A deep convolutional neural network for real-time analysis of big powder diffraction data

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X-Ray Diffraction Microtomography (XRD-CT)

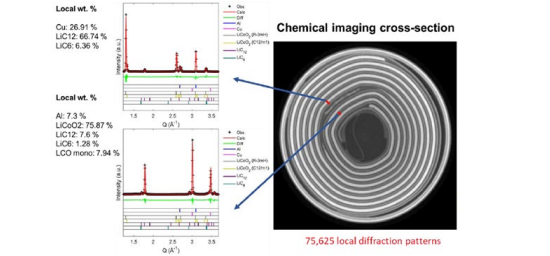

Fig. 1: An XRD-CT image acquired from a Li-ion battery. Each pixel has a corresponding X-Ray diffraction pattern.

- In an XRD-CT image, each pixel has a corresponding X-ray diffraction pattern which contains rich chemical information.
- It has been employed to study functional materials and devices, such as heterogeneous solid catalysts, fuel cells and batteries, under operating conditions.

The Challenges of XRD-CT

- Each XRD-CT image typically contains 10,000s of diffraction patterns. The current diffraction data analysis pipeline normally takes days to weeks for an expert.
- Therefore, we used a convolutional neural network (CNN) to develop a new tool for real-time full profile analysis of diffraction patterns, which we termed as the Phase Quantification Neural Network (PQ-Net).

PQ-Net Architecture

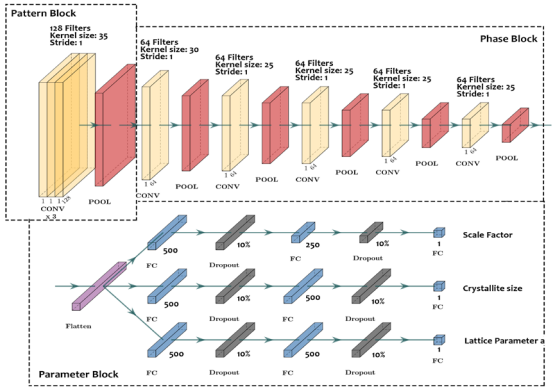

Fig. 3: PQ-Net architecture for a single-phase system with cubic symmetry. CONV represents 1-D convolutional layers, Pool with 10% represents max-pooling layers, FC represents fully connected layers, and Dropout represents dropout layers dropout rate.

- **Pattern Block**: It contains multiple convolutional layers to extract general information from the diffraction pattern.
- **Phase Block:** Each phase has its own phase block which is connected to the last layer of the pattern block. The size of the feature maps are reduced by the pooling layers.
- **Parameter Block:** Each phase has its own parameter block to extract chemical information from the feature maps created by the phase block.

Results & Performance

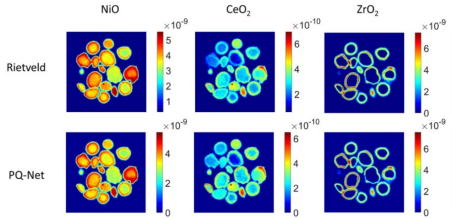

Fig. 5: The comparison between the PQ-Net result and the Rietveld result on scale factors for multi-phase problem.

- The PQ-Net is trained with simulated diffraction patterns, which can be done before new data are collected.
- The PQ-Net only takes 5% time of the current method
- A deep ensemble method also estimates the uncertainties of the results.
- The method can also be applied to other data (i.e., spectroscopic).

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Results & Performance

[1] Dong, H., Butler, K.T., Matras, D. et al. A deep convolutional neural network for real-time full profile analysis of big powder diffraction data. npj Comput Mater 7, 74 (2021). https://doi.org/10.1038/s41524-021-00542-4

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