Convolutional neural network analysis of x-ray diffraction data

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Abstract

A proof of concept was demonstrated in the previous work [1], illustrating the application of convolutional neural networks (CNN) in extracting strain profiles from x-ray diffraction (XRD) data. Numerically generated data has been employed to design, fine-tune, and train a specialized convolutional neural network (CNN) with the overarching objective of deducing spatial strain profiles exclusively from X-ray diffraction (XRD) data. Due to the impracticality of acquiring and analyzing a large set of XRD curves and strain profiles for training, the XRD curves were computed within the framework of the dynamical theory of diffraction, utilizing a recursive solution [2] to the Takagi-Taupin differential equations [3]. The corresponding strain profiles are generated by fitting a B-spline function [4] to an asymmetrical Gaussian function normalized to a unit maximum. The Debye-Weller factor is calculated using the equation [5]:

$$DW(z) = e^{(-\alpha \times (e(z)/e_{max})^2)}$$

where z is the depth coordinate from the surface, $e(z)$ and e_{max} are the strain profile and maximum strain value of the crystal.

In this subsequent study, the primary objectives are to bring the numerically generated training data closer to the experimental data (realistic data), subsequently adjusting the CNN architecture and to have the strain profiles predicted for all materials by this CNN. To accommodate counting statistics, a randomly generated Poisson distribution is incorporated into the computed XRD intensity. Additionally, random-valued noises (uniform noises) are introduced to consider the noises in the peaks of the computed intensity. A linear function with randomly generated slopes in the range of 1 to 100 is introduced as the background noise to induce deviation of the XRD curve base from being a straight line. The Debye-Weller profile is generated by fitting a B-spline function to an asymmetrical Gaussian curve, the same curve used to generate strain profiles thus decoupling it from the strain profile. The fitted weights are allowed to randomly deviate from their initial value within a specified range with a uniform probability.

References

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Figures

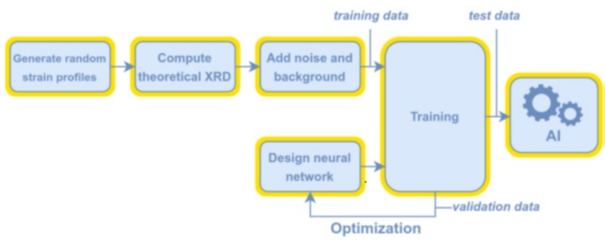

Figure 1. General Workflow [1]