Contribution ID : **115** Type : **Invited Oral**

Rapid multivariate analysis of 3D ToF-SIMS data: graphical processor units (GPUs) for large-scale principal component analysis

Wednesday, 15 August 2018 16:45 (30)

Principal component analysis (PCA) and other multivariate analysis methods have been used increasingly to analyse and understand depth-profiles in XPS, AES and SIMS[1]. For large images or three-dimensional (3D) imaging depth-profiles, PCA has been difficult to apply until now simply because of the size of the matrices of data involved. We have developed two algorithms that improve the speed of PCA for large ToFSIMS datasets[2], and allow these datasets to be of unlimited size. We apply these to perform PCA on full 3D time-of-flight SIMS data for the first time[3]. An example is the processing of a 128 × 128 pixel depth-profile of 120 layers, each voxel having a 70 439 value mass spectrum associated with it. This forms over a terabyte of data when uncompressed. We have implemented this algorithm on a PC having a graphical processor unit (GPU) card containing 2880 individual processor cores. This increases the speed of calculation by a factor of around 4.1 compared with what is possible using a fast commercially available desktop PC having central processing units alone, and full PCA of this terabyte of ToFSIMS data is performed in less than 7 seconds. We show a number of datasets and PCA results, including biological examples and 3D "tomographic" views of the PCA results[4].

[1] M S Wagner, D G Castner, Langmuir 17 (2001) 4649–4660
[2] P J Cumpson et al, Surface and Interface Analysis 47 (2015) 986–993
[3] P J Cumpson et al, Surface and Interface Analyis 48 (2016) 1328-1336
[4] www.youtube.com/watch?v=bUT0kYuad2E

Primary author(s) : CUMPSON, Peter (Newcastle University)

Co-author(s) : BARLOW, Anders (La Trobe University); Prof. SANO, Naoko (Nara Womens University); Prof. FLETCHER, Ian (Newcastle University UK)

Presenter(s) : CUMPSON, Peter (Newcastle University)

Session Classification : Speaker Sessions and Seminars

Track Classification : Applied Surface Science