Data-driven spectral analysis method in electron-beam based techniques

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1. Introduction

Popular surface analysis techniques and operating procedures have seen little improvement in recent decades. These techniques take measurements on the surface of a material and then data are analysed by identifying weak features in core-level signals against strong secondary electron (SE) background with the naked eye. Is there any method that is able to obtain information about nanomaterials from SE background signals?

2. Abstract format

Surface analysis techniques such as x-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES) are widely used for a broad range of materials, and provide quantitative elemental and chemical state information from the surface of the material being studied. Nowadays, these techniques are intensively employed to study nanomaterials and focus on a sole target, mapping the surface elemental composition of nanomaterial. However, the capabilities of these techniques to play a greater role in nanomaterial studies are limited owing to the lack of analysis

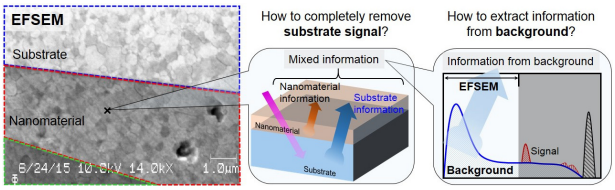

Fig. 1. The main question when studying substrate-supported nanomaterial by electron-beam based techniques.

approach that could make the full use of SE signals obtained from the nanomaterial samples.

In most electron spectroscopic data analyses the SE background signals are neglected as noise and are not quantitatively analyzed. The main reason for this is that the widely used physics-driven spectral analysis approaches on which the analysis is based, describe the measured data in terms of physically meaningful parameters, i.e. physically defined (PD) descriptors designated from an informatics point of view. Therefore, the currently available physics-driven spectral analysis approaches are only able to analyze the peak signal and generally do not make use of the SE background signal

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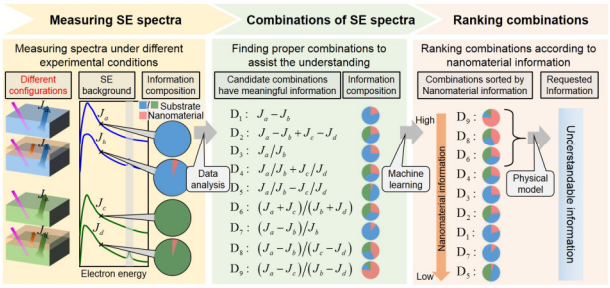

Fig. 2. The process of heuristic data-driven analysis method. First the SE spectra are measured under slightly different experimental conditions; then, these spectra are extensively combined with algebra; finally, those combinations that have large percentage of nanomaterial information are selected, and further interpreted.

owing to the difficulty in modelling accurate physical mechanisms of SE excitation and emission, despite it being known that the SE background signals must involve quantitative information about the electron transport properties. To extract meaningful information from the SE background signal, a new method is required that is fundamentally different to the conventional physics-driven spectral analysis approaches in which only peak signals can be analyzed.

In this work, we propose a new heuristic data-driven spectral analysis technique [1,2] to overcome current limitations. Instead of interpreting individual measurements in terms of only PD descriptors, analytically defined (AD) descriptors obtained through the data analysis of many slightly different conditions, are used to describe the background data. These AD descriptors are ranked according to specified scores so that those with high scores may be effective for describing the measurements under slightly different experimental conditions.

3. Conclusions

In summary, the Data-driven method represents a benchmark to provide ‘free-standing’ nanomaterial information from measurements of substrate-supported samples, which does not demand extra investment in equipment.

References

1) B. Da, et al. Phys. Rev. Appl. **13**, 044055 (2020).
2) B. Da, et al. Nature Commun. **8**, 15629 (2017).