Kinetic-Energy Discrimination for Atom Probe Tomography: Concepts and Potential Detectors

Thomas F. Kelly

Cameca Instruments, Inc., 5500 Nobel Drive, Madison, WI 53711

The purpose of mass spectroscopy is to discriminate among species of atomic or molecular ions sufficiently well to unambiguously identify them. In time-of-flight mass spectroscopy, the ion time of flight is converted to ion mass-to-charge-state ratio, m/n, where m is the ion mass and n is the charge state, Fig. 1a. This approach works well except when two distinct ion types have nominally the same m/n, e.g., ²⁸Si⁺⁺ and ¹⁴N⁺ at m/n = 14 Da. If additional information can be obtained, namely the ion kinetic energy, then such interferences could readily be discriminated as shown in the simulation of Fig. 1b [1]. The benefits of using kinetic-energy information to aid ion discrimination in atom probe tomography are explored in this paper with an eye toward new detector technologies.

Ion peak interferences in time-of-flight mass spectra are first categorized by difficulty of discrimination using time-of-flight and kinetic-energy information. Several of these categories which are intractable interferences when only time-of-flight information is available may be discriminated when kinetic-energy information also is available. Furthermore, many opportunities for removing noise from composition determinations and 3D images are enabled. Modest kinetic-energy resolving powers of 10 or so should be sufficient to have a major impact on atom probe tomography. With kinetic-energy resolving power of about 100, the energy deficits in voltage pulsing may be resolved to enable high-ion-discriminating power in a straight-flight-path voltage-pulsed instrument, Fig. 2. Current detectors do not provide the kinetic energy of incoming ions but there are prospects for building such detectors. A Kinetic-Energy Atom Probe (KEAP) should offer superior performance by reducing both peak ambiguities and noise while potentially enabling 100% detection of ions.

Position-sensitive detectors (PSD) for APT are very challenging and sophisticated devices: they are required to provide an ion arrival location in two dimensions with better than one-part-in-one-thousand precision and an ion-arrival time to better than 100 ps. They must also do this for each of several simultaneous hits that may be separated by only a few pixels on the detector, and they must be able to reset and handle the next barrage of ions in less than a microsecond. Today's PSDs are not configured to discriminate the kinetic energy of incoming ions but it is reasonable to pursue this prospect with superconducting detectors [2, also see 3 for a brief overview]. Programs to create a kinetic-energy detector should be pursued.

Irwin [3] points out that superconducting detectors are useful precisely because they are so fragile: the binding energy of Cooper-paired electrons is on the order of 3 to 5 meV. 10 keV ions should therefore produce signal magnitudes of $> 10^6$ electrons in superconductors. In principle, there appears to be the opportunity to configure a detector which has a) full areal coverage (100% detection efficiency), b) a physical process which is fundamentally fast enough to allow sub-100 ps timing, and c) a signal that may be proportional to the kinetic energy of the incoming ion. It is possible to envision a detector with 1000 by 1000 striplines (or blocks of striplines) where the perturbation in any line is detected by its influence on a dark supercurrent coursing through each line [4] or the change in high-frequency impedance in the line [5]. A serious challenge will be to make the impact position detectable in X and Y but it might be achieved by latching the top stripline such that the normal zone grows and activates a perpendicular sub-surface Y stripline. Achieving all of this while also extracting a signal that is related to the kinetic energy at impact may be a tall order. The path to superconducting detectors for atom probe tomography is uncertain today. However, such revolutionary detectors should be explored especially since advances in both basic understanding and sophisticated technology have been occurring at a high rate in this field.

References

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FIG. 1. a) Simulated mass spectrum with interferences between Si and N at m/n = 14 and oxygen species at m/n = 16. The peak heights are not scaled to naturally occurring isotope ratios and the peak width is exaggerated for clarity. b) Simulated mass-energy spectrum for a) where the ion peaks are fully discriminated.



FIG. 2. a) Actual data from a steel in a straight-flight-path voltage-pulsed LEAP. b) Simulated mass-energy spectrum for a) where the peaks are fully discriminated. Flight times in the two spectra do not correspond.