Max Planck Society for the Advancement of Science (Germany)
Artificial Intelligence in Materials Science

The amount of data produced by detectors has increased exponentially. Automated tools to process and analyze the data are necessary. Artificial intelligence (AI), in particular machine learning (ML), has been exploited by an increasing number of disciplines to automate complex problem-solving tasks. Progress in ML has led to decision rules that can in some cases be automatically derived by data extraction from 3D-FIM but also to identify and characterize various material defects. Currently, the physics of image formation in FIM are still not completely understood, but it is our firm belief that ML can be a powerful tool in this direction.

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Machine-learning-based extraction of crystalline information from atom probe data

Machine learning (ML) applied to atom probe tomography (APT) will enable new high-impact materials science at the nanoscale, including tracking orientation gradients with changes in chemistry, linking grain structure and segregation of different atomic species. Such information is particularly valuable for understanding the mechanisms governing changes in nanostructure and the influence on displayed mechanical and functional properties of engineering materials.

Fig. 1: Computed values of the yttrium-similarity index, YsI (eq. 1) for the 2850 solute probe. Image processing and machine learning techniques were used to identify the similarity of each atom to the pure Mg. Subsequent processing allowed the extraction of atom maps obtained from pure-Al specimens.

References:
[1] C. Briones, M. Ashton, M. Herbig, B. Gault, C. Freysoldt, J. Neugebauer: “Machine learning from atom probe data: towards large databases from which the machine learning algorithms will automatically learn and refine the data analyses, as well as systematically explore the ultimate limits of APT crystallography in multi-phase multi-component systems.”

Fig. 2: Engineering stress-strain curves of the new Mg-Al-Ca alloy in comparison with not pure Mg and Mg-Al-0.3Ca. The new Mg-Al-Ca alloy exhibits improved mechanical properties.

References:

Fig. 3: Machine-learning (k-nearest neighbour) classification result: the machine learning algorithm is able to identify pure Mg and Mg-Al-0.3Ca well. The performance of this approach is highly promising for the automation of large-scale materials science datasets in an automated, fast and accurate manner.

References:

Acknowledgments

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Fig. 4: 3D-FIM datasets of the Mg-Al-Ca alloy a set of the images recorded on an atom probe detector map.

References:

Fig. 5: Pole identification via machine-learning for electron probe crystallography (EM-APC).

References:

Fig. 6: Machine learning (k-nearest neighbour) classification result: the machine learning algorithm is able to identify pure Mg and Mg-Al-0.3Ca well. The performance of this approach is highly promising for the automation of large-scale materials science datasets in an automated, fast and accurate manner.

References:

Fig. 7: Machine-learning (k-nearest neighbour) classification result: the machine learning algorithm is able to identify pure Mg and Mg-Al-0.3Ca well. The performance of this approach is highly promising for the automation of large-scale materials science datasets in an automated, fast and accurate manner.