

Application of artificial intelligence algorithms for phase analysis

Gábor Ribárik^a and Bence Dajka^a

^aDepartment of Materials Physics, Eötvös University Budapest, Hungary
^aribarik@elte.hu

X-Ray Diffraction (XRD) is an efficient technique to determine the crystal structure of materials. The method of qualitative phase analysis can be used to identify the phases of crystalline materials and it also provides the relative proportion (fraction) of the phases. This problem is usually solved manually, but due to the rapid evolution of artificial intelligence algorithms, it is now possible to use automated methods for this task. Machine learning is a subfield of artificial intelligence, which is broadly defined as the capability of a machine to imitate intelligent human behaviour. A recently developed method gives the number and type of the phases from experimental XRD patterns. The code uses a branch of machine learning called artificial neural networks and gives the number and type of the phases from experimental XRD patterns. The results (e.g. the number of phases, the lattice type and lattice parameters for each phase and the hkl indices for each XRD peak) can be used directly as input parameters for the Convolutional Multiple Whole Profile fitting (CMWP) method, an experimental whole pattern modelling method which gives the relevant parameters of the microstructure. The information about the crystal structure and the correct indexing of the peaks is a prerequisite for the CMWP method. The code is implemented into the CMWP software as an automated phase and structure recognition module. By using this module in CMWP, the input parameters related to the crystal structure are automatically guessed and the procedure of peak indexing is also automated, which makes the evaluation procedure more robust.

Keywords: X-ray diffraction, line profile analysis, phase analysis, artificial intelligence, machine learning, neural networks