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«Assessment of software for the analysis of electron diffraction patterns obtained by transmission electron microscopy and modeling»

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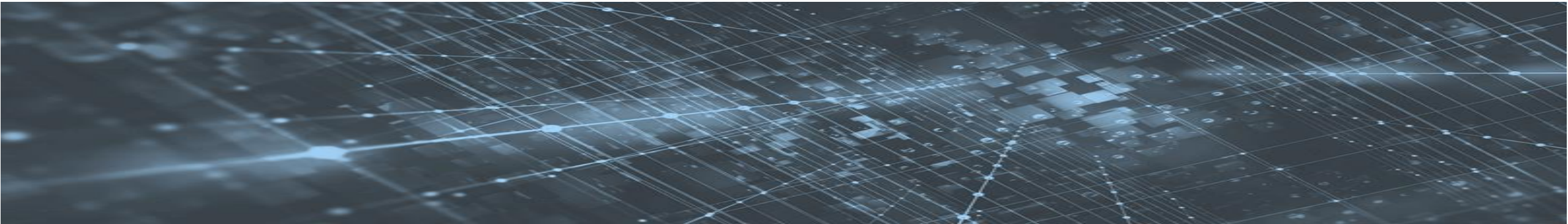
Problem statement

There are various methods for the analysis and processing of electron diffraction patterns obtained using transmission electron microscopy.

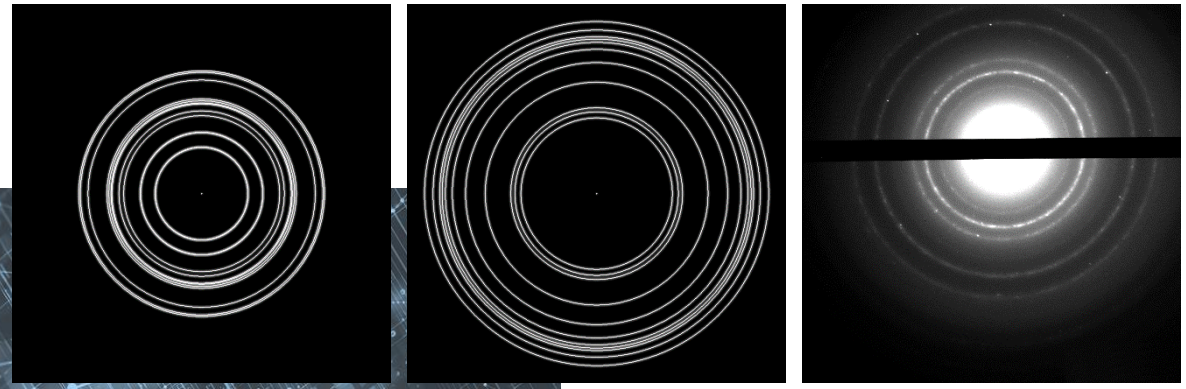
Manual processing with the subsequent search for matching data in crystallographic reference books is a traditional approach that has been used for many decades. New ways to solve this problem began to appear due to the development of new technologies and digitalization. These methods can be divided into semi-automatic and fully automatic processing of electron diffraction patterns using specialized software.

The data obtained by different methods may not converge, which is due to the peculiarity of the software functioning. Thus, it is necessary to determine (evaluate) the advantages and disadvantages of these methods.



Solution methods

- Electron diffraction patterns of TiO_2 and ZnO were obtained by crystal structure modeling using the Electron Diffraction software. Electron diffraction patterns of synthesized copper-containing nanoparticles samples were obtained by TEM.
- The following methods were used for the analysis of electron diffraction patterns:
  - manual measurement
  - processing using ImageJ (Calc d-space) and DigitalMicrograph (DiffTools)
  - automatic processing in CrysTBox and ProcessDiffraction software.
- PDF-2 and Crystallography Open Database were used as sources of crystallographic data.



Electron diffraction patterns used for analysis (from left to right): modeled TiO_2 and ZnO, synthesized copper-containing nanoparticles (Cu_2O).

Conclusions

This study shows that:

1. the measurement results by various methods are in good agreement with the reference values and data obtained using traditional methods
2. the error of determination in all the methods used was less than 0.07 Å
3. during automatic processing of electron diffraction patterns, errors in the identification of diffraction rings are possible due to their low contrast or too dense arrangement.

It should also be added that software for electron diffraction patterns automated processing do not provide the possibility of detailed customization of the results display.

This affects the ability to publish the results without additional processing.

However, all the methods studied are generally suitable for use and allow for sufficient accuracy of the analysis.

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