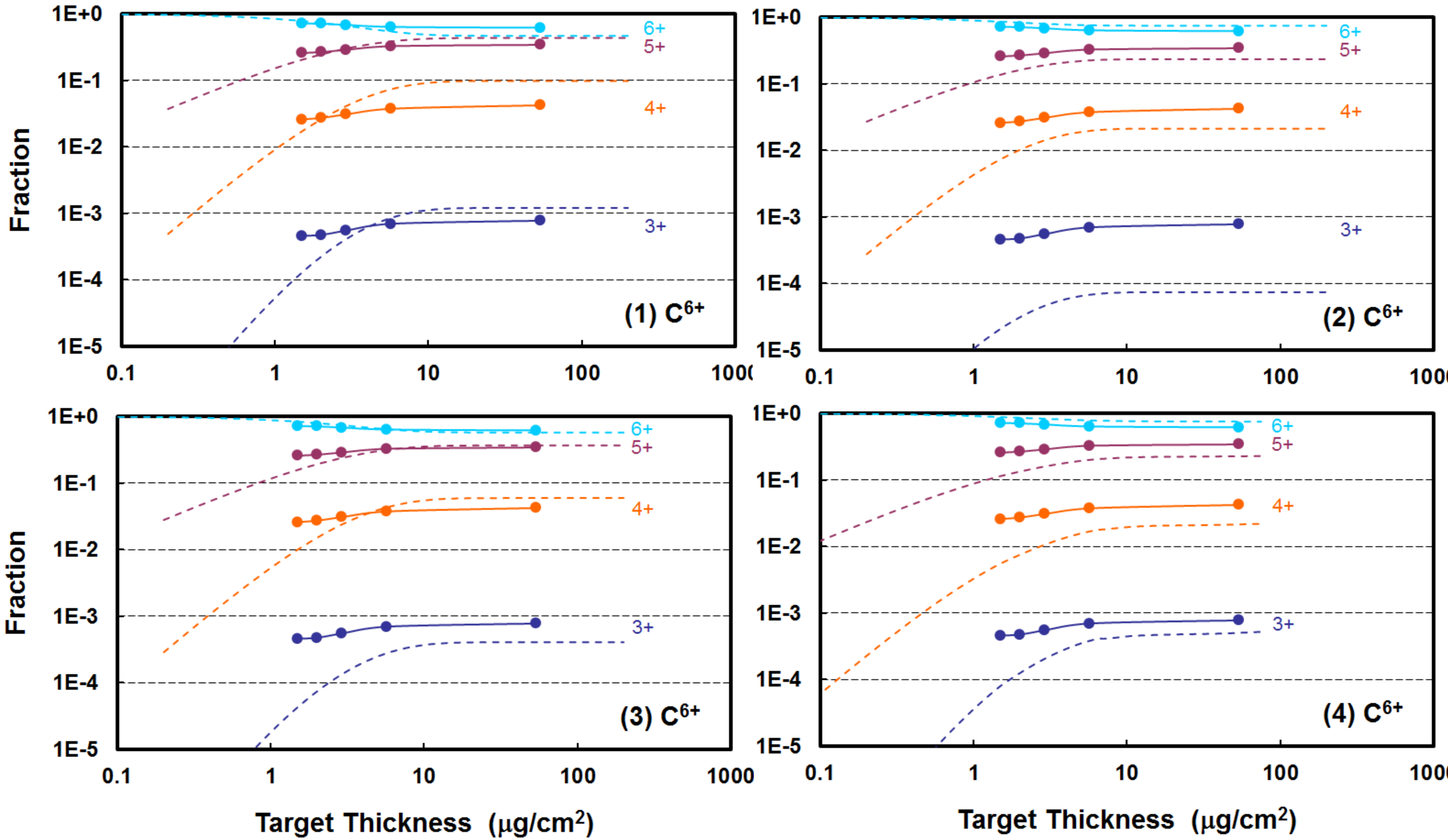
Model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



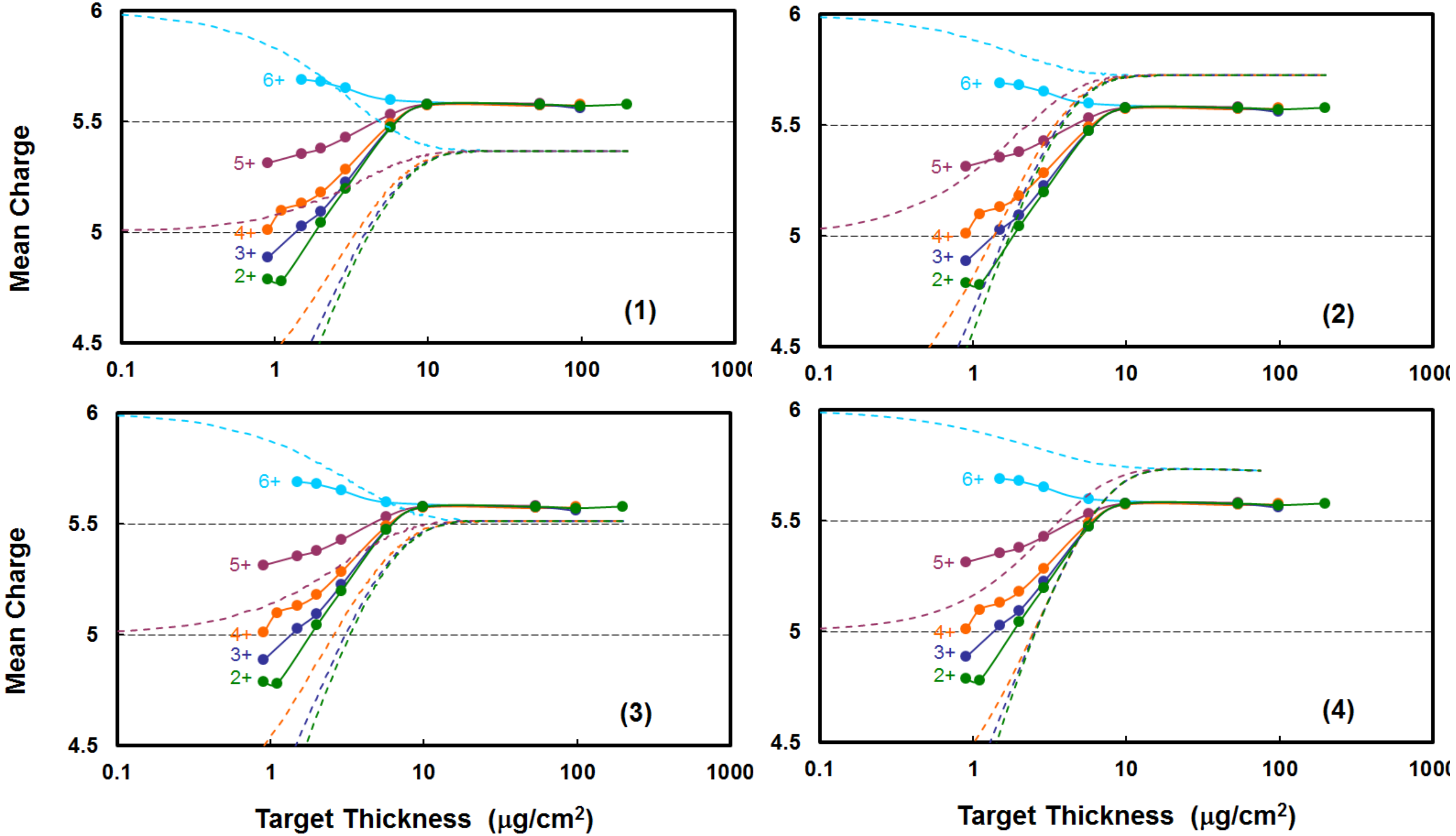
Model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



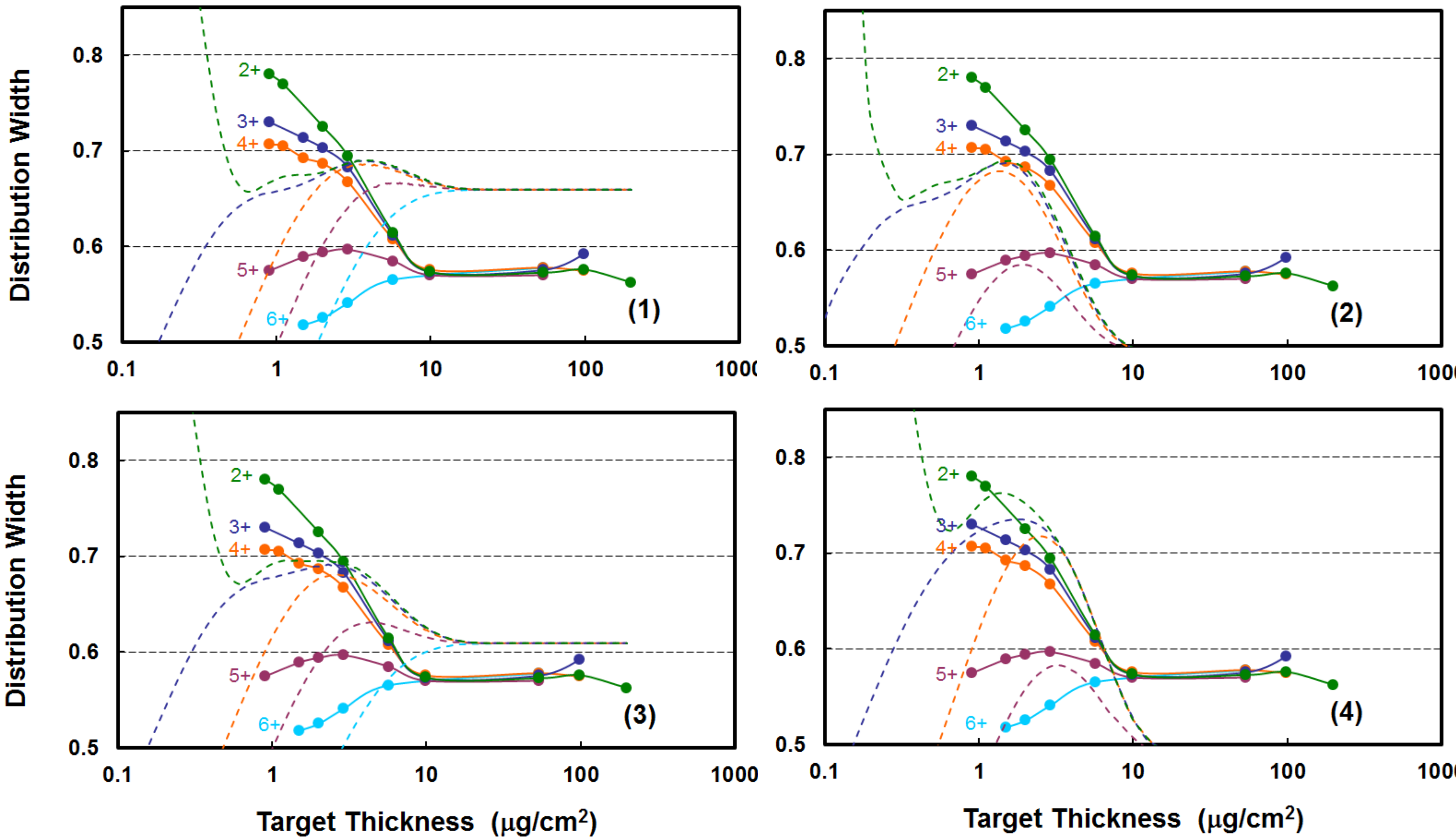
Model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



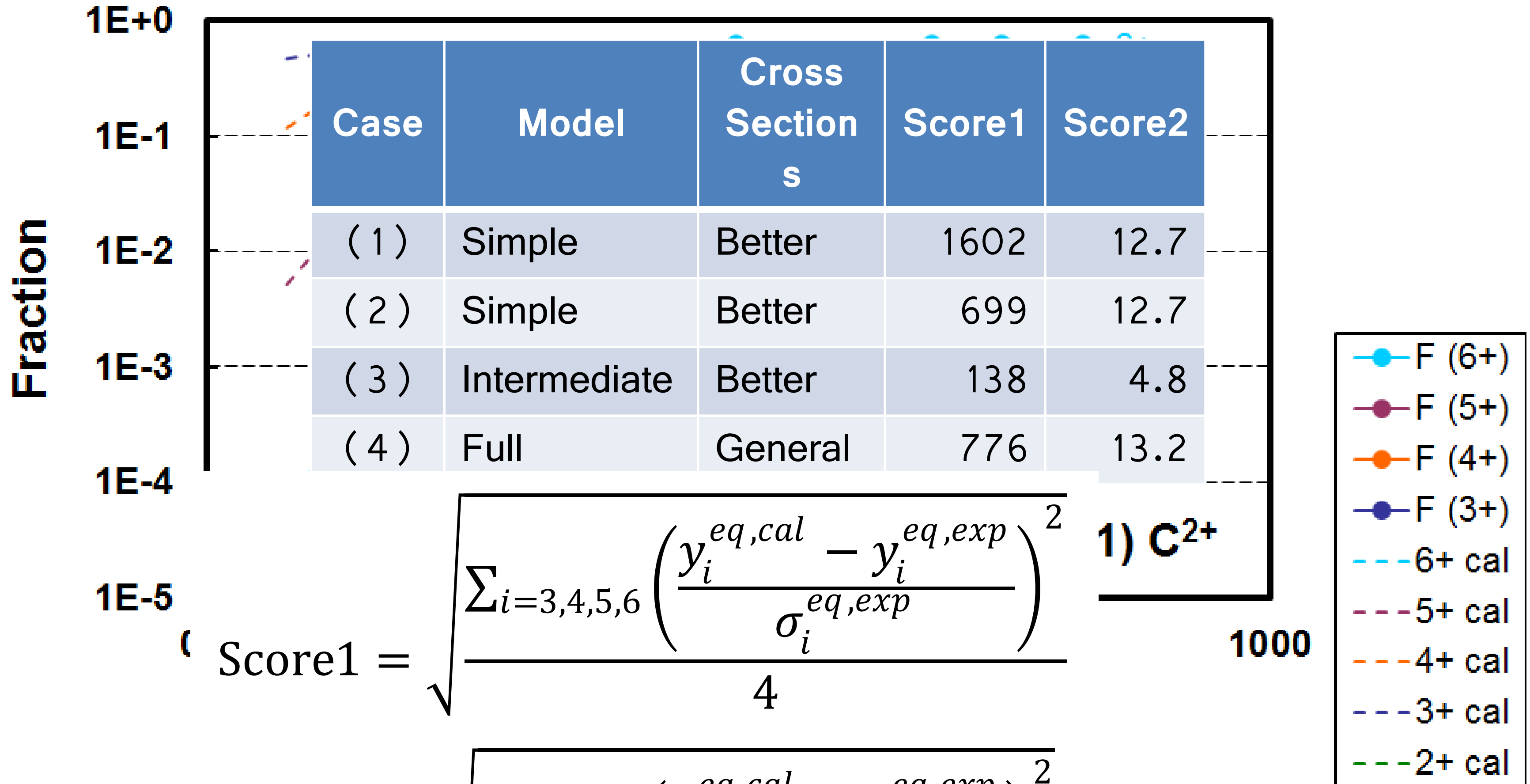
Model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



Model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



Scores for reproducibility of the **equilibrium charge-state distributions** of 2.0 MeV/u C ions after C-foils

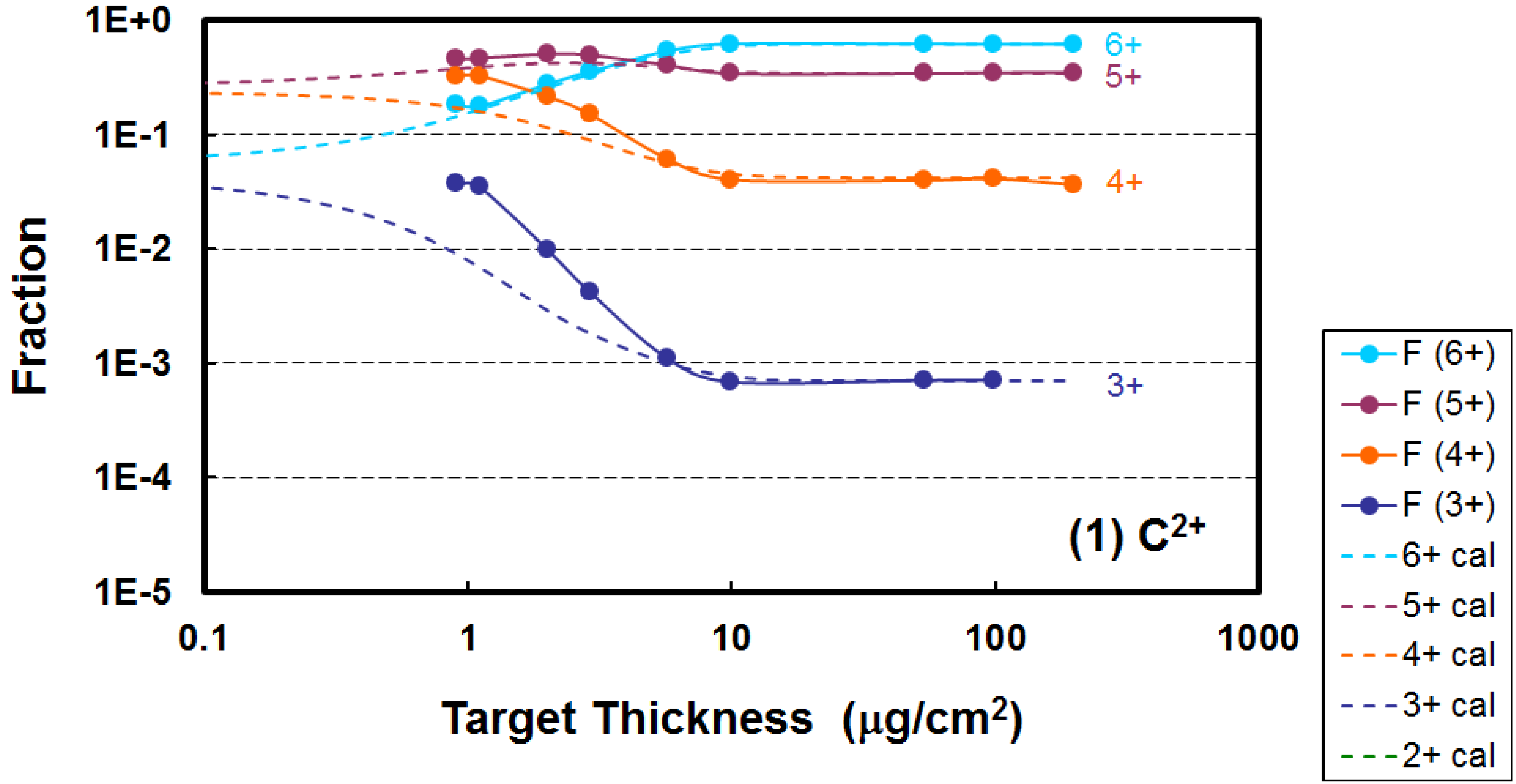


Case	Model	Cross Sections	Score1	Score2
(1)	Simple	Better	1602	12.7
(2)	Simple	Better	699	12.7
(3)	Intermediate	Better	138	4.8
(4)	Full	General	776	13.2

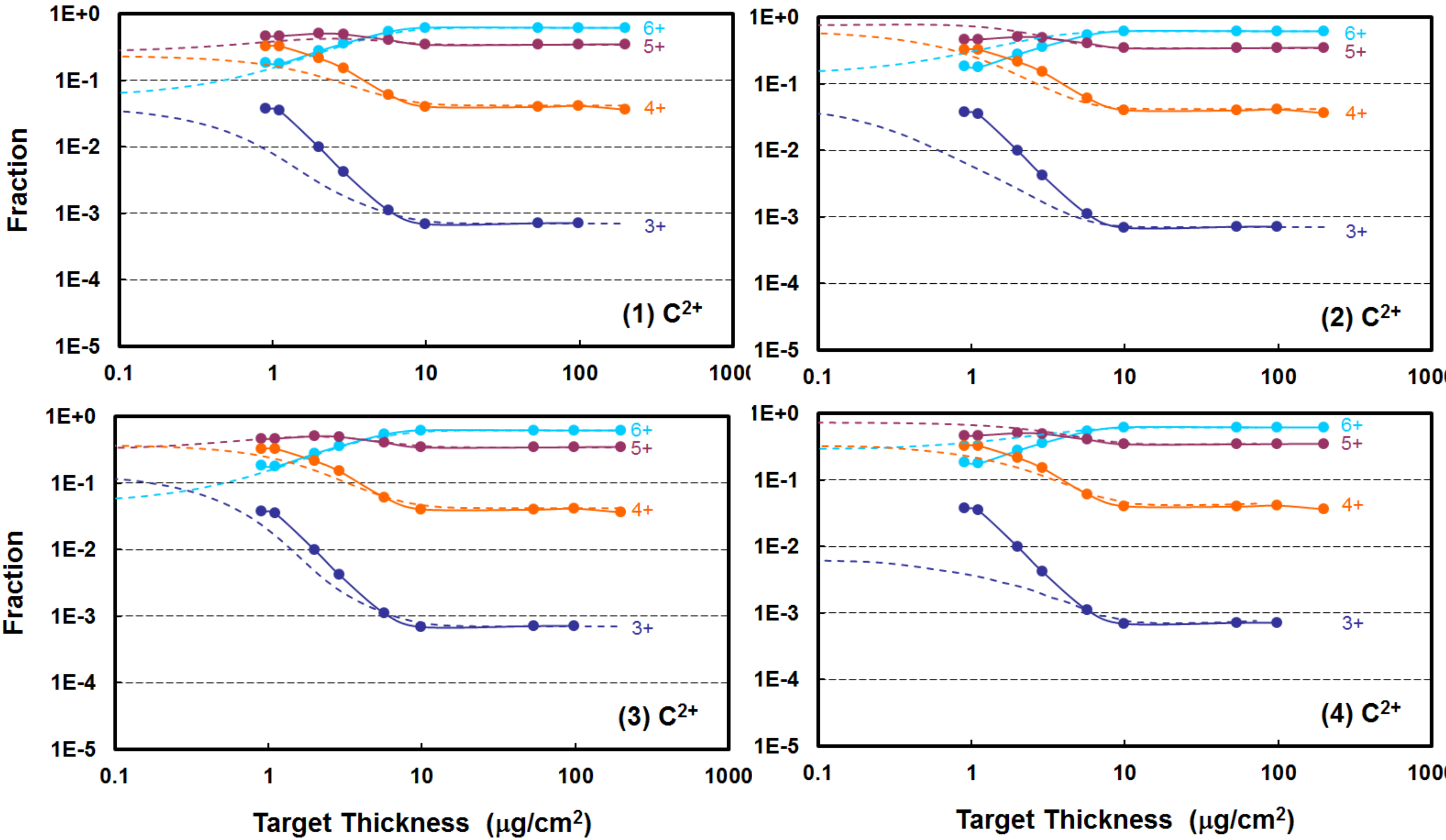
$$\mathrm{Score1} = \sqrt{\frac{\sum_{i=3,4,5,6}\left(\frac{y_i^{eq,cal} - y_i^{eq,exp}}{\sigma_i^{eq,exp}}\right)^2}{4}}$$

$$\mathrm{Score2} = \sqrt{\frac{\sum_{i=\bar{q},d,s}\left(\frac{y_i^{eq,cal} - y_i^{eq,exp}}{\sigma_i^{eq,exp}}\right)^2}{3}}$$

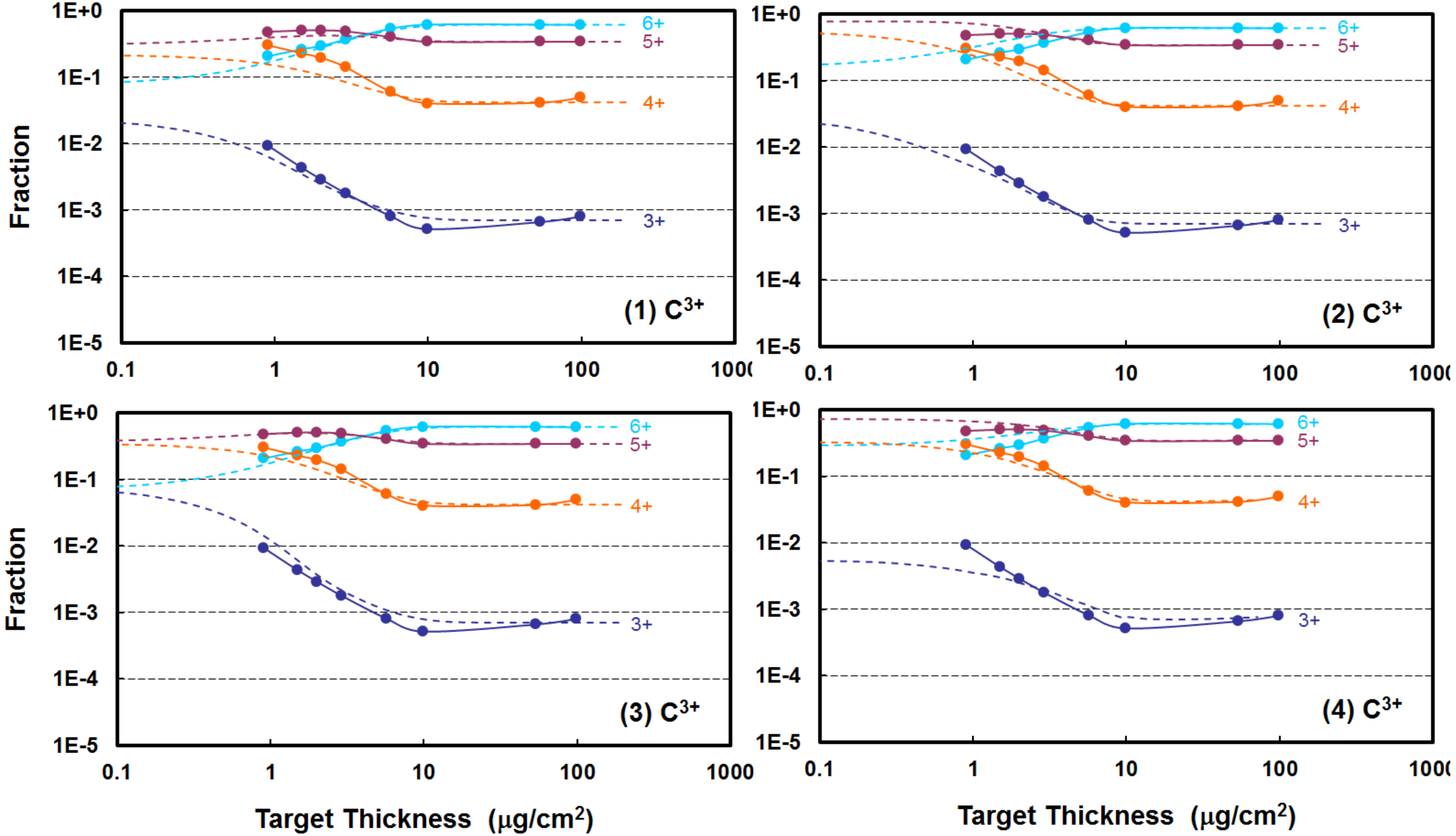
Shifted model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



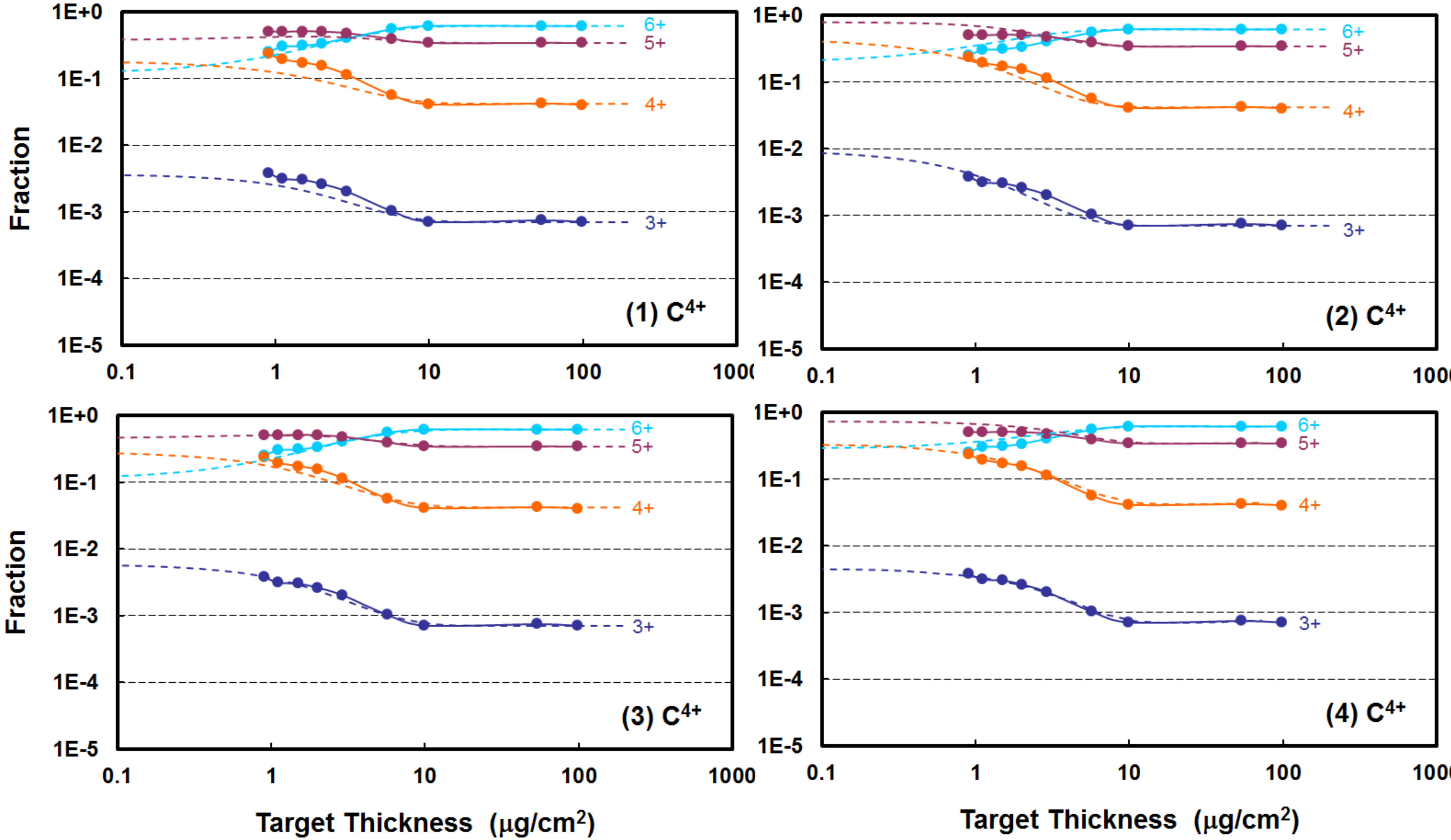
Shifted model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



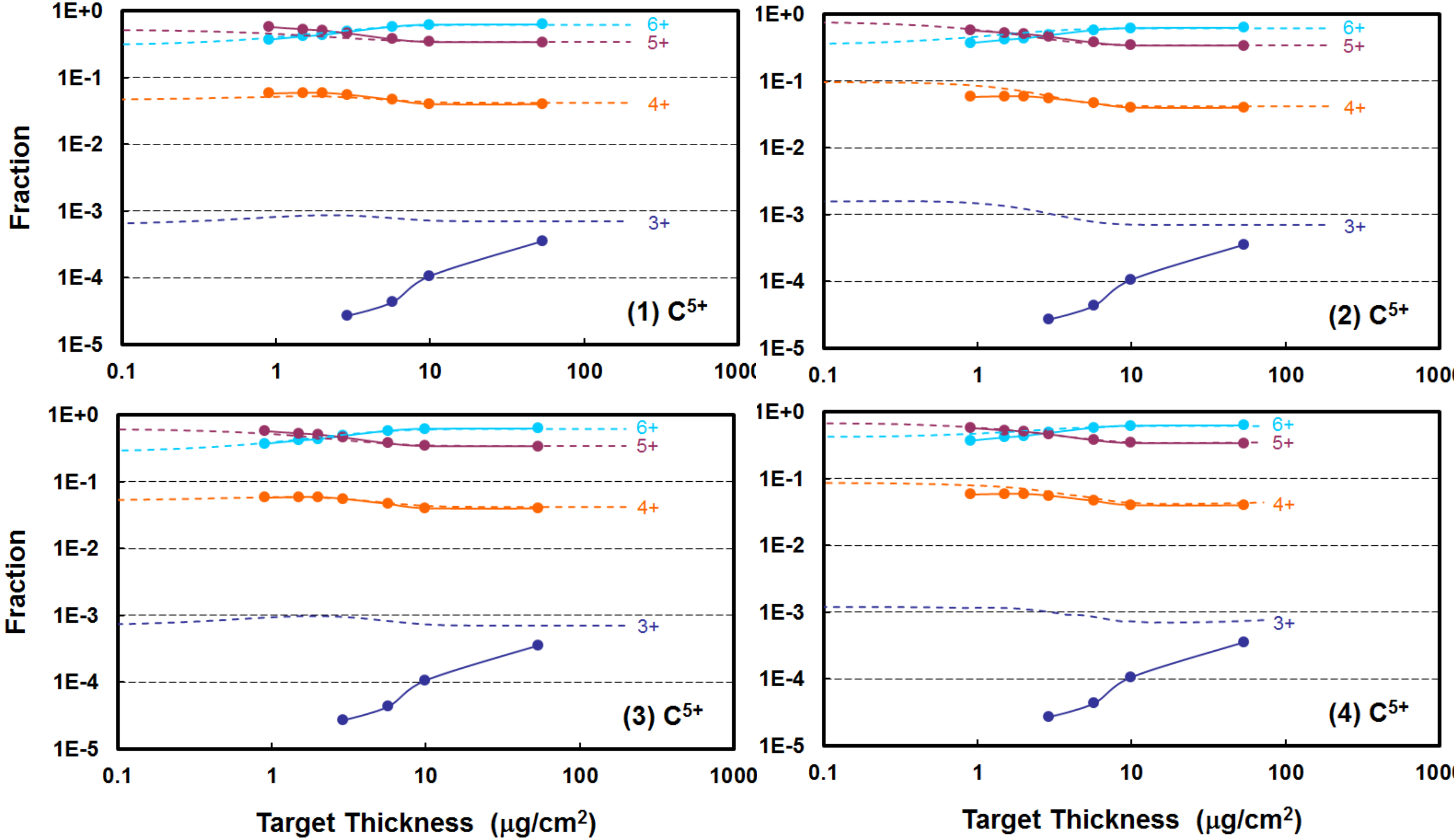
Shifted model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



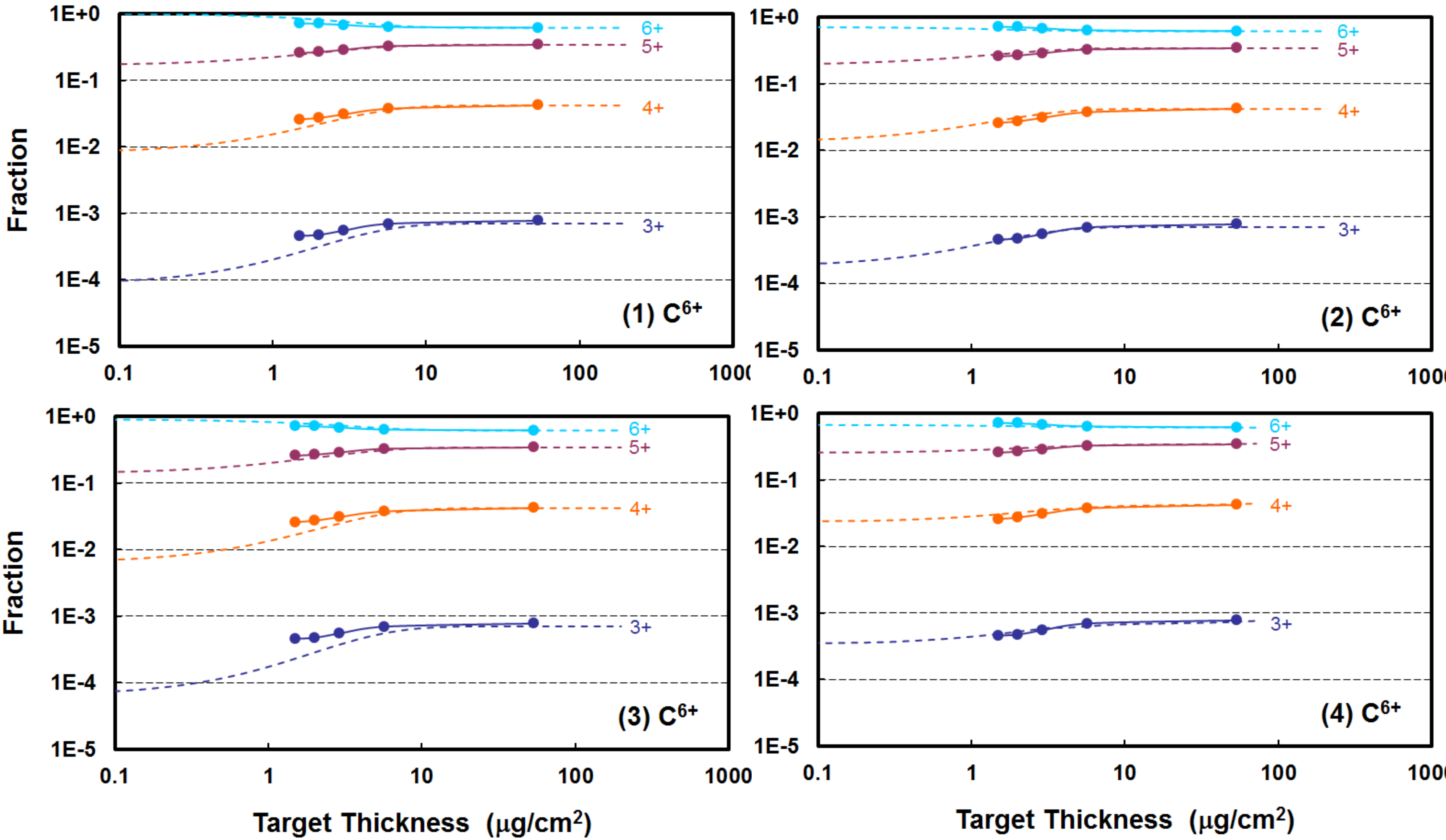
Shifted model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



Shifted model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



Shifted model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



Scores for reproducibility of the **pre-equilibrium charge-state distributions** of 2.0 MeV/u C ions after C-foils

$$Score = \sqrt{\frac{\sum_i \left(y_i^{pre-eq,cal} - y_i^{pre-eq,exp}\right)^2}{N}}$$

$$N = 97$$

Case	Model	Cross Sections	Score	Score1	Score2
(1)	Simple	Better	0.0570	1602	12.7
(2)	Simple	Better	0.0792	699	12.7
(3)	Intermediate	Better	0.0282	138	4.8
(4)	Full	General	0.0747	776	13.2

Summary and outlook

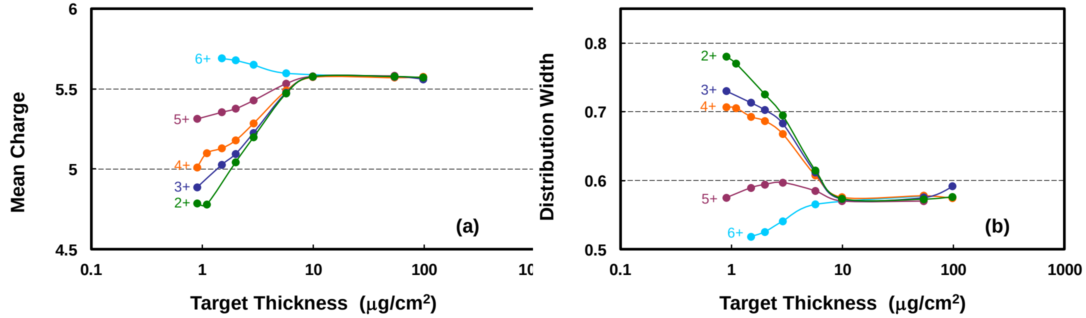
- You require not just accuracy of calculated cross sections but also their completeness.
- Experimentalists would like the evaluation of theoretical data to be done with experiments, but in many cases, there exist few experiments directly comparable to theories.
- Experimentalists are able to provide very accurate experimental results in some cases.
- It would be possible to evaluate set of calculated cross sections (e-capture, loss, excitation, de-excitation) using charge state evolution data.
- It would be also possible to reduce the collision energy by using dense gas targets.

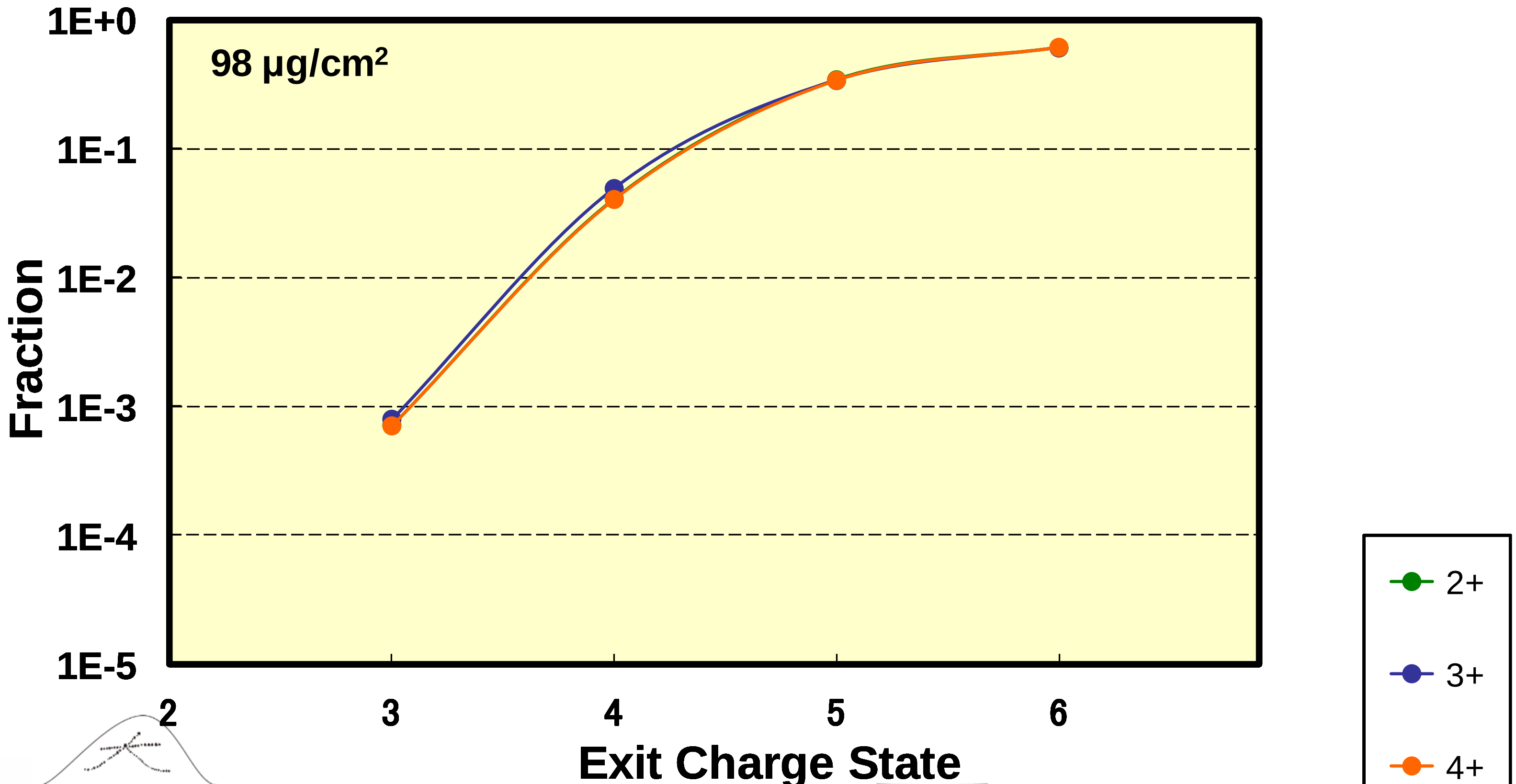
Vielen Dank und Frohe Weihnachten！

© Nakamura Jakuemon V

www.youtube.com/watch?v=CChdGosT300

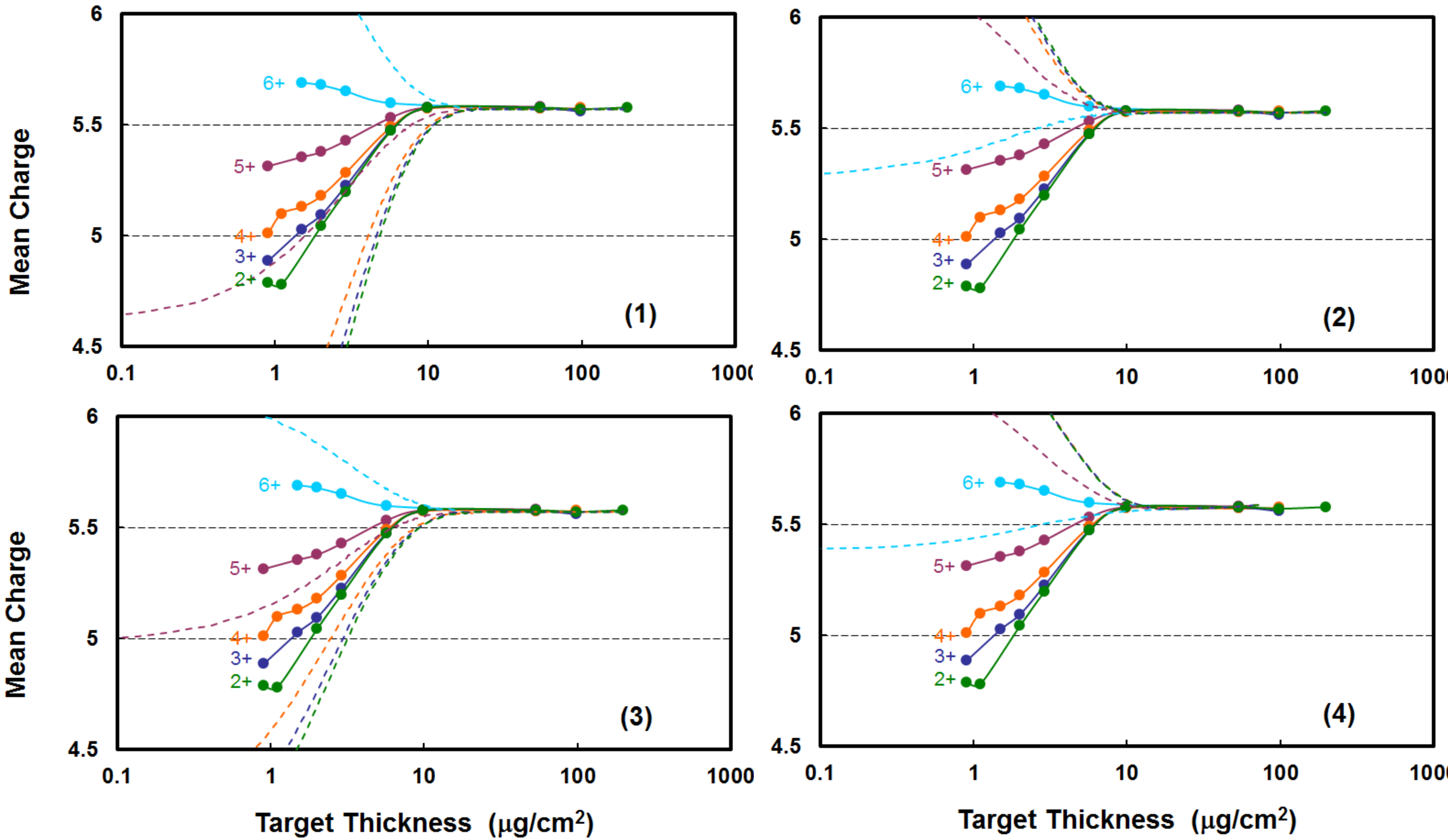
Charge-state distributions of 2.0 MeV/u C^{q+} ions after C-foils





M.Imai *et al.*, NIM B 354, 172 (2015).

Shifted model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils



Shifted model calculations using sets of cross sections for charge-state distributions of 2.0 MeV/u C ions after C-foils