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Title

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Permalink

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Journal

Berkeley Scientific Journal, 21(1)

ISSN

1097-0967

Authors

Tokumaru, William
Talukdar, Ishan
Haeffner, Harmut

Publication Date

2016

DOI

10.5070/BS3211033746

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FOURIER TRANSFORM INFRARED ANALYSIS OF SURFACE ION TRAPS

Abstract: This study examines gold and copper-aluminum surfaces in air and vacuum via Fourier-transform infrared spectroscopy to learn more about the causes of electric surface noise in ion traps. The FTIR spectra show traces contamination, including unique fingerprints in the range of 4000 to 600 cm^{-1} . We study how the spectra change when the surfaces are exposed to controlled hydrocarbon contamination. We also study whether procedures commonly used in ion trapping such baking for establishing ultra-high vacuum, and exposure to blue to ultraviolet light radiation alter the surface. Spectra of individual surfaces are found to differ more from each other than they do under these procedures. This work is based off of the first author's honors thesis.

BY WILLIAM TOKUMARU, ISHAN TALUKDAR, & HARTMUT HAEFFNER

LAYOUT BY ELLIS VAVRA, REBECCA CHAN, AVANI VAID, HYEONJI SHIM, HARRISON RAMSAY

INTRODUCTION AND BACKGROUND

Quantum computing has exciting applications ranging from clever solutions for optimization problems to superior implementations of existing algorithms.^[1] It should enable cracking of traditional cryptography, while likewise protecting information. One of the most promising ways to create a universal quantum computer is using trapped ions.^[1]

While quantum computing with trapped ions is well advanced, surface noise prevents progress towards smaller and more compact systems which would allow for faster and more flexible quantum computing architectures.^[2, 3] Ion "qubits" are controlled by manipulating electronic and motional states of ions with lasers. Unfortunately, electric field noise limits the coherence of multi-qubit operations by destroying the quantum information in the quantum bus connecting the respective qubits.^[2] After eliminating technical noise, the remaining noise is too large to be explained by Johnson noise and unlikely to be a systematic or a measurement error. Instead, the noise has been reduced by cooling the electrodes to cryogenic temperatures, by increasing the distance of the ions from the surfaces, and by surface treatment with energetic Argon ions. Concentrated laser radiation has been reported to both decrease and increase heating rates.^[4-10]

In particular, surface treatment experiments suggest that surface contaminants play an important role in the observed

noise.^[6] Indeed, Auger electron spectroscopy shows that carbon and oxygen are present before treatment and are removed by the energetic Argon ions.^[7, 8] However, the experiments in Ref. [8] also report that subsequent re-contamination from molecules present in Ultra-High Vacuum (UHV) does not let the noise reappear. Carbon contamination may be either in the form of atomic carbon or of hydrocarbons deposited on the electrodes somewhere during the fabrication, assembly or baking procedures.

The studies in this paper aim at comprehending the noise mechanisms to help in future experimental planning. They also apply to numerous other fields studying electric noise near surfaces, including engineering nanoelectronics and superconducting electronics, detection of Casimir forces in quantum field theory, tests of general relativity, and hybrid quantum devices.^[11-15]

Organic materials present in air tend to adsorb onto metal and form nanostructures to reduce the free energy between surfaces and the environment.^[16] A common model for these contaminants is based around Self-assembled Monolayers (SAMs).^[17] These molecular structures are formed from exposure to fluids and gases with organic content and organize spontaneously into crystalline-like adatom structures. They commonly appear on gold and copper surfaces, both of which are common traps electrode materials.^[18-27] Many SAMs are "alkanethiols,"

characterized by single-bond hydrocarbon chains with sulfur heads.^[28] They can be removed by plasma cleaning.^[29] These observations make them a candidate for the contamination leading to the elevated electric field noise observed in ion traps. This study investigates whether or not certain ion trap procedures can change the structure of organic surface contamination.

EXPERIMENTAL METHODS

Auger spectroscopy identifies Carbon and Oxygen as the main contaminants.^[7, 8] However, Auger spectroscopy cannot detect Hydrogen nor is it very sensitive to the chemical structure of the surface. Hence, it is unknown in which form Carbon and Oxygen are bound to the electrode surface. One method of characterizing the Chemical composition is through Fourier Transform Infrared Spectroscopy (FTIR). Molecular bonds vibrate at specific frequencies, which correspond to particular vibrational energies, typically in the infrared (IR) regime. Analyzing an absorption spectrum of a sample excited by IR light allows one to identify specific bonds and function groups of the adsorbed molecules and thereby construct a description of the molecular structure of the sample.^[30]

The primary tool of our experiment is a Fourier Transform Infrared Spectrometer (Bruker Tensor 27 FTIR). It produces a spectrally broad IR beam, spectrally filtered by a scanning interferometer. Outside the FTIR, the beam reflects off of a plane mirror, followed by a parabolic mirror for focusing (see Fig. 1). It then passes through an automated wire-grid polarizer which sets the S or P linear polarization of the beam before arriving at the entry IR viewport of the vacuum chamber containing the sample. Upon entry, it grazes off of the trap

surface at approximately 10 μ m and exits the second IR viewport to meet the second parabolic mirror which directs the light onto the detector. Both parabolic mirrors have 30 cm foci with the sample positioned at the focus of both. Finally, the beam reflects off of a plane mirror and enters a Mercury Cadmium Telluride (MCT) detector, focused by a final parabolic mirror. Performing a Fourier transformation of the detector signal yields the desired spectrum.

The goal of the measurements is to learn more about the chemical compositions of adsorbates on the trap electrode surfaces, in particular under realistic conditions for ion trapping. Before ions can be trapped, vacuum chambers containing the trap are baked to typically 200Co to desorb water and other surface contaminations so that UHV can be achieved. Furthermore, ions are typically cooled with near ultraviolet (UV) light and hence the traps are often exposed to blue and ultraviolet radiation. This study mimics the steps taken to prepare the traps after manufacturing to understand whether and how these steps affect the trap surface.

INFRARED SPECTROSCOPY

Infrared spectroscopy identifies and characterizes molecules by measuring how light interacts with the molecular bonds. The specific molecular vibrations, stretches, rocks, wags, pinches, and other changes to relative atomic orientations manifest themselves as spectral features. Consider Fig. 2: The primary region of interest in most FTIR spectra ranges from 4000 to 2800 cm⁻¹, where most single hydrogen vibrational bonds are located. Common signals here include features of water, alcohol hydroxyls, alkanes, alkenes, and alkynes. The next region from 2800 to

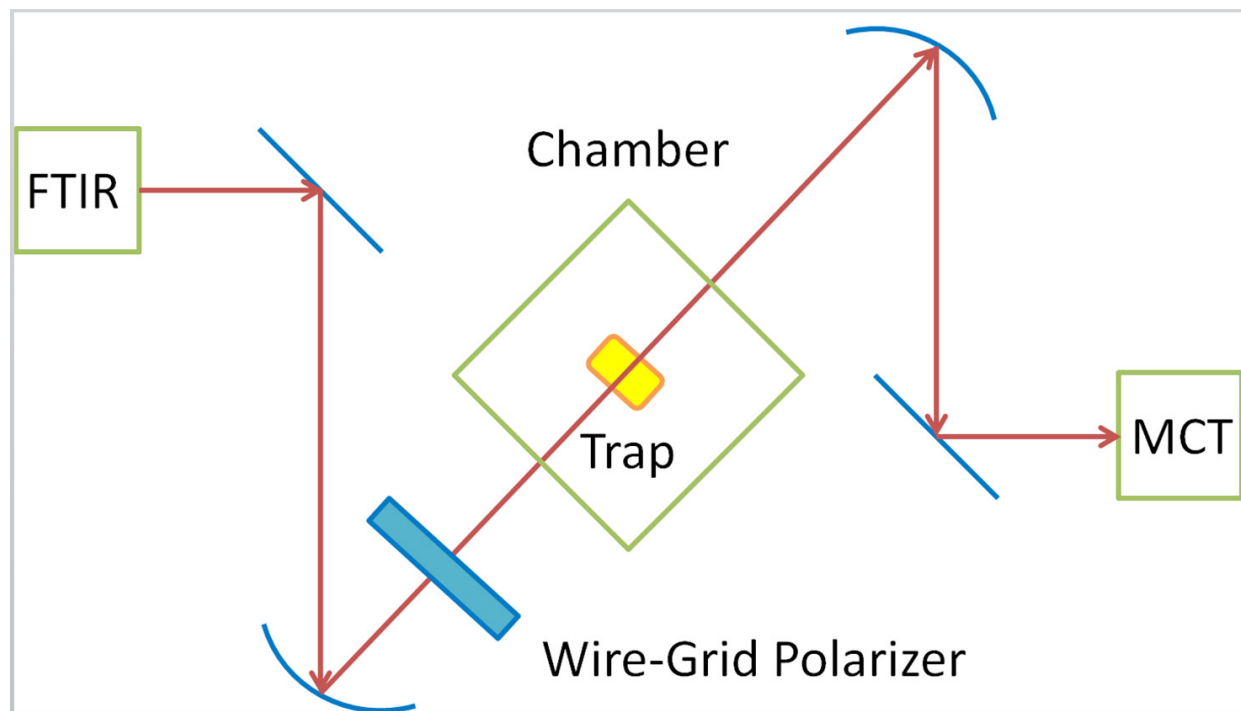
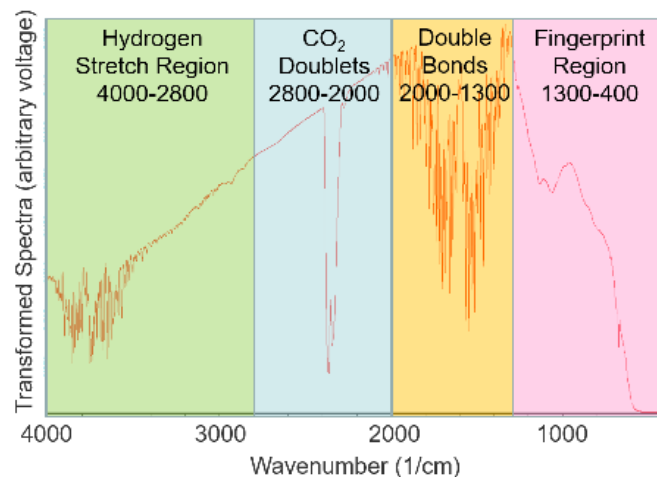


Figure 1. The optical setup displaying the FTIR and external instruments.

Figure 2. Common types of chemical bonds by region in IR spectra. As this has yet to be referenced to a background, the absorption is measured in arbitrary



2000 cm^{-1} includes triple bonds, as well as carbon dioxide doublet absorption due to the air between optical elements. Signals from 2000 to 1300 cm^{-1} include double bonds, most of which include at least one carbon, though single hydrogen bond stretches can be found here as well. Finally, from 1300 to 400 cm^{-1} , we choose to define the “fingerprint region,” which is best analyzed in terms of its overall shape because it is challenging to resolve bonds that can range from complex motions of alkanes to single bonds of uncommon elements.

Counterintuitively, even FTIR spectra of ideal surfaces show a wide variety of signals. To begin, the IR beam is not necessarily spectrally flat. Furthermore, the light passing through air can be absorbed by molecules present in ambient air. Similarly, the light passes through various optical elements which may contain contaminants. Hence, it is important to reference the taken spectra to a background to ensure that the actual signals stem from the sample. One method would be to compare the spectra of the contaminated surface under study to that of an ideal perfectly clean one. Apart from the difficulties in preparing a truly clean sample, this method becomes difficult if the sample is in vacuum as alternating between samples is not straightforward.

Another method for discerning surface absorption from other effects is to use the fact that most contaminants bound to the surface are aligned perpendicular with respect to the surface. In particular, Grazing Angle Polarization Modulation (PM) can take advantage of this by alternating between perpendicular (S) and parallel (P) components, using one signal as the background for the

other when collecting spectra.^[31] In particular, the fact that P polarized light interacts stronger with the surface layer than S polarized light allows one to differentiate between surface bonded molecules and the molecules in air which do not possess a specific orientation. Since switching between different polarization can be very fast, this method allows one also to efficiently remove background fluctuations.^[32, 33]

Figure 3 displays the absorption spectra AP and AS of P and S polarized light, respectively, as a function of the wavenumber k as well as their normalized difference, as a function of the wavenumber k : $(AP(k) - AS(k)) / (AP(k) + AS(k))$. Most of the signals are common to both polarizations, leaving only small differences except in the fingerprint region.

In theory, the spectra should be a flat line with absorption peaks dropping down. The drop in intensity at either end of the spectrum is due to limited infrared transmission through the optics. Spectra can also drift during and between scans due to the motion of equipment or change in detected intensity due to environmental factors. The interferogram mirror also takes imperfect step sizes or experience tilting due to hardware limitations. The amplitude of most of the spectra vanishes below 600 cm^{-1} so that region is not included in the analysis below.

The following specific features are also present in Fig. 3: From 4000 to 3400 cm^{-1} there are peaks that typically correspond to water vapor in the air and condensation on our optics. From 2400 to 2200 cm^{-1} , a pair of strong peaks corresponds to the instrument’s environmental carbon dioxide.^[34] This carbon dioxide signal in the doublet region is typically the signal most prone to this effect due to its relative strength and the volatility of the environment around the setup. Retaking background scans frequently limits the impact of this atmospheric noise. The entire double bond region here is clouded by water and carbon dioxide signals as well. Due to the complex nature of the fingerprint region, one can typically at best use it to recognize that surfaces are contaminated and distinguish between them as each con-

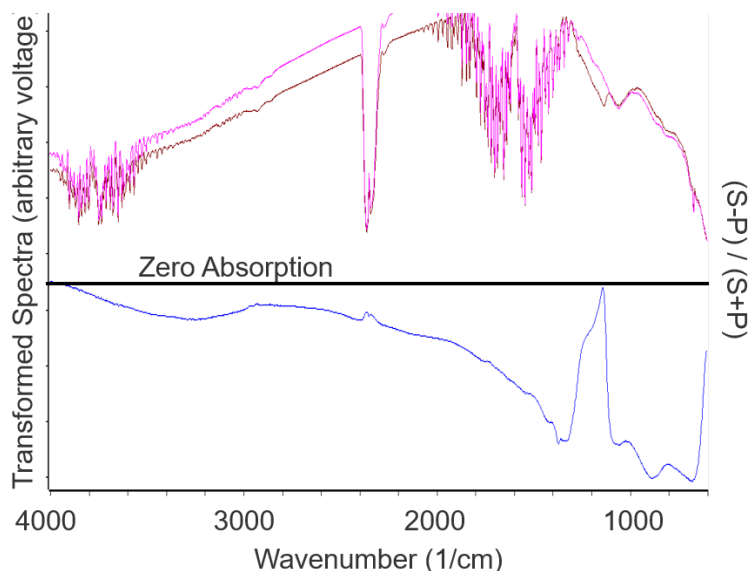


Figure 3. S polarized (violet), P polarized (burgundy) and difference over sum (blue) of a typical spectra. The normalized difference of these two polarizations is in-sensitive to atmospheric noise and noise from other non-polarizing sources. In this case, the only prominent feature is the signal from the silicon

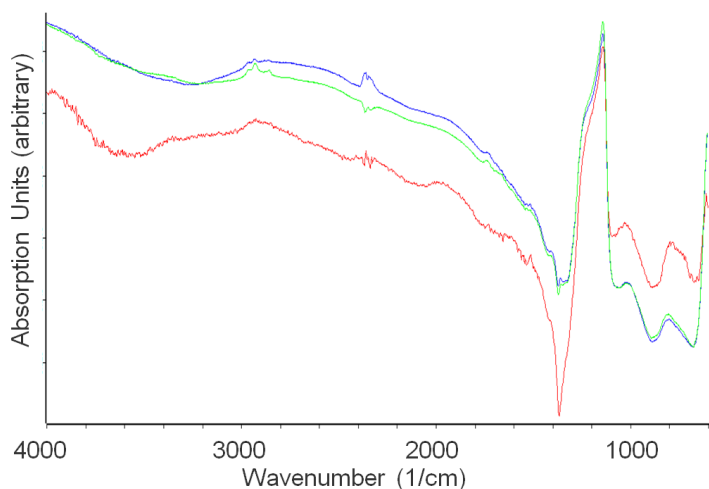
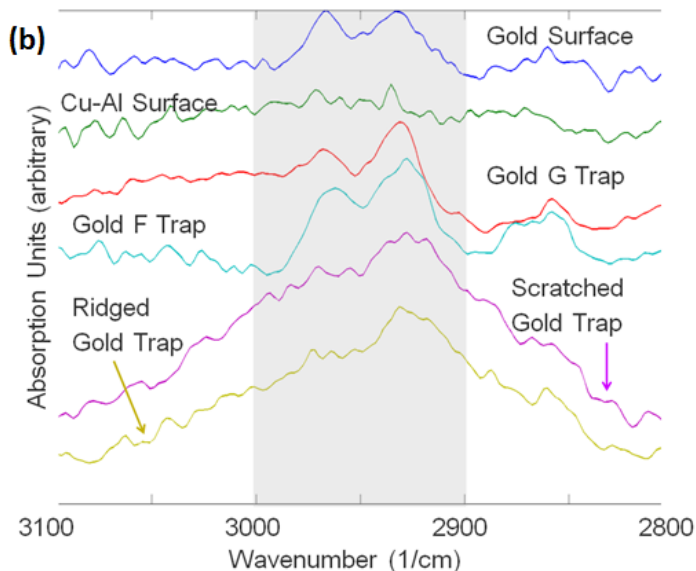
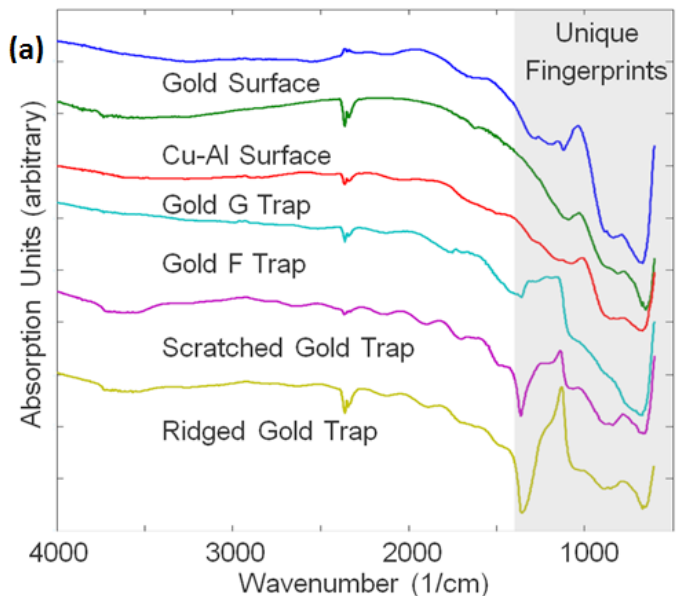


Figure 4. Difference over sum spectra of a surface (blue) subjected to water (red) and wiped dry (green). The primary change to observe is present around 3500 cm^{-1} , corresponding to the addition of hydroxide bonds. The signals around 2900 and 1400 cm^{-1} indicate that molecules with alkane bonds are now present at the surface. The overall baseline shift and the carbon dioxide signal around 2400 cm^{-1} are not as meaningful,

self should never get directly contacted to other tools except those for wire-bonding used to connect the trap electrically. All tools in close proximity are cleaned with isopropanol and distilled water.

Despite all care, we expect the sample surfaces to be contaminated. As stated in Ref. [35]: “any surface that has been exposed to the atmosphere will have a covering of adsorbents at least several monolayers thick. Additionally, trap electrode mate-



tamination will have a different fingerprint.^[30] Finally, it is possible to make out many narrow peaks clustered around 1700 cm^{-1} such as the carbon double bond.

When performing experiments, one compares the spectra before and after a specific attempt to modify the surface to check if there is any substantial change to the contamination. While it may not be always possible to determine exactly what the contamination is, one still can comment on its molecular structure by identifying particular bonds with high precision. For example, Fig. 3 displays the effects of applying tap water to a surface and then removing it.

This surface was open to the air, not in vacuum. We see a substantial water peak as well as signals in the fingerprint region around 1350 cm^{-1} . Most prominently, alkane bonds remain around 2900 and 1400 cm^{-1} while all other signs of the water are removed. The carbon dioxide peaks around 2400 cm^{-1} fluctuate as part of the environmental noise.

SURFACES UNDER STUDY

Each trap surface begins as a glass substrate. The trap electrodes are produced by evaporating first a titanium adhesion layer on the substrate, followed by evaporating either gold or a copper-aluminum alloy to a thickness of 500-1000 nm. The traps are handled in a clean room only and stored in plastic containers. After they are brought into the measurement laboratory, the traps are mounted inside a vacuum chamber with clamps. Any adhesive used is UHV-safe to avoid outgassing. During the initial pumping, heaters bake the chamber to about 200Co.

Extreme care is taken to keep all parts which go inside the vacuum chamber oil-free, including multi-step ultrasonic cleaning and wearing nitrile gloves while handling them. The trap surface it-

Figure 5. All surfaces tested are uniquely dirty. The upper figure displays the complete spectra. All spectra exhibit some degree of noise around 2400 cm^{-1} due to fluctuation in carbon dioxide content in the air. The signals of individual samples differ most in the fingerprint region. This lower figure displays the the region from 2800 to 3100 cm^{-1} of the same data. The spectra are baseline corrected again to the new bounds for clarity. All surfaces include alkane contamination as evidenced by the peaks around 2925 and 2975 cm^{-1} , except for the Cu-Al surface, which has peaks too small to

rials that react with oxygen will have a native oxide layer.” Fig. 5 verifies the existence of substances on numerous surfaces.

In addition to the fingerprint regions shown in Fig. 5a, some alkane bonds and the aforementioned instrument imperfections are relevant to the analysis. Of the single bonds displayed in Fig. 5b, most are alkanes, which would be expected for alkanethiol contamination, especially on metal surfaces.^[20, 36-38] There is a distinct lack of alkene, alkyne, carboxyl, and other common bonds in any spectra. When hydroxyl bonds are present, they are most likely to be water on the surface in addition to typical parasitic water signals from our instruments and optics. Despite their relative intensity, the bonds of the fingerprint region are too numerous and close together to be resolvable. Some fingerprints include stretches consistent with alkane “wag” and “rock,” while others have a broad signal centered around 1200 cm^{-1} that is associated with silicon dioxide peaks from the glass substrate or possibly plasmon resonance from the metal coating.^[39, 40]

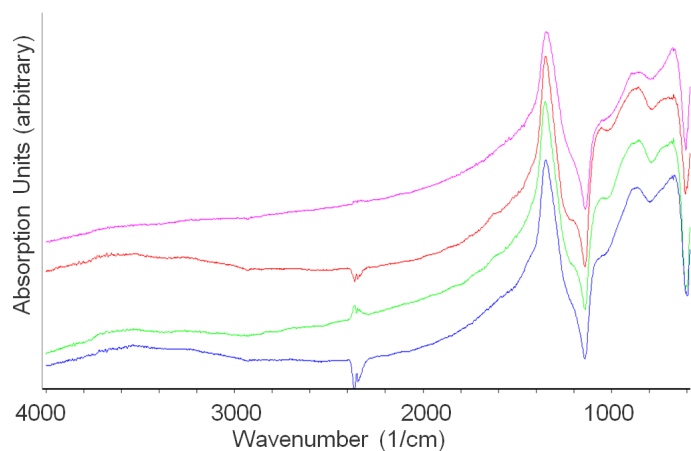


Figure 6. Initial surface (green), Isopropanol on surface (teal), and wiped-clean surface (red). Notice how the Iso-propanol adds hydrocarbon and hydroxyl signals around 3000 cm^{-1} and obscures the silicon dioxide fingerprint around 1200 cm^{-1} .

RESULTS AND ANALYSIS

The surface used for the first test is gold and is subject to cleaning by hydrocarbon chemicals (isopropanol and acetone) that are commonly used to clean parts used in ultra-high vacuum environments. The surface of the second test is also gold and subject to baking. The surface for the third test is an alloy of copper and aluminum and subject to blue laser, blue LED, and UV radiation.

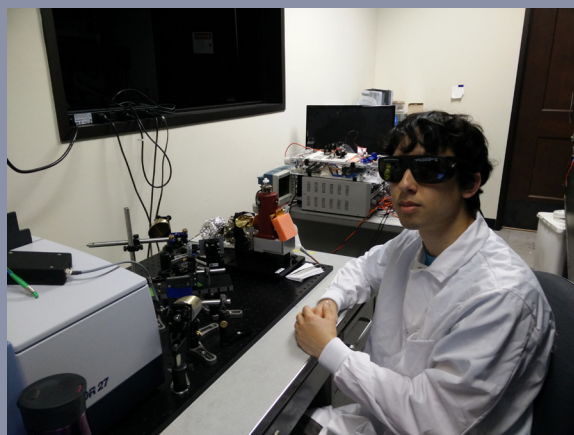
In the first test on a gold surface, we observe that applying standard cleaning Isopropanol changes the spectra drastically but almost all of its changes are undone when it is removed with a wipe. This is the same result as tap water except that Isopropanol reduces the alkane signature left by the water (around 2900 and 1400 cm^{-1}) rather than increasing it. We also observe that the liq-

uid Isopropanol temporarily obscures the 1200 cm^{-1} silicon dioxide signal in the fingerprint region, providing additional evidence that the signal is characteristic of the surface. The spectra shown in Fig. 6 demonstrate how clean the initial surface is compared to one covered in Isopropanol, how clean it is after Isopropanol is dried off, and how persistent the initial spectra of the trap is.

These tests reproduce easily and every additional experiment had the same effects. In fact, after determining that the alkane tests for this trap were complete, additional tests of all types of intentional contamination from contact with skin to application dust could all be removed with Isopropanol and return to the initial values of the spectrum. This suggests that cleaning with Isopropanol does not substantially alter the chemical composition of the initial surface contamination on traps in a way that can be observed here. We also test whether common baking procedures required for ultra-high baking have an observable effect on the surfaces. Baking is typically used to enable ultra-high vacuum conditions. However, it is known to modify the reflectance and can alter surface structures.^[41, 42] We find that the bakeout procedure does not significantly alter the spectra when compared to the difference between individual but nominally clean surfaces. Furthermore, as shown in Fig. 7, three sets of week-long exposures to 200 degrees Celsius environments during baking produces similar results.

The last procedure studied here investigates whether exposure to ultraviolet light can alter the surface. Because we use copper-aluminum traps in our laboratory extensively and

ABOUT THE AUTHOR



WILLIAM TOKUMARU

William is a recently graduated physics major from Southern California. His research is from work with Professor Haeffner in the Department of Physics. He began work there after an interesting lab tour and worked on numerous projects before this one. He and professor Haeffner realized that there was a need for studying anomalous heating so they acquired an FTIR for this project..

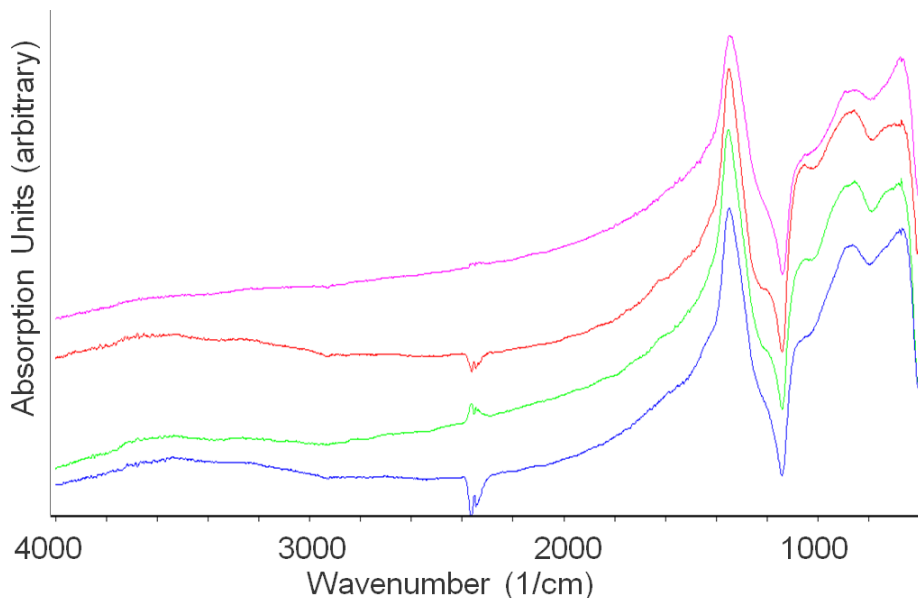


Figure 7. Initial surface in air (violet), after a week of baking (red), after two weeks (green), and after 3 weeks (blue). The relative vertical placement of each spectra is arbitrary and the vertical axis has been inverted relative to previous figures for clarity. Notice that the differences between spectra in this figure are far less significant than the differences between those depicted in Figs. 5 and 6.

because their FTIR spectra are cleaner than those for gold, we use copper-aluminum traps for this test. In the first test, we expose the traps to laser light near 397 nm, commonly used in our laboratory, with a total power of 130 micro Watts directed through a viewport onto the surface. The beam is focused to a spot approximately half a centimeter in diameter. The initial and final spectra are as similar as the typical variations of spectra ran back-to-back. Hence, we find no evidence that the laser caused any change. The second investigation uses a 365-400 nm blue-UV LED flashlight with 7~mW power. Even after shining it on the trap for over 12 hours, there is no effect. The third investigation uses a 290~nm UV LED at 800 micro Watts. It is attached inside the chamber about 2 millimeters above the surface of the trap. The LED is driven only for tens of minutes at a time in order to avoid damaging it. Again, there is no effect, even for in-situ UV radiation.

It is quite possible that the equipment and methods are not sensitive enough to detect the change to spectra. Meaningful signals may be obscured by water and carbon dioxide fluctuations in air. Additionally, some surface signals may be due to surface roughness and polarization-dependent Fabry Perot interference effects in addition to hydrocarbon. However, the observed signals, particularly in the fingerprint region, are many orders of magnitude stronger than background noise.

CONCLUSION

This study investigates the effectiveness of PM-FTIR methods for detecting contamination of surfaces of planar ion traps in air and vacuum. Different surfaces have different contaminations after the manufacturing process, possibly deposited upon brief exposure to air. Isopropanol cleaning, baking, and blue-UV radiation produce no noticeable changes to the trap spectra beyond the deviation between individual trap spectra of

nominally the same particular surface. It is possible that these three experiments may cause changes to surface contamination that are at levels below the sensitivity of our PM-FTIR measurements.

Future tests may include the effect of different temperatures of the surface, as well as annealing and argon treatment of the surfaces.^[7, 8] Furthermore, it is possible to add a photoelastic modulator to collect data with faster polarization modulation to minimize environmental noise by retaining the background on a kHz scale. Finally, FTIR spectroscopy of the surface of a planar trap can be combined with measurements of the motional heating of ions trapped by it, in order to compare and correlate the relationship between the detected contamination with heating rates.

ACKNOWLEDGEMENTS

We would like to thank the following people: Maya Lewin-Berlin and Sonke Moeller for fabricating surfaces. Shunlin Wang of Bruker for hardware assistance. Sepehr Ebadi and Henning Kaufmann for optical design and testing. This research was partially funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), through the Army Research Office grant W911NF-10-1-0284. William Tokumaru was supported by the Rose Hills Summer Undergraduate Research Fellowship program. Finally, we would like to thank Crystal Noel, Dr. Michael Martin, and Professor Robert Corn for assistance in editing the manuscript.

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