

## Analysis of Ion Evaporation Events through Data Mining: An Experimental Foundation for Interpreting Chemical Imaging in the Atomscope

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One of the key challenges in the use of the integrated atom probe and scanning transmission electron microscope (APT/STEM) system, known as the Atomscope [1], will be to ensure that there is a quantitative understanding of the mechanisms of image formation in the atom probe. This provides a basis to link such information to the well-established understanding of image and chemical analysis interpretation in STEM mode. This paper addresses the former issue by exploring ways to integrate advanced statistical learning tools with the analysis of ion evaporation maps to enhance the discrimination of isotopes in the mass spectra and to better track elemental changes within the material. Such information will provide critical insights into the coupling of the dual image/microanalysis modalities of the Atomscope.

As noted by Kelly [2], one approach to discriminate ions with similar time-of-flights (TOFs) is to map the ions based on their kinetic energy. The logic of this approach is that if descriptors for the voltage applied to the material, the evaporation events, and the material are assessed, the kinetic energy should be represented within the data. The challenge is to extract this information. To map the relationship between instrument operating parameters, material chemistry, and evaporation physics, a dimensionality reduction was done using principal component analysis (PCA), which maps the data in a new space based on maximizing the information captured [3]. The input into PCA was the applied voltage, material, and evaporation. The result of the PCA analysis is shown Fig. 1. The first principal component (PC1) primarily captures TOF, whereas PC2 captures a combination of voltages, mass-to-charge state ( $m/n$ ) ratio, and evaporation. The isotopes are clearly discriminated in Fig. 1. Additionally, when compared with the kinetic energy map [2], it is concluded that this combination of variables (PC2) represents the kinetic energy. Therefore, the combination of data mining techniques with existing atom probe data can be used to improve the discrimination of isotopes with similar TOFs. This demonstrates the value of advanced data mining methods to help enhance the information resolution of the atom probe. The approach of Saxey [4] has also been adapted in the present study for developing ion evaporation or atom maps to track the spatial correlations of the detection events back to the sample image, Fig. 2. This direct one-to-one correlation provides the basis for developing a larger multi-dimensional data set for further applications of data mining methods for quantitative interpretation of chemical imaging.[5]

### References

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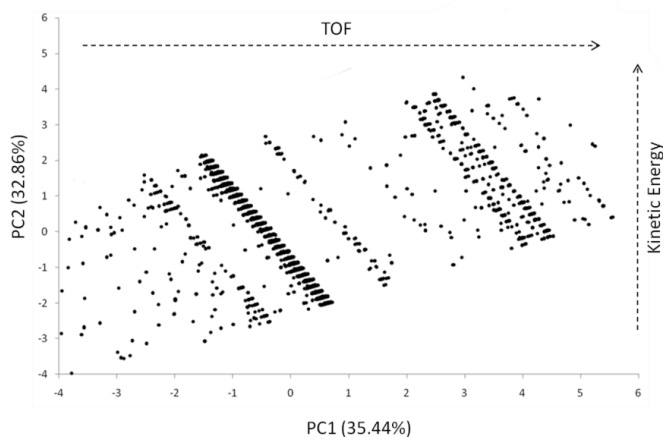


FIG. 1. A mapping of atoms after dimensionally reducing the parameters related with the sample and instrumental parameters. The axes represent a linear combination of these parameters, which capture the maximum amount of independent information. When compared with the kinetic energy map in [2], PC2 is identified as capturing kinetic energy, demonstrating the use of data mining for ion discrimination via mapping of kinetic energies.

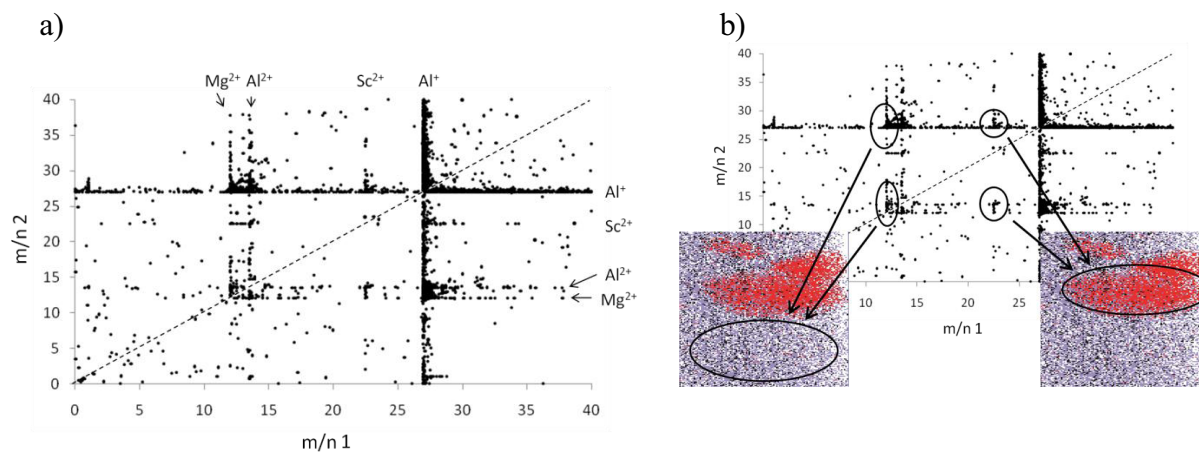


FIG. 2. Ion evaporation map, where each point represents a dimer comprised of two ions. The major ionic species present are labeled, where each axis is the  $m/n$  ratio of one of the two ions. For example, the points at coordinates (12,27) and (27,12) indicates a molecular ion containing an  $Mg^{2+}$  ion and an  $Al^+$  ion. Fig. 2b tracks the evaporation events back to the image.