National Aeronautics and Space Administration

Identifying Planetary Mixed Materials Through *In Situ* Mass Spectrometry

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Program: FY21 R&TD Topics **Strategic Focus Area: Planetary Science Data Analysis**

Objectives

We are demonstrating the identification of mixed planetary materials in the laboratory. Drawing on the world's largest set of impact ionization mass spectra of analog planetary materials, obtained over more than two decades at the University of Colorado's IMPACT dust accelerator lab and precursor facilities, we are (1) developing a procedure to identify materials and mixtures and determine statistical confidence levels using Gaussian mixture modeling, a convolutional deep learning network, and a neural network initially developed for electron-ionization mass spectroscopy, and (2) obtaining new laboratory mass spectra for planetary materials and mixtures, specifically including organics of the kinds expected in planetary and interplanetary contexts. The lab work is being carried out by continuing CU graduate student Zachary Ulibarri overseen by professors Tobin Munsat, Mihaly Horanyi, and Sascha Kempf, with input on the choice of materials from JPL researchers Valerie Kristof and Morgan Cable. The automatic identification process is being developed by JPL researcher Neal Turner and tested using synthetic mass spectra produced by new CU graduate student Ethan Ayari and Horanyi, his thesis advisor.

Background

In situ mass spectrometry of solids is a key measurement technique for missions targeting airless bodies' surface compositions (Europa Clipper-SUDA, mid-2020s launch), interplanetary and interstellar dust (IMAP-IDEX, 2024), the particles ejected from asteroids (DESTINY+, 2022) or comets (Comet Interceptor, 2027), the geysers of Enceladus, the aerosols of Titan, and the volcanos of Io and Triton. While technology for obtaining mass spectra of solid particles is advancing, there has been less attention to analyzing the data to reach science objectives. Mission proposal reviews have picked out this lack as a weakness. For example, reviewers of the FOSSIL 2019 Discovery concept found *"The proposal did not convincingly demonstrate that it would be possible to identify mineral composition and phases from bulk chemistry for polyphasic particles, particles of mixed composition, and glass phases, all of which are important components of the interplanetary dust particle population."*

Approach and Results

We are demonstrating composition measurement in three steps. First, spectra of single-material particles have been classified using Gaussian mixture modeling and will next be classified independently using a convolutional deep learning network (Thomas Albin, 2019 PhD thesis, Univ. Stuttgart). One of these two approaches will be selected based on performance for step 2, where the mixtures' spectra are classified by their similarity to those of the component materials. In step 3, the single-material and mixture spectra together will be used to train the neural net developed by Wei et al. (2019, doi:10.1021/acscentsci.9b00085) to predict new mixtures' spectra from those of individual materials. We are adapting Jennifer Wei's source code from http://github.com/brain-research/deep-molecular-massspec.

To the thousands of laboratory mass spectra already in the CU dataset from the calibration of the Europa Clipper-SUDA instrument and precursors such as LAMA, the lab work is adding new spectra from the next-generation prototype Hyperdust for a Titan tholin analog and various combinations of organic materials, metals, and minerals. Additionally, we are generating synthetic spectra by feeding particle-impact-generated ion clouds to the SIMION code where we compute the charged particles' trajectories through a model of the instrument's electrostatic fields. Subsets of the laboratory and synthetic spectral datasets will serve as the training sets for the machine learning methods.

Significance/Benefits to JPL and NASA

Impact ionization time-of-flight mass spectrometric instruments could return key measurements of Titan's aerosols, Enceladus' geysers, Io's and Triton's volcanos, comets, asteroids, interplanetary and interstellar dust, and airless bodies throughout the solar system. Demonstrating particulate composition measurements with prototype instruments in the laboratory will strengthen the cases for missions to these targets. The laboratory experiments' results when fed into the machine identification efforts will show what combinations of planetary and interstellar analog materials can be distinguished, and over what particle mass and speed ranges, enabling capability estimates to be made quantitative. The work will provide the evidence needed to show in mission proposals that impact ionization instruments perform well enough to meet science objectives. To enable citation in proposals, the results will be disseminated in the PhD theses of Ulibarri and Ayari and through publication in refereed journals.

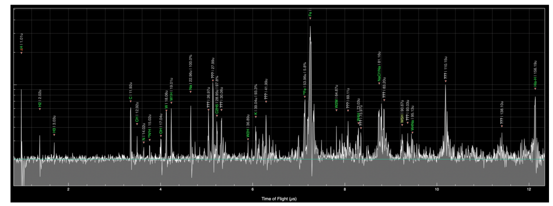

Figure 1. To demonstrate capability for measuring complex organics, we impacted micron-sized Fe particles into water ice with high molar (>1M) concentrations of the amino acid, histidine. This TOF mass spectrum shows the parent histidine molecule alongside fragments matching those produced when histidine is struck by energetic electrons in other laboratories. The parent and fragment mass peaks together unequivocally identify the amino acid. Our ongoing experiments explore how well we can determine from such dust-impact mass spectra the abundances of two amino acids in a mixture.

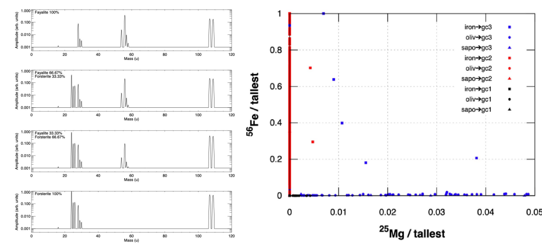

Figure 2. ***Left:*** Synthetic mass spectra covering the fayalite-forsterite mineral series. We will use such model spectra to train the identification algorithms in the project's second year. ***Right:*** Identification of SUDA laboratory calibration mass spectra using Gaussian component modeling of peaks including ^{56}Fe and ^{25}Mg. Red squares along vertical axis are correctly-identified Fe particles, blue circles along horizontal axis are olivine, and black triangles near origin are saponite.

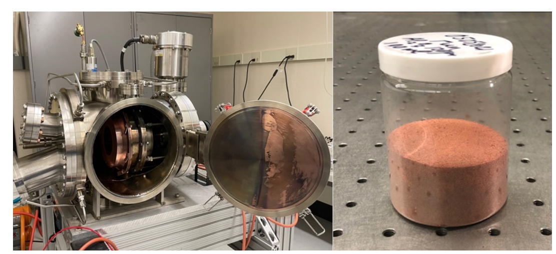

Figure 3. ***Left:*** The new vapor-deposition dust coater couples an evaporative metal source to a fluidized bed for handling fine powders of any type. We are now routinely applying conductive metal coatings to grains with sizes down to 1 μm, enabling insulating materials to be flown in the electrostatic laboratory accelerator. ***Right:*** Batch of particles of the refractory mineral corundum (Al_2O_3) vapor-coated with copper, ready for testing in the accelerator.

Clearance Number:

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