

## Recent Advances in SIMS

### Room Great Lakes Promenade & A1 - Session RA6-TuP

#### Recent Advances in SIMS Poster Session

**RA6-TuP-1 Experimental and Theoretical Analysis of Tricyclic Antidepressants Using 213 Nm Picosecond Laser Desorption Positionization Mass Spectrometry**, *T. Zagorac*, University of Illinois Chicago; *H. López Pena*, Virginia Commonwealth University; *J. Gross*, University of Illinois Chicago; *K. Moore Tibbets*, Virginia Commonwealth University; **Luke Hanley**, University of Illinois Chicago

Imipramine class tricyclic antidepressants have low ionization efficiencies that render them difficult to detect using secondary ion mass spectrometry [1]. Imipramine ionization efficiency was previously studied with 800 nm, ~75 fs laser desorption photoionization mass spectrometry (fs-LDPI-MS) [2] and a significant precursor ( $M^+$ ) ion was detected. Here we examine the use of 213 nm, ~30 ps-LDPI-MS for detection of imipramine, desipramine, amitriptyline and clomipramine via 7.9 eV single photon ionization.

Precursor and fragment ion signal for all four compounds are compared to electron impact mass spectral libraries and ps-LDPI-MS displayed higher  $M^+$  signal than electron impact for all four compounds. Furthermore, detection of imipramine by ps-LDPI-MS shows slightly less fragmentation than did fs-LDPI-MS [2]. A power study on the effect of desorption laser irradiance on the survival yield of the precursor ion shows that the desorption laser irradiances in the ps-LDPI-MS are significantly lower and  $M^+$  survival yields are slightly higher than those for fs-LDPI-MS. Ionization energies of imipramine, desipramine, amitriptyline, clomipramine, and several of their major fragments are predicted using density functional theory calculations and used to explain the observed ps-LDPI-MS data. Low mass amine containing fragments are calculated to have low ionization energies, so their experimental observation might arise at least in part from dissociation during laser desorption. Results are discussed in terms of the application of 7.9 eV single photon ionization to laser secondary neutral mass spectrometry of drug compounds.

1) Vorng, J.-L.; Kotowska, A. M.; Passarelli, M. K.; West, A.; Marshall, P. S.; Havelund, R.; Seah, M. P.; Dollery, C. T.; Rakowska, P. D.; Gilmore, I. S., *Anal. Chem.* **2016**,*88*, 11028.

2) Pieterse, C. L.; Rungger, I.; Gilmore, I. S.; Wickramasinghe, R. C.; Hanley, L., *J. Phys. Chem. Lett.* **2020**,*11*, 8616.

**RA6-TuP-3 Analysis of Organic Principal Component Distribution Using Orbitrap/TOF Hybrid SIMS**, *Y. Jeong, J. Lee, H. Moon, J. Sung*, Korea Basic Science Institute, Republic of Korea; *. Suh*, Pusan National University, Republic of Korea; **Jong Sung Jin**, Korea Basic Science Institute, Republic of Korea

An analysis method was presented to confirm the distribution of small molecules according to the depth in the organic multilayer thin film using the newly developed Orbitrap/TOF Hybrid SIMS. With the conventional TOF-SIMS analysis method, ions such as  $CN^+$ , which correspond to the nitrogen component present in the molecule, were observed. This method has a limitation in obtaining only the information of the molecule to be analyzed accurately. Using Orbitrap/TOF Hybrid SIMS, we developed an analysis method that can obtain information on only the relevant molecules whose distribution is to be reported. In particular, by identifying each characteristic peak from the results of MVSA statistical processing, it was possible to infer different mechanisms of behavioral change depending on the molecular structure.

**RA6-TuP-7 Epi SiGe Application using METRION® in-line SIMS System**, **Lawrence Rooney**, *S. Okada*, Nova

The epitaxial process is a well-established deposition technique in semiconductor fabrication because it enables the ability to achieve much higher doping concentrations than can be obtained via ion implantation. As we move toward <5nm technology, a key process for enabling gate-all-around FET (GAAFET) is the stacked multi-lattice of Silicon (Si) and Silicon-germanium (SiGe) epi process for constructing the nanosheets.

Germanium (Ge) content in SiGe correlates to channel stress, and the germanium fraction (Ge%) has been increasing steadily as we move towards smaller technology nodes. When stress is high, epi layers can suffer from multiple problems such as defect formation, facet formation, non-uniform strain, etc. The challenge is greater when moving from planar to 3D structures, where uniformity of strain and control of defect density are important. Often, multiple epi layers of SiGe with varying thicknesses,

Ge%, and Boron doping are deposited to optimize the device structure and process integration.

Enabling process control on the layer thickness, Ge%, and Boron doping concentration in these complicated SiGeB epi stacks is critical in high-volume manufacturing (HVM), and there is no single in-line metrology that is able to do the measurement.

This paper describes how in-line Secondary Ion Mass Spectrometry (SIMS) could be a solution to this problem by providing material composition profiles as a function of depth – resulting in thickness, Ge% and Boron concentration data from each nanosheet.

**RA6-TuP-9 Detection of Contaminants in Positive and Negative Ion Mode Using in-Line SIMS with an Oxygen Primary Ion Beam**, **Julia Hoffman**, *S. Okada*, Nova

Utilizing Secondary Ion Mass Spectrometry (SIMS) for in-line metrology is a newly emerging method of process control that requires contamination-free measurements, enabling SIMS on product wafers. SIMS measurements of negative ions are usually associated with a Cesium primary ion beam. Unfortunately, when Cesium is present in Silicon, it forms trap states in the Si band gap, which can cause serious leakage issues for Si-base transistors. Therefore, Cesium is considered a very damaging contaminant in semiconductor devices.

To enable contaminant-free inline SIMS a choice of Oxygen ion source is a preferable choice since it is generally benign and not considered a contaminant. This kind of source is typically used for positive secondary ion measurements. By switching the secondary spectrometer polarity between positive and negative ion modes, an Oxygen primary ion source can be used successfully to measure both positive and negative species.

While an Oxygen primary ion source may not provide the same sensitivity to negative secondary ions as a Cesium primary ion beam, the ability to directly measure a range of species without the risk of contamination creates a wide field for in-line SIMS applications.

In this paper, the use of an Oxygen primary ion source for positive and negative secondary ion detection is being investigated on an in-line SIMS tool. We evaluate sensitivity levels of detecting contaminants like O, F, Cl<sup>-</sup> in positive and negative ion mode with an Oxygen primary beam, as well as the use of proxy species or alternate isotopes for improved results.

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