Poster

Leveraging Deep Learning for smart sample alignment

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Development of new Deep Learning techniques have impacted a wide range of research areas [1]. One area where deep neural networks have proven powerful is the processing and interpretation of images [2]. We built on top of these methods to develop a novel technique to streamline the process of aligning crystal samples in the centre of a single crystal X-ray diffractometer.

The neural network is designed to mimic the decision-making process of an experienced crystallographer, going through the procedure of finding the most promising position for X-ray exposition, providing valuable feedback to novices and expert users alike. The method utilizes a two-stage model built on top of the ResNet family of convolutional neuronal networks and is trained on several millions of reference images [3]. The resulting model is lightweight enough to run on any modern desktop or laptop PC, providing seamless real-time feedback to users of Bruker's APEX and PROTEUM software suites (Figure 1).

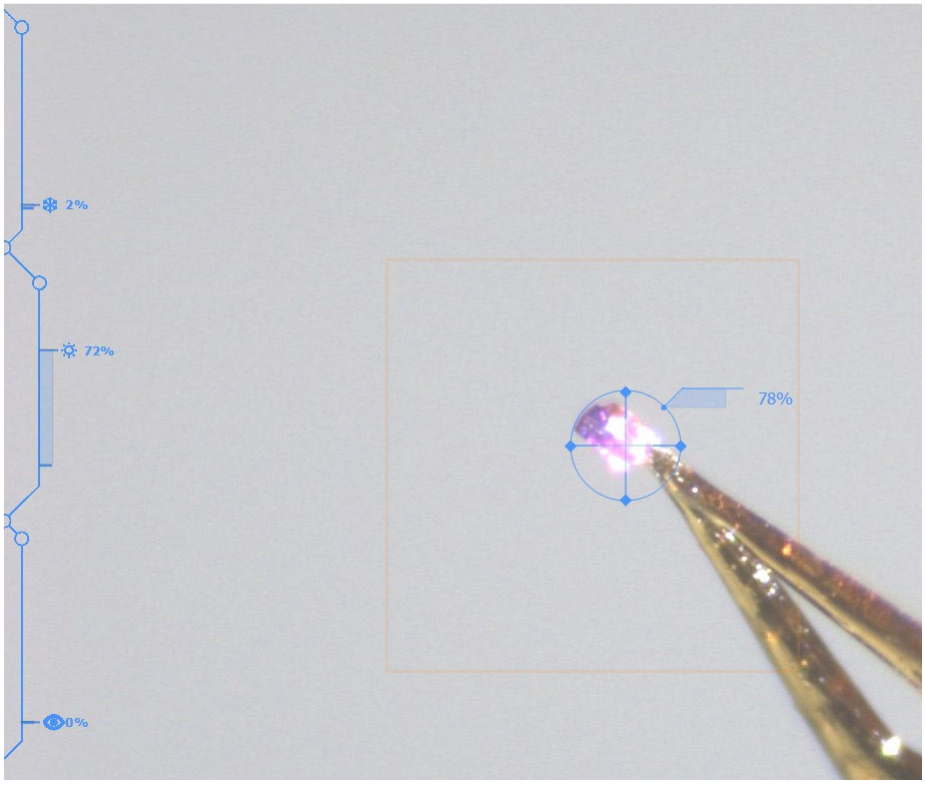

Figure 1. Direct visual feedback during Deep learning assisted crystal centering.

[1] Alzubaidi, L., Zhang, J., Humaidi, A.J. et al. (2021). *J Big Data.* **8**, 53.

[2] Ito S, Ueno G, Yamamoto M. (2019*). J Synchrotron Radiat.* **26(Pt 4)**, 1361.

[3] Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun (2015). Deep Residual Learning for Image Recognition. arXiv:1512.03385.