Contribution ID: **141** Type: **Talk**

Near-Surface Cation Diffusion in Magnetite studied by advanced Synchrotron and Neutron Methods

With their flexible stoichiometry, magnetic properties and wide abundance, iron oxides are used as catalysts and catalyst components, in medicine, magneto-electronic devices and composite materials. As the surface and interface properties of iron oxides are crucial for these applications, tuning their performance requires a precise understanding of structure and reactions in their near-surface region.
For the stable magnetite (Fe_3O_4) (001) surface, oxidative regrowth, (partial) lifting of the subsurface cation vacancy reconstruction and the element-specific incorporation of adatoms not only demonstrate a sensitive relation of environmental conditions and defect structure, but also highlight the importance of near-surface cation transport [1,2,3].
We studied the growth, defect structure and cation transport between an isotopically labelled $^{57}Fe_3O_4$ thin film and a Fe_3O_4 (001) single crystal substrate by a combination of surface X-ray diffraction (SXRD), neutron reflectivity (NR) and nuclear forward scattering (NFS) [4,5]. While NR provided information about the ^{57}Fe depth distribution, *in situ* NFS allowed to determine the lattice site-selective ^{57}Fe depth distribution and provided independent information about the density and stoichiometry of the near-surface region. The transport experiments are complemented with SXRD to characterise the Fe_3O_4 homoepitaxy, further emphasizing the link between structure, stoichiometry and transport processes in Fe_3O_4.
Combining advanced sample preparation at CXNS with methods available at synchrotron and neutron facilities such as PETRAIII, FRMII and SOLEIL allowed to derive characteristics of near-surface cation transport in Fe_3O_4 that might as well be relevant for the class of spinel-type oxides as a whole.

References: [1] S. Nie *et al.* JACS **135**, 10091 (2013); [2] R. Bliem *et al.* Science **346**, 1215 (2014); [3] B. Arndt *et al.* Surf. Sci. **653**, 76 (2016), [4] S. Tober *et al.*, Phys. Rev. Res. **2**, 023406 (2020), [5] S. Tober *et al.* Phy. Rev. Lett. **134**, 236203 (2025).

Authors: TOBER, Steffen (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany Universität Hamburg, Fachbereich Physik, Luruper Chaussee 129, 22607 Hamburg, Germany, Jülich Centre of Neutron Science (JCNS-2), Forschungszentrum Jülich, Wilhelm-Johnen-Str., 52428 Jülich, Germany, Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany); SCHOBER, Jan-Christian (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany Universität Hamburg, Fachbereich Physik, Luruper Chaussee 129, 22607 Hamburg, Germany); CREUTZBURG, Marcus (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany Universität Hamburg, Fachbereich Physik, Luruper Chaussee 129, 22607 Hamburg, Germany); JACOBSE, Leon (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany); CHUNG, Simon (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany); ARNDT, Björn (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany Universität Hamburg, Fachbereich Physik, Luruper Chaussee 129, 22607 Hamburg, Germany); BECK, Esko Erik (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany Universität Hamburg, Fachbereich Physik, Luruper Chaussee 129, 22607 Hamburg, Germany); VLAD, Alina (Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, 91192 Gif sur Yvette, France); WILLE, Hans-Christian (Deutsches Elektronen-Synchrotron); STEINBRÜGGE, René (Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany); SERGEEV, Ilya (Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany); KOUTSIOUBAS, Alexandros (Jülich Centre of Neutron Science (JCNS-2), Forschungszentrum Jülich, Wilhelm-Johnen-Str., 52428 Jülich, Germany); PÜTTER, Sabine (Jülich Centre of Neutron Science (JCNS-2), Forschungszentrum Jülich, Wilhelm-Johnen-Str., 52428 Jülich, Germany); MATTAUCH, Stefan (Jülich Centre of Neutron Science (JCNS-2), Forschungszentrum Jülich,

Wilhelm-Johnen-Str., 52428 Jülich, Germany); NOEI, Heshmat (Deutsches Elektronen-Synchrotron DESY); LEUPOLD, Olaf (Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany); LOTT, Dieter (Helmholtz-Zentrum Hereon, Max-Planck-Strasse 1, Geesthacht, 21502, Germany); SCHLAGE, Kai (DESY); VONK, Vedran (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany); STIERLE, Andreas (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany Universität Hamburg, Fachbereich Physik, Luruper Chaussee 129, 22607 Hamburg, Germany)

Presenter: TOBER, Steffen (Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany Universität Hamburg, Fachbereich Physik, Luruper Chaussee 129, 22607 Hamburg, Germany, Jülich Centre of Neutron Science (JCNS-2), Forschungszentrum Jülich, Wilhelm-Johnen-Str., 52428 Jülich, Germany, Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany)

Session Classification: Plenary 2

Track Classification: RT2