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Hough Transform Based Accurate Composition Extractions From Correlation Histograms in Atom Probe Tomography

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Atom probe tomography (APT) has enabled key insights into material properties and design, by providing accurate nanoscale chemical composition in three dimensions. APT uses a time-of-flight-based mass-spectrometry to decipher the chemical identity of the atoms. The field evaporated ions are collected at a position-sensitive detector, and later back reconstructed in to a three dimensional point cloud. The times of flight are measured in a pulsing window, where the field evaporation of an ion (ideally) is triggered by the application of a single high-voltage pulse or a fast laser pulse. Experimentally, the rates of evaporation are kept actually as low as 0.01 ion(s) per pulse on average. However, the field evaporation triggered by either a high voltage pulse or a laser pulse usually have a decay time. This leads to multiple evaporations not only at the peak of one pulse but also during the decay of the pulse. This causes the departed ions to have a deficit compared to the highest possible kinetic energy or simply a delay, and, these ions are registered with a time of flight incommensurate with their mass-to-charge, making it impossible to label them properly. Field evaporation from phases that are ionically or covalently bonded also often lead to the formation of metastable molecular ions that can dissociate during the flight [1,2]. Such dissociations also cause kinetic energy deficiencies leading to inaccurate identification of the ions. These inaccuracies can cause bias in the extracted compositions.

These effects can be observed and corrected for by plotting a correlation histogram of the multiple events [3]. The effects described above appear as distinct lines and curves in correlation histograms. Here, we plot the correlation histograms with square roots of mass to charge ratios, which is a proxy for the time of flight. Then, a series of image processing algorithms including morphological operations are applied to enhance the contrast of these features. After that, a Hough transform is applied on the images to identify the lines with unit slope. These lines originate from hotspots corresponding to the element's correct mass-to-charge ratios, which tend to evaporate correlatively. These lines are constituted by atoms leaving during the decay of the pulse. Due to the aberrated time of flight, the hits constituting the lines are not counted in the appropriate mass ranges used to associate a mass-to-charge ratio to an elemental identity.

Once these lines are identified through the developed algorithm, a filtering protocol is then applied to identify the lines originating from the hotspots. Then, the hits constituting the line are reverted to their actual times-of-flight. This way, the times-of-flight are correctly labelled, which leads to a more accurate determination of the composition, in the cases where it is strongly effected by multiple events.

The developed protocol is applied on a simulated mass spectrum, which is strongly influenced by multiple events. The measured composition from the simulated data using a conventional mass spectrum ranging shows an inaccurate composition. The application of the protocol is shown to improve the composition and brings it closer to the actual composition. The method is also applied on an experimental dataset. The data is obtained on a local electrode atom probe (LEAP) 5000 XS with a

straight flight path. Alumina (Al_2O_3) is used as the expected composition is stoichiometric. The correlative histogram is shown in Figure.1 (a), with distinct lines originating from various hotspots. The identification of the lines is shown in Figure.1 (b). The composition extracted by the application of the current protocol has shown improvement compared to the default ranging. In the future work, we would extend the current protocol to identify the molecular dissociation tracks.

References:

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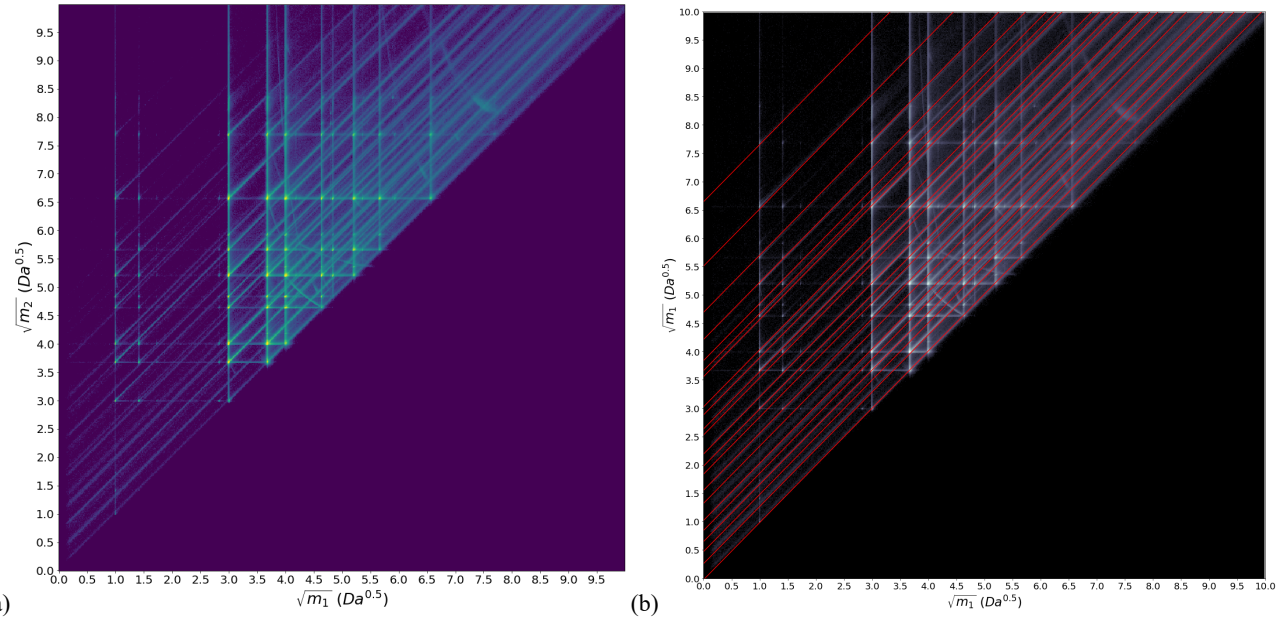

Figure 1. (a) A correlative histogram plotted in square roots of mass to charge ratios of an Alumina sample. (b) Hough transform applied to the histogram to identify the lines at 45°.

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