Seeing hydrogen in matter

Sprawozdania

Informacje na temat projektu

SHINE

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Strona internetowa projektu

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Podsumowanie kontekstu i ogólnych celów projektu

The main aim of SHINE is to push the boundaries of quantitative analysis of hydrogen in materials in three-dimensions and at near-atomic resolution using atom probe tomography.
The materials of interest to SHINE find applications in the scope of a ‘low-carbon-emission economy’ either for hydrogen storage, or for light-weight transportation where hydrogen embrittlement is a

crucial limiting factor.
The project officially started in Feb 2018 and finished in January 2023.
SHINE built on the expertise and world-unique infrastructure in the Atom Probe group at MPIE along with the expertise in atomistic simulations. SHINE was the prime user of the Laplace Project established at MPIE in 2017, and that is still being developed.

Prace wykonane od początku projektu do końca okresu sprawozdawczego oraz najważniejsze dotychczasowe rezultaty

Following on preliminary results on H in Ti published in Acta Materialia, we used the uncontrolled ingress of H during specimen preparation to load samples of Ti-Mo alloys with different microstructures (Scripta Materialia Volume 162, 15 March 2019, Pages 321-325), highlighting the influence on the initial phase composition on the H-behaviour. Crucially, we demonstrated that H-introduction during specimen preparation could be avoided by performing the final steps of the specimen preparation at cryogenic temperatures, as shown in Nature communications 10 (1), 942, borrowing techniques from biologists. In parallel, we started studying stable hydrides and deuterides of Zr, in a collaboration with Dr Ben Britton from Imperial College London, and we revealed interesting processes taking place between the hydride and the metallic matrix, namely a redistribution of Sn and the presence of an interfacial region with a different crystal structure and composition – published in Scripta Materialia. We went on to perform a systematic study of how well hydrogen or deuterium could be quantified in Zr-based hydrides and Ti-hydrides, with publications in Microscopy & MIcroanalysis and New Journal of Physics. We also designed a gas charging chamber for atom probe specimens (Plos one 17 (2), e0262543) and explored the many possible paths for specimen preparation and analysis (Open Research Europe 1 (12), Acta Materialia 188, 108-120) to optimise the results in the analysis of both austenitic and ferritic/martensitic steels. The working group also made substantial contributions in the analysis of how hydrogen causes embrittlement of high-strength Al-alloys (Nature 602 (7897), 437-441, Nature Communications 13 (1), 4290), Ti-alloys (Scripta Materialia 213, 114640) but also bulk magnets (Advanced Materials 33 (5) 2006853). We also made strides in the analysis of catalyst materials for the hydrogen cycle - either for the electrolysers or fuel cells, and with an empahsis on the role of impurities on the durability (Journal of the American Chemical Society 144 987-994) and dopants on the performance (Advanced Materials 34 2022 2203030) of nanocatalysts. We branched out and initiated the analysis of processes taking place during the reduction of iron ore by hydrogen (Acta Materialia 212, 116933), leading in principle to the possibility of making 'green steel'.

Innowacyjność oraz oczekiwany potencjalny wpływ (w tym dotychczasowe znaczenie społeczno-gospodarcze i szersze implikacje społeczne projektu)

Now that the project is finished, I can provide some perspective as to the work from the SHINE group advanced the field. We have made significant progress in the detection of H and the clean preparation of specimens for H-quantification and their transfer into the instrument. As expected, some unforeseen hurdles came our way, but we have understood many of the limitations and have developed paths to circumvent those issues. Amongst the key issues is the uncontrolled introduction of H during the preparation of specimens, during conventional electrochemical polishing or FIBbing. We showed that cryo-enabled techniques can be necessary, which limits the throughput but improves the data quality. Experiments are still not routine, but are much better established. We have also worked on a broad range of different materials in which H is known to play a role in limiting the service lifetime of engineering parts (Al, Ti, steel) but also many materials that find application in the hydrogen economy cycle. With regards to these, we have made good progress on the front of analysing nanoscale materials by APT, and enabling new, facile approaches to get these complex samples into an analysable shape. The approach that I had outlined in the proposal of the need to push the limits on the experimental side and to jointly work with experts in atomistic simulations to help rationalise the observations and measurements.

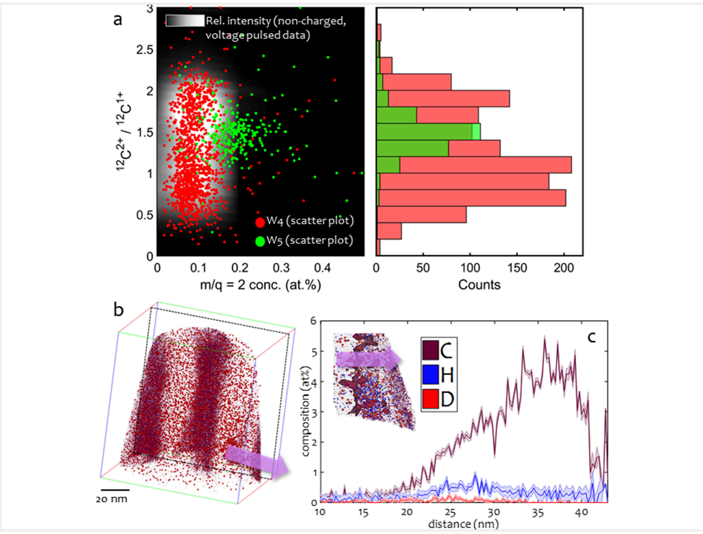

Figure from our artciel showing the detection of deuterium segregated at an in a high-strength steel

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