Supplementary material: Solving Peak Overlaps for Proximity Histogram Analysis of Complex Interfaces for Atom Probe Tomography Data

Jens Keutgen1, Andrew J. London2, Oana Cojocaru-Miredin1,*

1 RWTH Aachen, I. Physikalisches Institut (1A), Aachen, Germany

2 UK Atomic Energy Authority, Culham Science Centre, Oxfordshire OX14 3DB, UK

*corresponding author: cojocaru-miredin@physik.rwth-aachen.de

In this supplementary material, we show the complete mass spectra for the two analyzed materials with all defined overlaps for both regions of the interface. Additionally, you'll find further information about the effect of voxel size on the steepness of the proximity histogram. Finally, we added the code used to create the simulation data and information about the EPOSA software suite.

To get hold of the EPOSA software suite just write an e-mail to keutgen@physik.rwth-aachen.de. An extended demonstration of the program is available at: https://youtu.be/k_SOyi-RlWw

CIGS case study mass spectra and overlap diagram

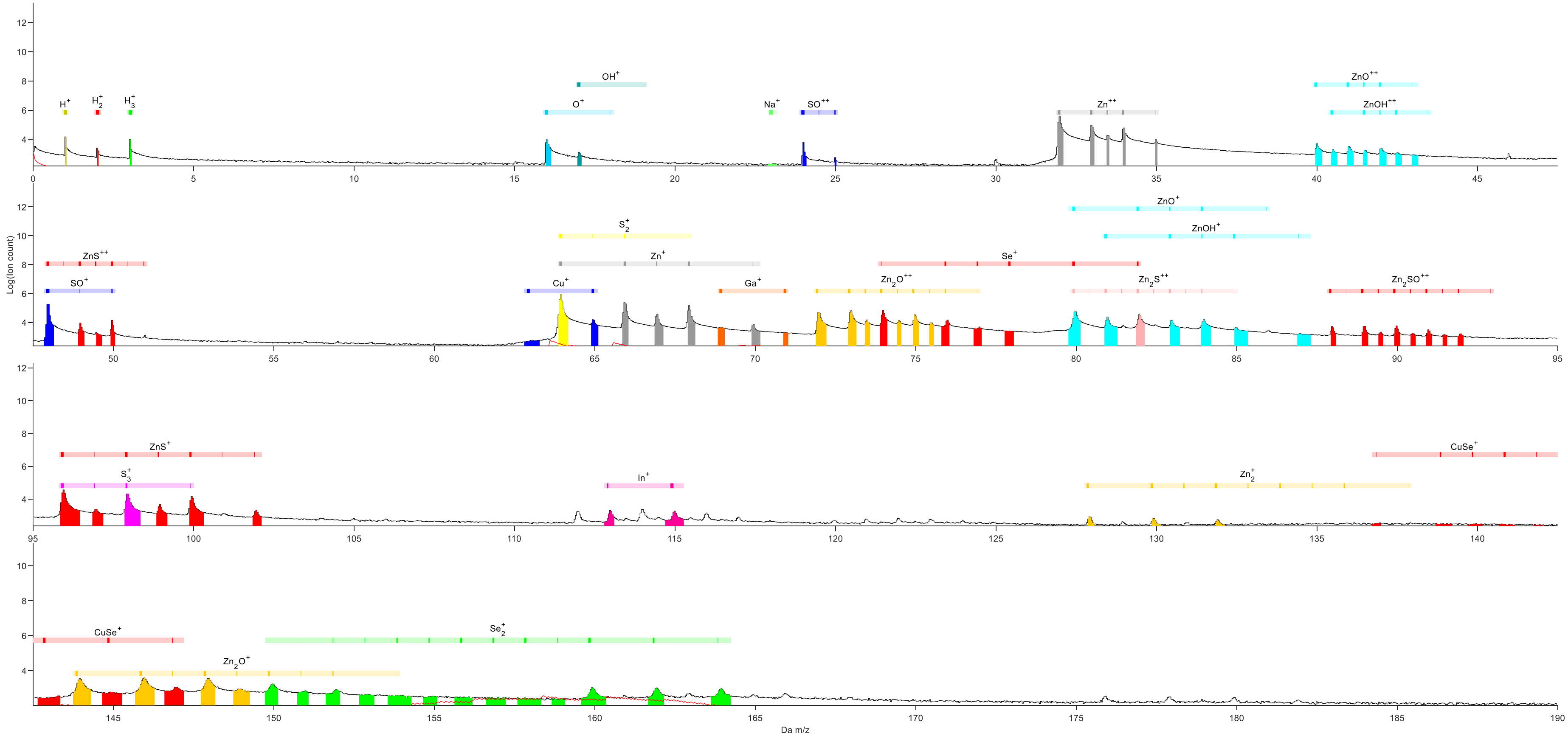

Figure S.1: Mass spectrum of the Zn(O,S) buffer inside the CIGS solar cell. Coloured ranges indicate the mass windows used, labeled bars above the plot indicate the theoretical peak positions of different ions used in the overlap solving and the red line indicates the background subtraction.

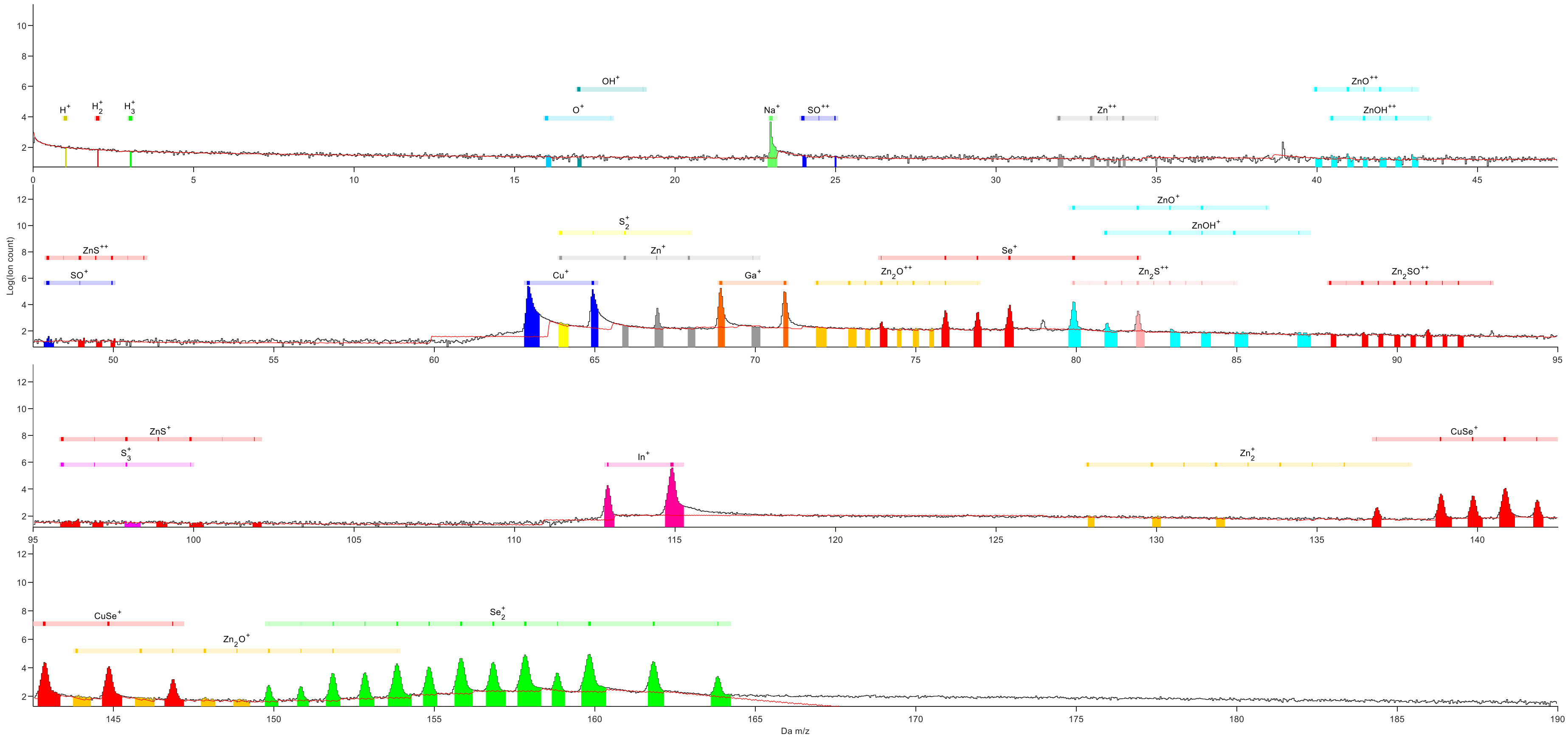

Figure S.2: Mass spectrum of the $Cu(In,Ga)Se_2$ absorber inside the CIGS solar cell. Coloured ranges indicate the mass windows used, labeled bars above the plot indicate the theoretical peak positions of different ions used in the overlap solving and the red line indicates the background subtraction.

ODS case study mass spectra and overlap diagram

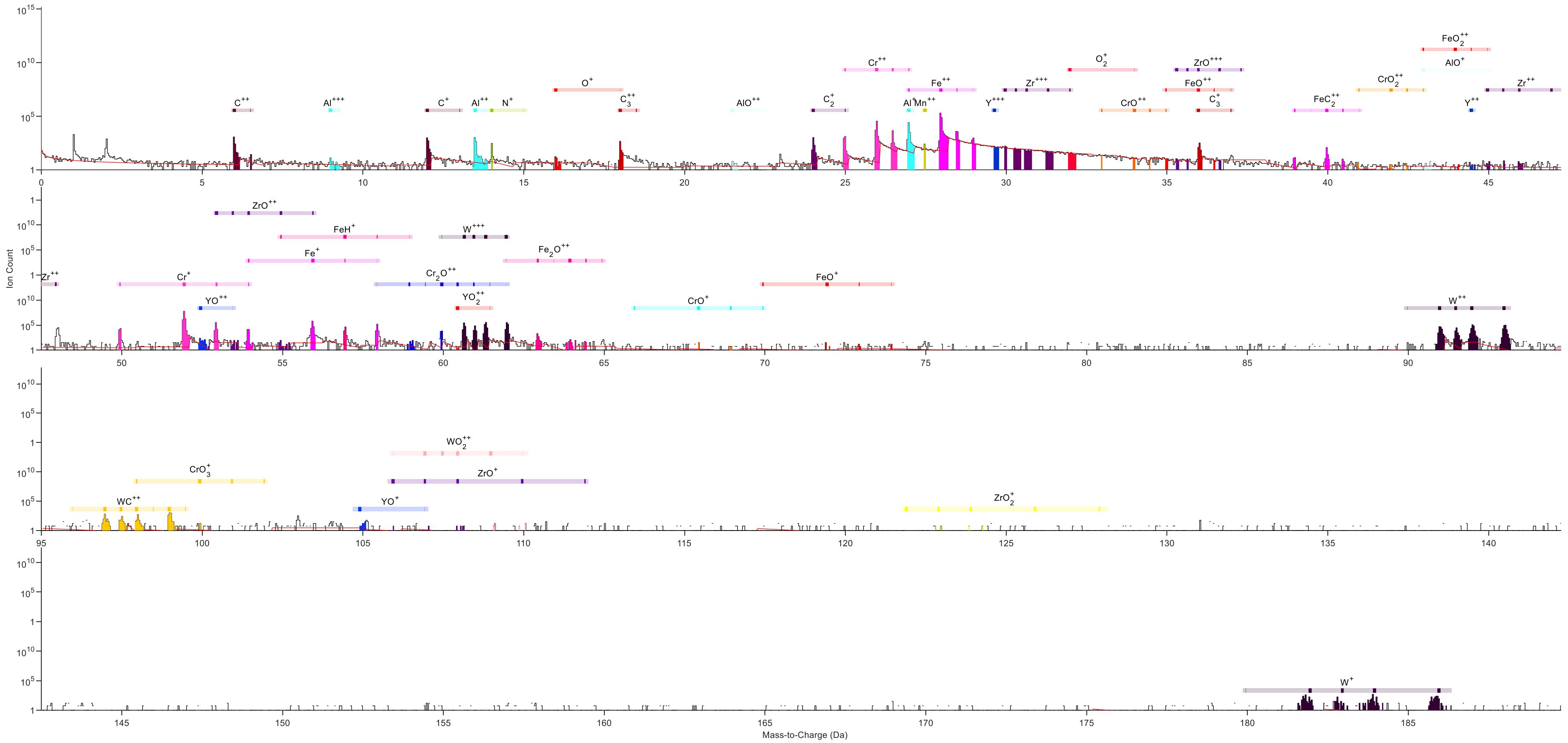

Figure S.3: Mass spectrum of the Fe-Cr matrix of oxide dispersion strengthened material. Coloured ranges indicate the mass windows used, labeled bars above the plot indicate the theoretical peak positions of different ions used in the overlap solving and the red line indicates the background subtraction.

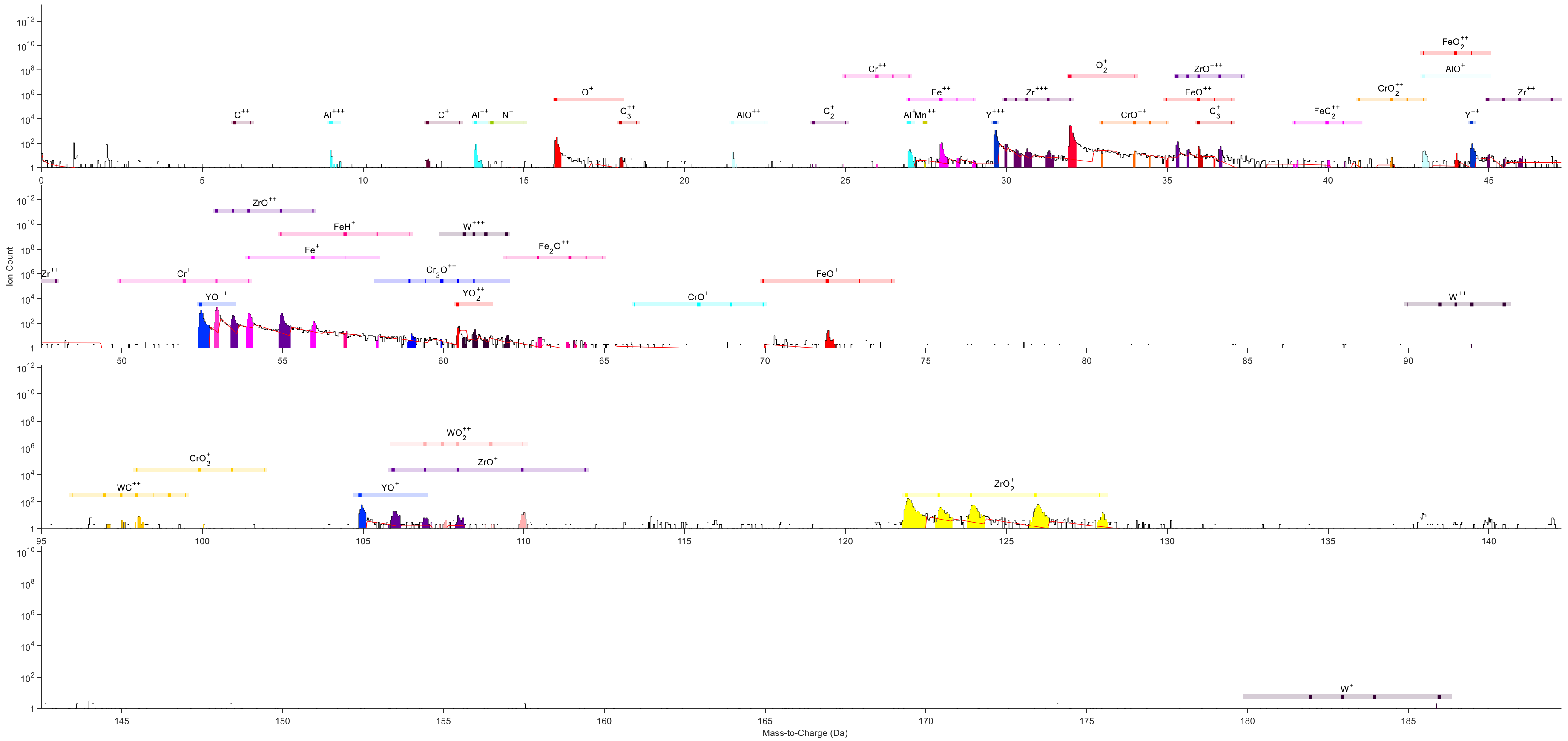

Figure S.4: Mass spectrum of the Zr-Y-oxide particle section of oxide dispersion strengthened material. Coloured ranges indicate the mass windows used, labeled bars above the plot indicate the theoretical peak positions of different ions used in the overlap solving and the red line indicates the background subtraction.

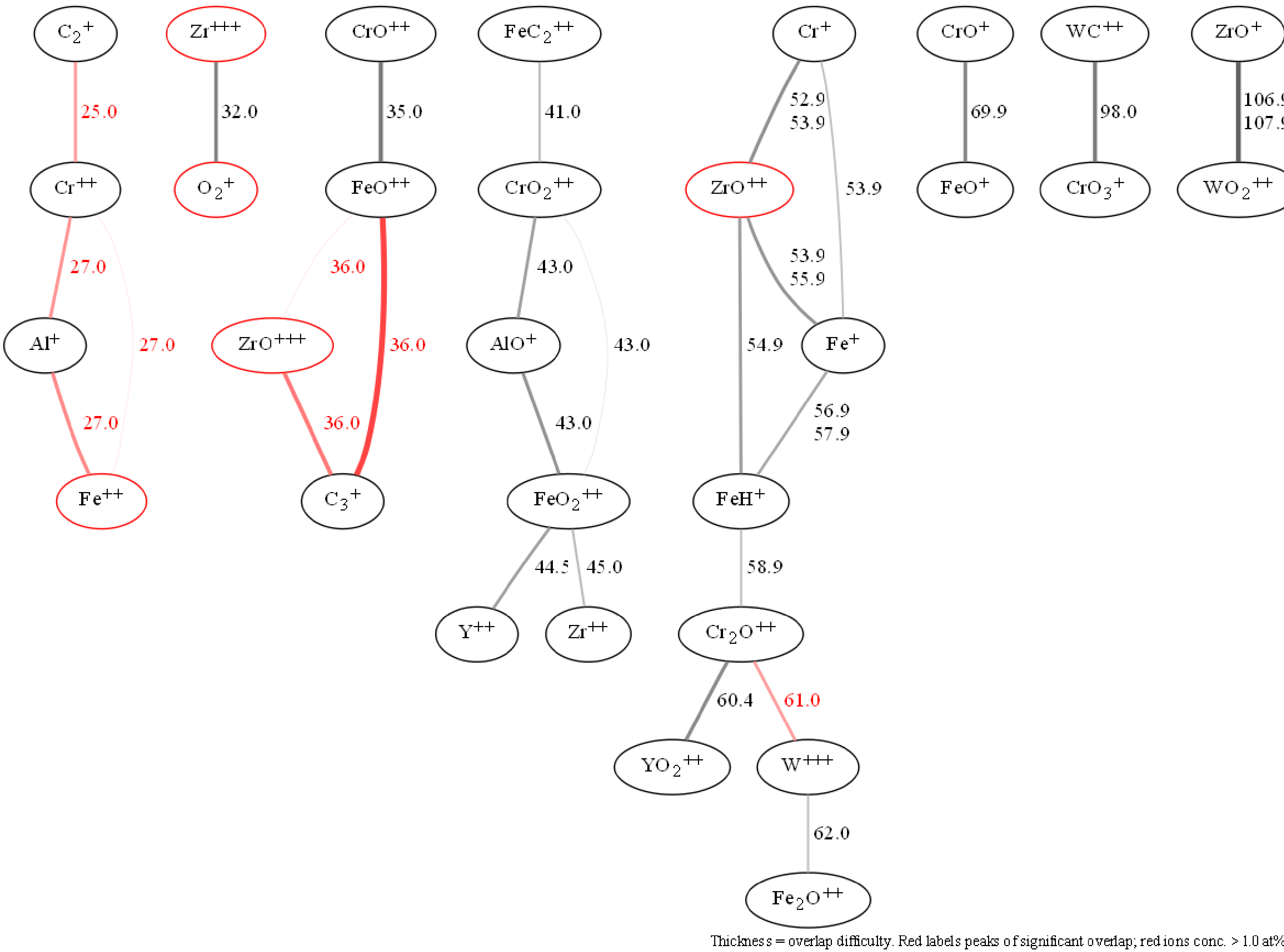

Figure S.5 : Overlap diagram for the ODS example. Bubbles show the ions involved, links show which ions have direct overlaps and the value of the line indicates the overlapping mass positions. The line thickness is proportional to the uncertainty introduced by the presence of the overlap. Red lines are mass positions with a significant contribution from multiple ions and red ions indicate ions with a concentration > 1.0 at%.

Impact of voxel size on iso-concentration surface accuracy

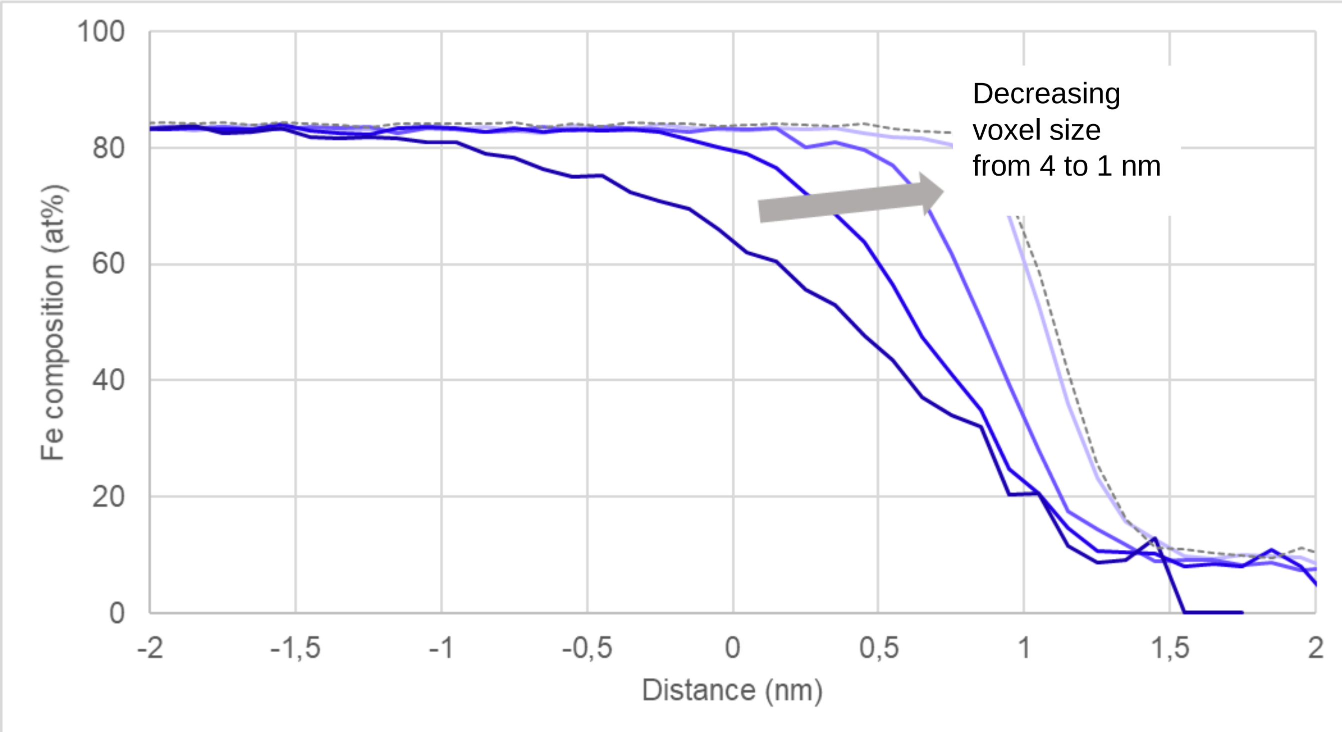

Figure S.6: Effect of voxel size on iso-concentration surface and proximity histogram analysis. The steepest curve (right most) is for 1 nm sized voxels. In all cases the delocalization is half the voxel size. Position of the proximity histograms has been shifted on the x-axis for clarity of the figure. All proximity histograms made using a 15% concentration of Al+Ni.

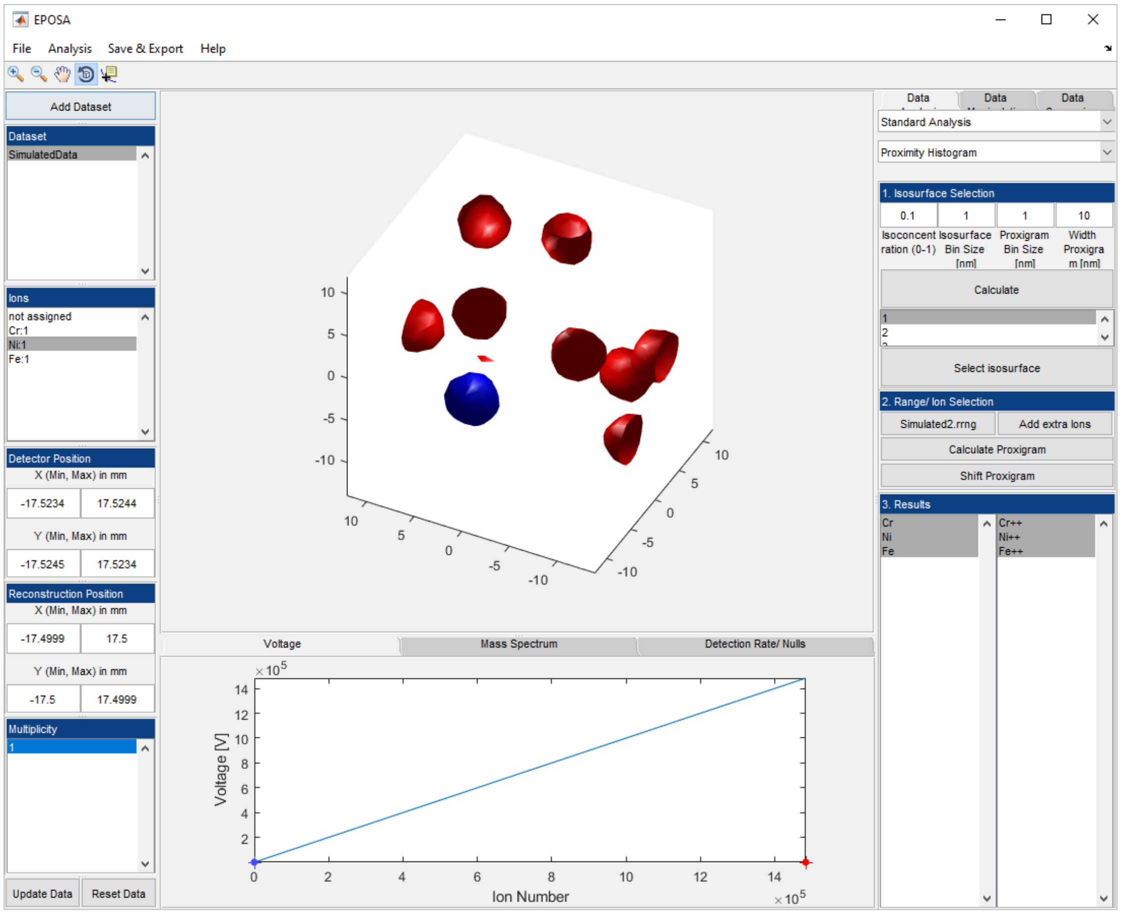

Figure S.7: Overview of the EPOSA software. It allows easy loading and selection of the desired dataset for further investigation.

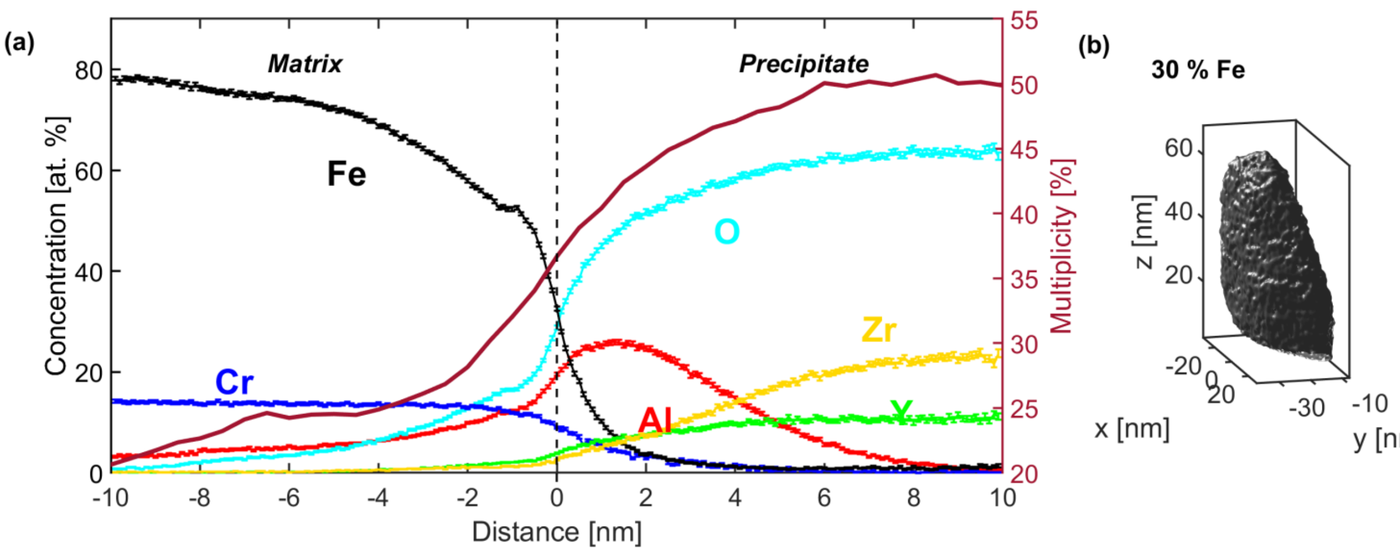

Figure S.8: Propability of multiple hit (Multiplicity) plotted for the interface of ODS steel dataset (compare Figure 6).

POSGEN SCRIPT SIMULATION:

https://rwthaachende-my.sharepoint.com/:u:/g/personal/jens_keutgen_rwth-aachen_de/EUvjlCzeEQtLhHuxnHQz9g8BrfVeToqzmzGwQtLlPEI7Dg?e=0CJnVE