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# Soft X-Ray Interferometry 

## Report of the Workshop

Lawrence Berkeley Laboratory
June 25, 1993

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720
September 1993

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## Soft X-Ray Interferometry

## Report of the Workshop

at
Lawrence Berkeley Laboratory
June 25, 1993

Organized by:
Malcolm Howells and Zahid Hussain

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

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# ALS WORKSHOP ON SOFT X-RAY INTERFEROMETRY 

PRELIMINARY PROGRAM

## June 25, 1993

Building 2, Room 100B


# Workshop on Soft X-ray Interferometry 

June 25, 1993<br>Lawrence Berkeley Laboratory<br>Berkeley, CA

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## Executive Summary

The purpose of the soft x-ray interferometry workshop held at Lawrence Berkeley Laboratory was to discuss with the scientific community the proposed technical design of the soft x-ray Fourier-transform spectrometer being developed at the ALS. Different design strategies for the instrument's components were discussed, as well as detection methods, signal processing issues, and how to meet the manufacturing tolerances that are necessary for the instrument to achieve the desired levels of performance. Workshop participants were encouraged to report on their experiences in the field of Fourier transform spectroscopy.

There are a number of problems in the physics of atoms and small molecules that challenge the resolution of the diffraction grating spectrometers that are traditionally used for vacuumultraviolet (VUV) and soft x-ray experiments at synchrotron radiation facilities. An interesting example is the helium absorption spectrum in the region from 60 to 80 eV near the double ionization threshold. Helium is the archetypal electron-exchange and three-body system and its spectrum exhibits many Rydberg series that correspond to the possible two-electron excitations with both negative and positive parity states involved. Fundamental studies of photoabsorption processes in helium go back to the 1960's. ${ }^{1}$ Using the monochromators of today, however, scientists can only resolve about twenty of the infinite number of members of the double-excitation Rydberg series below the $\mathrm{N}=2$ threshold of $\mathrm{He}^{+}$. Furthermore, the transitions from the negative parity states can hardly be seen because of very small natural line widths even though they are believed to have very high oscillator strength. Although the present technology has been pushed to the limit ${ }^{2,3}$ (resolving power $\cong 16000$ ), it has allowed only limited studies of the interactions between the Rydberg series that should show an interesting transition to chaotic states at sufficiently high values of the principal quantum number. Similarly, the study of the lowest-order negative-parity states, which are predicted to have widths in the microvolt range or lower, has been severely restricted by present day monochromator performance. The information from these studies is needed for comparison with the many theoretical analyses of the helium spectrum.

To address the types of problems described above, the ALS is developing a Fourier transform spectrometer that is intended to operate up to 100 eV . The motivation is solely improved resolution and not the throughput (Jaquinot) or multiplex (Fellgett) advantage, neither of which apply for the sources and detectors used in this spectral range. Our proposed implementation of this is via a Mach-Zehnder geometry that has been (1) distorted from a square to a rhombus to get grazing incidence of a suitable angle for 100 eV and (2) provided with a mirror-motion system to make the path difference between the interfering beams tunable. The experiment consists of measuring the emergent light intensity $(I(x))$ as a function of the path difference ( $x$ ). The resolving power of the system is limited by the amount of path difference obtainable that is 1 cm (one million half-waves at 200 $\AA$ wavelength) in our design thus allowing a resolving power of one million. The free spectral range of the system is limited by the closeness with which the function $I(x)$ is sampled. We propose to illuminate a helium absorption cell with roughly $1 \%$-band-width light from a monochromator thus allowing one hundred aliases without spectral overlap even for sampling of $I(x)$ at one hundredth of the Nyquist frequency.

1. P. Madden, K. Codling, "New Autoionizing Atomic Energy Levels in $\mathrm{He}, \mathrm{Ne}$, and Ar," Phys. Rev. Lett. 10, 516-8 (1963).
2. Domke, C. Xue, A. Puschmann, T. Mandel, E. Hudson, D. A. Shirley, G. Kaindl, C. H. Greene, H. R. Sadeghpour, "Extensive Double-Excitation States in Atomic Helium," Phys. Rev. Lett., 66, 1306-9 (1991).
3. Domke, G. Remmers, G. Kaindl, "Observation of the ( $2 p, n d$ ) ${ }^{1} P^{0}$ Double-Excitation Rydberg Series of Helium," Phys. Rev. Lett., 69, 1171-4 (1992).

## Discussion Notes:

Mirrors and Beam Splitters. Anne Thorne asked if beam dispersion had been considered. Malcolm Howells replied that a milliradian is ok and typical of synchrotron radiation. A question arose about the thickness of the mirrors. Howells pointed out that molybdenum is only used as the optical coating, while the material used for the substrate must be thick enough to polish. Madden asked if the phase changes of the light upon reflection had been considered. Wenbing Yun replied that theta-critical is such that phase changes are small.

Anne Thorne reported that they originally used two separate pieces for beam splitters. Then they tried a solid piece of silicon which worked as both beam splitters-this worked well. When they tried a solid piece of magnesium fluoride, they had problems because of inhomogeneity. Now they are back to using two separate pieces with the drift of the system requiring adjustments every few hours. The moral of the story being that the beam splitters should be adjustable so that they can be realigned easily.

Flex Hinges. Robert Madden suggested considering vertical design as an alternative. One drawback of this is that second order terms become important. Dave Shirley brought up the possibility of making the translation system three-dimensional (3D). This provides improved stability for motion along one dimension. Anne Thorne suggested making the optical system 3D by adding a roof to the structure to reduce the influence of pitch.

Inchworm Drive. Roger Carr said with inchworm drives the thermal drift is quite high and the creep can reach $10 \%$ per second. Robert Madden reported that the space-based VUV systems had abandoned the use of inchworm drives because of creep. Anne Thorne said that a magnetic drive doesn't jerk and has very smooth motion.

Position Indexing. Someone pointed out that you can expect [(1.25 nm) x (" n " factor)] resolution at the lower limit, but polarization alignments must be done very carefully or nonlinearities will drive the value of " n " way up.

Data Sampling. Anne Thorne said one must measure the amplitude and phase and "both" sides of the interferogram because absorption lines are not symmetric.

## Post-Workshop Comments from Anne Thorne

Two problems discussed-how to avoid pitch error on the moving mirrors and how to keep the beam splitter and recombiner aligned to within the micro-radian tolerance-are obviously crucial. Interestingly, the microradian alignment tolerance is almost identical with ours, since we have 10 times the beam diameter at 10 times the wavelength. But we do have the advantage that our two beam-splitter elements are immediately adjacent.

As regards scanning and sampling, I do think you will have to get a laser reference beam through your interferometer somehow, close to and parallel to the signal beam so that it sees exactly the same path differences. Sub-dividing the laser fringes to the required accuracy I do not see as an enormous problem. I think it will turn out to be not very different from what we already do, although the sampling tolerance does depend on the signal to noise ratio you are aiming to achieve. I'suggest that you consider continuous scanning so that you can put your signal frequency where you want it, within limits, and make yourself a nice sanitary digital filter to eliminate the out-of-alias noise. You can then make up your time integration by coadding, with the laser fringes as reference. Admittedly you lose the "fly-back" time, but you save on settling-down time, and most importantly you do not rely on everything staying in perfect alignment with perfect performance for hours on end. If something goes wrong or breaks down you can save the pile you already have, start again next day, and co-add the spectra, whereas if the same thing happens 5 hours through a 6 hour scan you lose everything. The criterion for continuous scanning is a smooth scan velocity-it does not have to be very constant. I think you should look at the possibility of a magnetic drive. We have found that linear motors work well.

# The Scientific Origins of the LBL Soft X-Ray Interferometer Project 

David Shirley
Pennsylvania State University

SCIENTIFIC ORIGINS OF THE LB SOFT X-RAY INTERFEROMETER PROJECT (DAVID A. SHIRLEY)
OUTLINE
I. $E / \Delta E$ us. $E:$ Is high -res ne cessaty?
II. History of our interest in high-res.
III. Achieving $E / \Delta E=10^{4}$ with
A. SGM [Mostly $\left.N_{2} \pi^{*}\right]$.
B. PGM [Mostly molecules, and $H_{e}{ }^{* *}$ ]
C. TGM [At BL 8-1, $55 R L$ ]
IV. More on He ${ }^{* *}$ : on to $E / D E=10^{6}$ !

$$
\begin{aligned}
& \text { I. EiDE US. E: } \\
& \begin{array}{lll}
\leqslant 10 e V & \leqslant 30 \mathrm{eV} & 30 \mathrm{eV}<E<1000 \mathrm{eV} \\
\text { [lasers] } & \text { Norm. Ifc. Optics } & \text { Grazing Inc. Optics }
\end{array} \\
& E / \Delta \sqrt[2]{2} \sim 10^{7} \sim 10^{5} \sim 10^{3} \text { until } \\
& \text { recently }
\end{aligned}
$$

For soft $x$-rays, - Is high te solution $\begin{aligned} & \text { necessary? }\end{aligned}$ necessary?
[MNSWER a VES!]

As stueley docebly-excited systems in the continuer:

$$
\Rightarrow e^{-}-e^{-} \text {correlations }
$$

II. History of our interest in high-resolution: photorecection satellites
[The improvement of $E / \Delta E$ with time]

PHOTOELECTRON
SATELLITES



From D.P. Spears, H.J. Fischbeck, and T.A. Carlson Phys. Rev. A 0, 1603 (1974)

From H. Kossmann, B. Krässig, V. Schmidt and J.E. Hansen


FIG. 2. Satellite lines of argon measured at the quasimagic angle. Upper part: Experimental spectrum obtained in this work. Lower part: Same spectrum convoluted by a Gausian distribution with I CV FWHM.
a)

Extraction

b)


XBL 866-2147
P.A. Heimann, U. Becker, H.G. Kerkhoff, B. Langer, D, Szostak, R. Wehlitz,
D.W. Lindle, T.A. Ferrett, and D.A. Shirley Phys. Rev. A 34, 3782 (1986)


III. Achiering $E / \Delta E=104$ with
A. $\underline{S G M '}$
[sGme spectra, mesotly $N_{2} \pi^{*}$ ]



Schematic of the Rense and Violeti spherical grating monochromator system. The condensing mirrors MI and M2 are designed so iilnt M1 Socuses in the horizontal plane to the exit slit, and M2 focuses in the verical plane to the entrance slit. Each mirror has essentially zero focusing effect in its sagitinl direction.


Detailed plots of the resolution of the $3^{\circ}$ spherical grating monochromator of Beam line C. 'Tle plots ate for $10-\mu \mathrm{m}$ stits and are derived fiom computer ray traces of the whole beam line. The solid lines correspond to revions where the Rowland condition is exaclly satislied and where resolution


Fig. 4-5. Photon flux from (a) a $10^{\circ}$ spherical grating monochromator, in conjunction with undulator U9.0: (b) a $3^{\circ}$ SGM, in conjunction with undulator U5.0: and (c) a $2^{\circ}$ SGM, in conjunction with undulator U3.65. For each. more detailed paramerers appear in Tables 4-2 and 4-3. The curves shown here assume that the monochromators are set for best resolution.


Fig. 2


$\mathrm{N}_{2} 1 \mathrm{~s}->1 \pi_{\mathrm{g}}{ }^{*}$
$\hbar \omega: 236.5 \pm .9 \mathrm{meV}$
$\hbar \omega_{\mathrm{x}}: 2.8 \pm .3 \mathrm{meV}$
$r_{0}: \quad 1.186 \pm .003 \AA$
$\Gamma: \quad 125 \pm 5 \mathrm{meV}$
III. $B$. $E / \Delta E=10^{4}$ with a PGM (SX-700II@BESSH)
M. Domke, G. Kaindl, E. Hudron,...






- XBL 912-129








Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH

III. C. $E / \Delta E=10^{4}$ with \& $T G M$ (M.Howells, Z. Hussain, T.Reich,...)


Exit slit position [cm]

IV. Mote on $H e^{* *}$, and on to $10^{6}$ !



Figure 1. Diagram showing increasing number of channels in the spectrum of helium and their interconnection by autoionisation and other processes (Fano 1969).

arinem








ever, the upper entries in the families remain physically meaningful-identified, in fact, by an experimental amangement that detects the electron at infonity togecher with the state of excitation of the residuewhereas che lower entries are now no longer eigenstates. The difference lies in that, for the top entries, the two electrons are separated to infinity where $e^{2} \hbar_{12}$ vanishes, whereas for the bottom entries $r_{12}$ is finite, thus invalidating the independent electron labels. Bottom entries drawn from different families in Eq. 2 that share the same $\{S, L$, $J$. $\pi\}$ but differ only in $N$ and $n$ are mixed by the electron-electron interaction with the result that the physical eigenstates are linear combinations of various independent particle configurations. (Incidentally, only the nonseparable portion of the interaction is responsible for this mixing and therefore for the contrast between top and bottom encries.) Tuming to the quark families, we see again that the top members are unchanged (this is a standard choice), only the bottom ones getting mixed as in Eq. 3 upon the superposition of electroweak and strong interactions. The analogy may suggest a dynamical explanation in terms of an underlying substructure of quarks ("urquarks"?). Suppose, as in the atomic example of chree charged particles, the quarks themselves are composites of three urquarks. A distinction can then be made between two types of composites of the three ur-quarks, depending on whecher one pair of relative discances vanishes (recall an inversion in the nature of chromodynamics relative to electrodynamics, that the interaction vanishes when distances go to zero rather than to infinity). One type, with a pair of ur-quarks having zero separation, would comespond to the $u, c$, and $t$, while a second, in which all pairs are finitely separated, to the $d, s$, and $b$. In the language of atomic physics, the switching on of interactions between the ur-quarks causes "configuration mixing" of the $\mathrm{d}, \mathrm{s}$, and b as given by the KM matrix in Eq. 3.

## Experimental Data on Doubly Excited Atoms

This section gives a brief review of experiments on doubly excited states over the last 20 years. It is designed to highlight those key features of the data that will be picked up in the next section to draw lessons on the family structure and on the hierarchical coupling between families of states of the three-body atomic system.

Exciration by photors. The simple sketch in Fig. 1 of two-electron states also shows how they may be excited and observed in the laboratory. One method is photoabsorption from the ground state of $\mathrm{H}^{-}$, or He , in an energy range below the detach-
ment or ionization thresholds $\mathrm{H}(\mathrm{N})$ or $\mathrm{He}^{+}(\mathrm{N})$. Against the background of the absorption into the one-electron continuum of the first family, structures appear in the absorption cross section at specific energies marking the positions of doubly excired states. The first doubly excited states in atoms were observed in chis way in He (13), utilizing synchrotron light from electron synchrotrons that provide photons of the. requisite energy ( $\sim 60 \mathrm{eV}$ or 20 nm ). Seates of ${ }^{1} P_{1}{ }^{\circ}$ symmetry of the $N=2$ faroily in Eq. 2 were observed as a Rydberg sequence of resonances converging to the $\mathrm{He}^{+}(\mathrm{N}=2)$ limit, which lies $24.6+$ $54.4(1-1 / 4)=65.4 \mathrm{eV}$ above the ground state of He. Experiments with synchrocron light in many ocher atoms have since been designed to study such sequences of doubly excited states, typically with relatively small values of $N$ (14). The most recent data (15) through $N=6$ are shown in Fig. 3. Seates of much larger $N$ have not been observed. This is not because of any lack of photon energy in synchrotron sources but more a reflection of the weakness of exciration to such $N$ as will be discussed.

Lasers provide much higher resolution, and stepwise absorption of multiple laser photons has reached doubly excited states in more complex atoms, particularly in the
alkaline earths such as barium. However, the lowest quasi-bound states within a family when $N$ is large have remained out of reach. As typical examples, when $N$ is 4 or 5 , the states observed can be atributed to principal quantum numbers $n$ larger than 10 for the second electron (16), or, when $N$ is 20, the values of $n$ are 40 or larger (17). That is, the doubly excited states of high excitation that have been studied through multiple laser photoabsorpcion bave a very unequal energy sharing berween the two electrons. States in which the two dectrons have comparable radial excication, which are the lowest members of each column in Eq. 2 or in Fig. 1, have remained elusive to such laser experimental searches, the best results being those in (18).

The longest sequence of comparably excited states seen in photoabsorption is from a very recent study on $\mathrm{H}^{-}$at LAMPF (3, 4). (In such particle physics latoratories, $\mathrm{H}^{-}$is often the initial charged species that is accelerated. Later, upon stripping of the two clectrons, proton beams and subsidiary meson or neurino beams are generated.) In a very innovative use of che relativistic beam of $\mathrm{H}^{-}(\sim 800 \mathrm{MeV})$ for atomic physics studies, Howard Bryant and his colleagues have studied various aspects of this atomic negative ion (19). The recent ex-

Fig. 3. (A) $\mathrm{He}(N=3, n)$. (B) $\mathrm{He}(N=4, n)$, and (C) $\mathrm{He}(N=5, n)$ and $\mathrm{He}(N=$ 6. n) ${ }^{1} P 0$ doubly excited states seen in protoabsorption with synctrotron light. Panels ( $A$ ) and ( $B$ ) include on the right a magnified high $n$ region. from (15), with permission]


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# Fourier Transform Spectroscopy: A Sketch Map to Lyman Alpha and Beyond Anne Thorne <br> Imperial College, U.K. 

FTS: a sketch map to Lyman $\alpha$ and beyond .-

Anne Thorns; Imperial College

Basics of FTS
resolution + Wavenumber accuracy
sampling $\alpha$ aliasing signal to noise ratios
Practical points about interferometers tolerances sampling accuracy field of new band limiting
Progress towards Lyman $\alpha$ problems a results to date Beyond Lyman a??

7ourier transform spectrometryy


Monochromatic:

$$
I(x)=B\left(\sigma_{0}\right)\left(1+\cos 2 \pi \sigma_{0} x\right)
$$

Source distrib. $B(\sigma)$ :

$$
I(x)=\int B(\sigma)(1+\cos 2 \pi \sigma x) d \sigma
$$

Subivact mean $\int B(\sigma) d \sigma$ :

$$
\begin{gathered}
I(x)=\int_{\Downarrow F F T} B(\sigma) \cos 2 \pi \sigma x d \sigma \\
B(\sigma)=\int I(x) \cos 2 \pi \sigma x d x
\end{gathered}
$$

Practical moditications
(1) The interferegram is digitally sampled at intervals $\Delta x$, so $\int \Rightarrow \Sigma$
(2) The interferepram is never eutively symmetric, so it is necessary to take the complex F.To

$$
B(\sigma)=\sum_{n=-M}^{n=N} I(n \Delta x) e^{-2 \pi i \sigma n \Delta x}
$$

Nobe In continuons scanning node The interferometor canverts optial frea. $\nu$ to audiofrequency $f$
ahere

$$
f=\frac{v}{c} \nu \quad \text { (ov }=\frac{1}{2} \text { mivivor vel.) }
$$

and $f=v \sigma$

Grating vs. 7.1. Spectrometer
Crating

$\Delta x \rightarrow$ spectral resolution $\delta \lambda$
ITS

$$
R=N
$$

$$
150 \text { der }
$$


$1+\infty \infty 11000013$

Spatial modulation freq. $\propto \sigma(=1 / \lambda)$
$L \rightarrow$ spectral resolution

$$
\delta \sigma=\frac{1}{2 L} \mathrm{~cm}^{-1}
$$

$\Delta x \rightarrow$ free spectral range

$$
N_{\text {samples }\left(=\frac{L}{\Delta x}=\frac{\Delta \sigma}{\delta \sigma}\right) \quad \Delta \sigma=\frac{1}{2 \Delta x} \sin ^{-1} 1 N_{\text {alas }}^{\prime}}
$$

The principal advantages of FTS

1. Multiplex (Fol leet) (venus grating

X Multiplex. (Fellgett) speciomeity)
$X$ applies in I.R. where detector noise is independent of signal gain $\sqrt{N}^{\text {in }}$ signal/nose
2. Throughput (Jacquinot)
$x$ affien in vis/UV when noise is photor-linited - also in I.R. gain $\sim 100$ in signal/aose $1 R$
3. Wavelength (Tonnes) always applies
all wavelength in Terms of reference (HerNe) laser
4. Resolution
can always be made to exceed grating

$$
\mathbb{R}=\lambda / \delta \lambda=L / \lambda
$$

$\pm$ Spectral coverage
All lines ( + badegurnhd) necessarichy

The principal disadvantages
(t) Spectral coverage
can be disadvantage if only 1 or 2 lines of interest
(土) Norse distribution
Random noise is "white": spectrum has almost uniform noise everywhere


ATS


Grating
relatively worse
for weak ines
Crosuct of doing a $F T$ of the noise- not the multiplex diradvacutare

The wavelength (Conner) advantage
The wave number scale in the $F T$ is denied directly from the sampling intervals - in practice from the wavelength of the reference laser
$\Rightarrow$ accurately linear wovenumber scale There is still a scaling factor for absolute accuracy of order $1 / R$ ie. scaling factor $\frac{\Delta \sigma}{\sigma} \sim 1: 10^{5}-10^{6}$

Calibration

$$
\begin{aligned}
& \text { Plot } \frac{\sigma_{\text {meas }}-\sigma_{\text {ref }}}{\sigma} \text { vs. } \sigma \\
& \frac{\Delta \sigma}{\sigma} \xlongequal{-\underline{x}-x-\frac{x}{7} \hat{\imath}-x-}{ }_{\text {calif. cost }}
\end{aligned}
$$

Note in contrast to grating in principle one line required as ref. for whole spectrum.

Resolution - how high?
Doppler width $\frac{\delta \lambda_{D}}{\lambda}=7 \times 10^{-7} \sqrt{\frac{T}{M}}$
so for $T \sim 2000$
with $M \sim 60$

$$
\frac{\lambda}{\Delta \lambda_{\Delta}} \sim 250000
$$

For negligible instrumental contribution

$$
\begin{aligned}
\delta \lambda \leqslant \frac{1}{2} & \Delta \lambda_{D} \\
& \Rightarrow \mathbb{R} \Rightarrow 500000
\end{aligned}
$$

For heavy elements or for gases at room temereature

$$
\mathbb{R}>1000000
$$

$\Rightarrow$ resolving power

$$
300000 \text { to } 1500000
$$

Relation between $\left(\frac{s}{n}\right)_{\text {intarf. }}$ and $\left(\frac{s}{n}\right)_{\text {spect. }}$
For $N$ points (independent) in both intorf. and spedrumi and for white nose: (modependunt of frequency)

$$
\left(\frac{\bar{s}}{n}\right)_{s p}=\frac{1}{\sqrt{N}}\left(\frac{s_{0}}{n}\right)_{\text {int }}
$$

$\therefore$ for a local signal $s$,

$$
\begin{aligned}
& \frac{s}{n}=\frac{s}{s} \frac{1}{\sqrt{N}}\left(\frac{s_{0}}{n}\right)_{\text {int }} \\
& \frac{s}{F}=\frac{\text { peak }}{\text { mean }}=\frac{1}{\text { filling factor }}=\alpha \\
& 1 \leq \alpha \leq N
\end{aligned}
$$

Quasi-continuum: $\alpha=1 \quad \frac{s}{n}=\frac{1}{\sqrt{N}}\left(\frac{s_{0}}{n}\right)$ int
The single unresolved line: $\alpha=N \quad \frac{s}{n}=\sqrt{N}\left(\frac{S_{0}}{n}\right)_{\text {int }}$
Normal" cmircion spedrum: $\alpha<1 \%, \frac{s}{n} \sim\left(\frac{S_{0}}{n}\right)$ int

Noise distribution
Grating nose is where the lines are


FTS "White" noise - the same everywhere


Sampling \& aliasing
Free spectral range $\sigma_{\max }$ determined by sampling interval $\Delta x$

$$
\sigma_{\text {max }}=\frac{1}{2 \Delta x} \quad(=F S R \Delta \sigma)
$$

(cf Nyquist: $\Delta x=\frac{1}{2} \lambda_{\text {min }}$ )
Discrete FT repeats $+\ldots$ - spectral pairs at intervals $1 / \Delta x$, or $2 \Delta \sigma$.


Under sampling $\Rightarrow$ aliasing


Nyquist sampling

$3 x$ undersampled

BEWARE

- Superposition of SIGNALS frame other aliases
- Superposition of NOISE f ion all aliases

Final sin for the photan-limited sase
Envision
resolution $\delta \sigma \mathrm{cm}^{-1}$
modulation $m$ fitter transom. $\tau$ total time $T$


$$
\frac{S_{p}}{n}=m \cdot \delta \sigma \varphi_{p} \sqrt{\frac{\tau T}{\int_{f_{i} \tau_{m}} \psi^{\delta}}}
$$

Absorption

$$
\begin{aligned}
& \frac{s}{n}=m \delta \sigma \sqrt{\frac{\varphi_{c} r T}{m T}} \\
& =m \cdot \delta \sigma \cdot \varphi_{\sigma} \sqrt{\frac{\tau T}{-\varphi_{L} W} \varphi_{c}}
\end{aligned}
$$

Tolerances for UV FTS (each give $N 80 \%$ modulation)
optical surfaces $(\lambda / 8)$
Suse of catseyes instead of plane nuivors reduces tilt requirement by $\sim 10$.)



Sampling accuracy
Periodic errors. generate ghosts
l.g. for period associated isth laser fringes


Random errors generate noise
Aim is to keep sampling noise below photon noise.
Criterion depends on type of spectrum $\sigma$ on signal - typically $\lambda / 100$


Field of view a band-lumiting
Path diff.

$$
x^{\prime \prime}=2 t \cos \theta
$$

so phase diff. between
 normal a extreme rays

$$
\begin{aligned}
& \delta \varphi=2 \pi \sigma \delta x=2 \pi \sigma x_{0} \frac{\theta^{2}}{2} \\
& \therefore \delta \varphi<\pi \Rightarrow \theta<\sqrt{\frac{2}{R}} \\
& R=500000 \Rightarrow \theta<2 \mathrm{mrad}
\end{aligned}
$$

Miducsin int. E determine size of entrance. aperture (circular.)
Rayleigh lit St width
Edetermane sit height
Bandpars monochromator
$\theta$ depends on $\lambda$
$\Rightarrow$ string phase effects
 actors band pass
$\Rightarrow$ distorted $\lambda$ scale




depurge
$x: 47393.9648 \mathrm{c-1}: y: \quad .5000 ; 4$ points/px

9 d2mfnew

Fourier Transform Spectroscopy Using Synchrotron Radiation

## Dieter Möller

Fairleigh Dickinson University

1) Wavefront Dividing Beamsplitters.

Interferometry in the IR at the Synchrotron at BNL. Projections for Interferometry in the X-ray region.
2) High Resolution Spectroscopy in the IR. Folding the spectrum to reduce the number of points. Errors from unequal sampling intervals.
3) Interferometers without moving parts. Interferogram displayed in Space. Michelson and Mach-Zender Array Interferometers. Array Interferometer with Gratings.

MICHELSON INTERFEROMETER:
AMPLITUDE DIVISION
STANDING WAVE PATTERN

CONSTRUCTIVE INTERFERENCE: MAX. AT DETECTOR: DESTRUCTIVE INTERFERENCE: MAX. AT SOURCE

SPECTRAL RANGE DEPEND ON BEAMSPLITTER RESOLUTION DEPEND ON DISPLACEMENT OF MMPRROR


DETECTOR

## LAMELLAR GRATING INTERFEROMETER WAVEFRONT DIVISION

## DIFFRACTION PATTERN

CONSTRUCTIVE INTERFERENCE: MAX. AT DETECTOR DESTRUCTIVE INTERFERENCE: MAX. AT FIRST ORDER DIFFRACTION
SPECTRAL RANGE DEPEND ON REFLECTION PROPERTIES OF REFLECTORS.

## RESOLUTION DEPEND ON DISPLACEMENT OF MIRROR

source


DISPLACEMENT


WAVEFRONT DIVISION (FRESNEL DIFFRACTION)

TWO REFLECTORS
INCDENT LIGHT


## WAVEFRONT DIVISION (FRAUNHOFER DIFFRACTION)




MOST IMPORTANT: THE SLIT

## TWO MIRROR WAVEFRONT DIVIDING INTERFEROMETER

##  <br>  <br> DIFFRACTION PATTERN FOR VARIOUS PATH DIFFERENCES

CONSTRUCTIVE INTERFERENCE

## PATH DIFFERENCE n. $\lambda$

DESTRUCTIVE INTERFERENCE

PATH DIFFERENCE $n \cdot \lambda / 2$


OTHER PATH DIFFERENCES
$\lambda / 6,2 \lambda / 6,4 \lambda / 6,5 \lambda / 6$






BEAMSPLITER: WIDTH OF SLOTS
$5 \mu$
$10 \mu$


SEPARATION OF ZEROTH AND FIRST ORDER AFTER I METER

$Y=(X / d) \lambda$
$Y=4 \mathrm{~mm}$

WIDTH OF EXIT SLIT OF MONOCHROMATOR IS .6 mm X-RAYS OF 1 A AT 5 MICRONS GRATING GAVE FRINGES MOVEMENT OF TABLE WTH VARIOUS METHODS

FOR VERY HIGH RESOLUTION AND NARROW BAND WIDTH SAMPLING OF THE ENVELOPE

$M_{2}$

SCHEMATIC


MYIAR BEAMSPITTTER

BEAMSRITTTER
BEAMSPITTTTER
CARACITIVE DOTS GRTD

## POINT-LIKE SOURCE

## EXIT APERTURE DETERMINES SPECTRAL RANGE FOR MODULATION



LIGHT OF $\lambda / 2$

For shorter wavelength more light of destructive interference enters the exit slit and reduces "modulation".

## FOUR REFLECTOR LAMELLAR GRATING "MINIGRATING"

CONSTRUCTIVE INTERFERENCE

PATH DIFFERENCE $n \cdot \lambda$ DESTRUCTIVE INTERFERENCE

PATH DIFFERENCE $n \cdot \lambda / 2$


OTHER PATH DIFFERENCES
$\lambda / 6,2 \lambda / 6,4 \lambda / 6,5 \lambda / 6$


## EXTENDED SOURCE

## SIZE OF APERTURES LIMIT MODULATION



LIGHT OF $\lambda$ FROM ONE POINT


LIGHT OF $\lambda$ FROM TWO POINTS OF THE SOURCE

When light from two points separated by a distance enter the exit slit, more light of destructive interference. arrives at the detector and reduces "modulation".

## ZERO ORDER --- FIRST ORDER --. GAP




# SPACIAL INCOHERENT LIGHT 

## TO ENLARGE THROUGHPUT AND SPECTRAL RANGE

WE NEED TO DISTRIBUTE THE DIFFRACTED LIGHT OF DESTRUCTIVE INTERFERENCE

NOT AT A SPECIFIC ANGLE
BUT OVER A RANGE OF ANGLES IN SPACE

INTERFERENCE FOR REGULAR AND DECREASING DISTANCES OF SOURCE POINTS

SAME DISTANCE BETWEEN SOURCE POINTS

$\delta_{1}=\delta_{2}=\delta_{3}=\delta_{4}=\delta_{5}=d \sin (\theta)$
PHASE DIFFERENCES ARE ALL EQUAL
SUPERPOSTTION WLL ADD UP IN A CONSTRUCTED WAY

DECREASING DISTANCE BETWEEN SOURCE POINTS


## DISK AND 3 RINGS





PERIODIC BEAMSPXITTIER
DIAMETER OF SECTION
3 mo 5 micron

RANDOM PATTERN BEAMSPITGTER OPENINGS SMAITER OR EQUALE TO 3 TO 5 mun





TRANSMISSION


Fourier transíosm with randomly unequal sampling intervals.
We superimpose :wo cos-wares with frequencies 13/1:3 and 17/128:

where $x$ runs $\because=n \pi 1$ to 123 itength and 8 is inisially equal 1.

The sampling interval (equal : may be aultiplied j; sunequal i to represent chanzes of =he sampling interval. We taine the following dieferent values ior $\delta$ :

| $A=(1-.005:$ | $A A=(1+.005)$ |
| :--- | :--- |
| $B=(1-.01)$ | $B B=(1+.01)$ |
| $C=(1-.015:$ | $C C=(1+.015)$ |
| $D=(1-.02)$ | $D D=(1+.02)$ |
| $E=(1-.025:$ | $E E=(1+.025)$ |
| $\mathrm{F}=(1-.03)$ | $\mathrm{FF}=(1+.03)$ |
| $G=(1-.035:$ | $G G=(1+.035)$ |
| $H=(1-.04)$ | $H H=(1+.04)$ |

These values have been randomly distributed and iow much each was used is given ir histogram A.





Fig. 3 Upper graph: Transformation for $8=1$.
Lower graph: black squares: values of histogram $A$, white squares: values of; histogram. B.



Points $1^{\prime}, 1,1^{\prime \prime}$ have same optical path difference
Points 2, 1, 3 have different optical path differences
At 2 and 3 beams meet which are "counter parts" of splitting at B1.


Optical path difference introduced at B2


Introduction of optical path difference by tilting

MIRRORS HORIZONTALI Y DIMDED


Mitrors with horizontal steps (large)

MIRRORS VERTICALIY DIVIDED


Mirrors with vertical steps (small)


PROFILE OF HORIZONTAL GROOVES


PROFILE OF VERTICAL GROOVES


TIME RESOLVED SPECTROSCOPY

PROFLIES




## BEAMSPLITER

$$
Y=(X / d)
$$



# Toward a Soft X-Ray Fourier Transform Spectrometer Malcolm Howells <br> Lawrence Berkeley Laboratory 

## TOWARD A SOFT X-RAY FOURIER TRANSFORM SPECTROMETER

## PARTICIPANTS:

| K. Frank | LBL |
| :--- | :--- |
| M.R. Howells | LBL |
| Z. Hussain | LBL |
| E. Moler | LBL |
| D. Möller | Fairleigh Dickenson |
| T. Reich | LBL |
| D.A. Shirley | Pennsylvania State |

## CONTENTS:

## Scientific motivation

Description of method and advantages
LBL technical proposal
Optical system and components
Mechanical motions
Signal processing
Model calculations
Noise estimates
Summary of main challenges

TWO-ELECTRON STATES IN HELIUM
Dome et al

$$
\begin{aligned}
& \text { PAL } 66,1306 \text { (1991) } \\
& \text { PRS } 69,1171(1992
\end{aligned}
$$



Minus (antisymmetric) and "d" series.
interference between $N=n$ principle term and the $N-1$ series


FIG. I. Auto ionizing resonances of doubly excited He below the $N=2$ threshold (I P2) of $\mathrm{He}^{+}$

## MOTIVATIONS FOR CONTINUED STUDIES OF HELIUM <br> AND FOR ATTEMPTS AT MUCH HIGHER RESOLUTION

1. THE GENERAL IMPORTANCE OF HELIUM EXPERIMENTS IN STUDIES OF ELECTRON CORRELATION INTERACTIONS

- Important advances made following the SURF experiments in the 1960's (new quantization scheme and selection rules for two-electron systems)
- Generally high level of interest and activity following the BESSY experiments in the 1990's

2. PRACTICAL GOALS NOT YET ACHIEVED DUE TO RESOLUTION LIMITATIONS

- Quantitative measurements on the Rydberg series for higher $\boldsymbol{N}$ and $\boldsymbol{n}$
- More detailed study of the interferences between an $N=n$ term and an $N-1$ series
- Observe and measure Fano parameters for higher members of the antisymmetric series and for the " d " series (not yet done at all)
- Detection and measurement of parameters for corresponding series for $N>2$ (hardly seen so far)
- Effects of applied fields

3. DESIRE TO USE MEASUREMENTS OF HIGHER ORDER EFFECTS AS SENSITIVE TESTS OF THEORETICAL TREATMENTS

FOURIER TRANFORM SPECTROSCOPY


By Weiner-Khinchin theorem. autocorrelation of ot

$$
\begin{aligned}
& I(\tau)=\frac{I(0)}{2}+\int_{0}^{\infty} B(f) \cos (2 \pi f x) d f \\
& \text { desired spectrum }
\end{aligned}
$$



ADVANTAGES OF FOURIER TRANSFORM
SPECTROSCOPY
THROUGHPUT:
Jacquinot advantage
doesu't apply for bright sources

MULTIPLEX:
Fellgett advantage
doesn't apply for a. shot-noise rather than detector -noise-limited system
RESOLVING POWER:

- Equal to number of waves of path difference between the interfering beams
- Can be very high, but spectral range is normally low does apply!

FREQUENCY RANGE TRANSFORMATION:

$$
\begin{aligned}
& I(\tau)=\frac{\dot{I}_{0}}{2}+\int_{0}^{\infty} B(f) \cos 2 \pi f x d f \\
& x=v t, \quad f_{0}-\Delta<f<f_{0}+\Delta \\
& I(\tau) \sim \cos \left(2 \pi f_{0} v t\right) \\
& f_{0}=\frac{1}{\lambda_{0}}=\frac{\nu_{0}}{c} \\
& \sim \cos \left(2 \pi \nu_{0} \frac{v}{c} t\right) \\
& \text { optical reduction } \\
& \text { frequency factor } \\
& \lambda_{0}=100 \AA \\
& v=20 \mu \mathrm{~m} / \mathrm{s} \\
& \downarrow \\
& 1 \mathrm{kH}_{3} \\
& \text { (optical } \rightarrow \text { audio) }
\end{aligned}
$$



BEAMY SPLITTERS


Issues - manufacture: silicon microfab.

- Thermal load
- density driven by order rejection




Figure 2. Construction of traverse units TU used with $\Delta s$ - and $\Delta x$-traverses.

(b)

Deslattes
1969


Figure 2. Linear motion devices used in $P T B$ (a) and NBS (b) measurements of Si 220 lattice periods.


Bild 2. Ansicht der gefertigten Doppelparallelfeder mit Adapter für den Antrieb


Biid 5. Winkeländerung in Abhängigkeit vom Federweg.
Feder in horizontaler Lage, Drehung um die $y$-Achse
I Kraftangriffspunkt $1,77 \mathrm{~mm}$ unterhalb der Mittelachse
II Kraftangriffspunkt $1,47 \mathrm{~mm}$ unterhalb der Mittelachse
III Kraftangriffspunkt $1,22_{1}$ ㄱm unterhalb der Mittel-

FLEXABLE HINGES
better
hinge

lower stress

$$
\begin{aligned}
C(y) & =\frac{\tau_{\text {hinge }}}{\tau_{\text {beam }}}=\frac{2 f^{2}}{\frac{1}{g}+\frac{1}{f^{2}}\left(g+\frac{8 y^{2}}{g}+\frac{12 g y}{f} \tan ^{-1} f\right)} \\
f & =\sqrt{4 y+1} \\
g & =2 y+1 \quad y=p / t
\end{aligned}
$$



ELEMENT SHAPE

$\square$

TORSIONAL RIGIDITY

$$
\tau_{\text {beam }}=\frac{Y b t^{3}}{24 p}
$$

$C(\mathrm{y}) \tau_{\text {beam }}$
$\frac{C(2 y)}{8} \tau_{b e a m}$
$2 C(y) \tau_{\text {beam }}$
$\frac{C(2 y)}{4} \tau_{\text {beam }}$

MAXIMUM STRESS

$$
\sigma_{b e a r i}=\frac{Y t \theta}{4 \rho}
$$

$C(y) \sigma_{b e a m}$

$$
\frac{C(2 y)}{8} \sigma_{b e a m}
$$

$2 C(y) \sigma_{\text {beam }}$
$\frac{C(2 y)}{4} \sigma_{\text {beam }}$


| FATIGUE PROPERTIES OF CANDIDATE FLEXURE MATERIALS |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |
| Class of material | Tool steel | Alloy steel | Maraging steel | Aluminum |
|  |  |  | (Vascomax) |  |
| Type | S7 | 4340 | C-300 | 7075 |
| Tempering temperature ( ${ }^{\circ} \mathrm{F}$ ) | 1000 | 200 | 900 |  |
| Temper designation |  |  |  | T651 |
| Tensile strength (ksi) | 264 | 287 | 294 | 77 |
| 0.2\% Yield strength | 200 | 270 | 287 | 67 |
| Elongation (\%) | 10 | 11 | 10 | 6 |
| Reduction in area (\%) | 33 | 39 | 47 | 12.7 |
| Elastic modulus (Msi) | 30 | 29 | 27.5 | 10.3 |
| Strain range (10^5) universal slopes | 0.008314 | 0.009356 | 0.010160 | 0.006874 |
| Strain range( $10^{\wedge} 7$ ) universal slopes | 0.004488 | 0.005048 | 0.005457 | 0.003801 |
| Fatigue endurance limit (ksi) |  | 140 | 125 | 23 |



$$
\Delta_{\epsilon}=3.5 \frac{\sigma_{u}}{E} N_{f}-0.12+D^{0.8} N_{f}-0.6
$$

where

$$
\begin{aligned}
& \sigma_{u}=\text { ultimate tensile strength, psi } \\
& D=\text { ductility, } \ln \frac{1}{1-R A} \\
& R A=\text { reduction in area, percent } \\
& N_{f}=\text { number of cycles to failure }
\end{aligned}
$$

$$
I(x)=\frac{I(0)}{2}+\int_{0}^{\infty} B(\sigma) \cos (2 \pi \sigma x) d \sigma
$$

Following Chamberlain [2] we represent wavefront errors by allowing $x$ in (2) to be a function of the position ( $u, v$ ) in the aperture and summing the contributions of all the separate "elementary interferometers" corresponding to each area dudv. Thus the total effect when (2) is evaluated is

$$
I(x)=\frac{I(0)}{2}+\int_{0}^{\infty} d \sigma \frac{B(\sigma)}{A} \iint_{A}[1+\cos (2 \pi \sigma x(u, v))] d u d v
$$

where $B(\sigma) / A$ is the power per unit area per unit bandwidth in the exiting beam. If we represent $x(u, v)$ as $x+\delta(u, v)$ then (3) can be written

$$
I(x)=\frac{I(0)}{2}+\int_{0}^{\infty} D(\sigma) B(\sigma) \cos (2 \pi \sigma x) d \sigma
$$

where

$$
D(\sigma)=\frac{1}{A} \iint_{A} \cos [2 \pi \sigma \delta(u, v)] d u d v
$$

$D(\sigma)$ is called by Chamberlain the "spectral distortion factor": a name which makes sense in view of the first of equations (4).

GENERAL TOLERANCE:

$$
D(\sigma)>0.9 \text { for } \sigma=10^{6} / \mathrm{cm}(\text { same as } \lambda=100 \AA) \text { and } R=1 \mathrm{~mm}
$$

## TILT OF ONE OF THE INTERFERING WAVEFRONTS WITH RESPECT TO THE OTHER:

Consider a wavefront tilt of $e$ so that $\delta(v)=v e$. Substituting again into the second of equations (4) we find

$$
\begin{aligned}
D(\sigma) & =\frac{1}{A} \int_{-R}^{R} d v \int_{-\sqrt{R^{2}-v^{2}}}^{\sqrt{R^{2}-v^{2}}} \cos (2 \pi \sigma v e) d u \\
& =\frac{2 R}{A} \int_{-R}^{R} \sqrt{\left(1-\left(\frac{v}{R}\right)^{2}\right)} \cos (2 \pi \sigma v e) d v \\
& =2 \frac{J_{1}(2 \pi \sigma e R)}{(2 \pi \sigma e R)}
\end{aligned}
$$

Where the last line is obtained using a standard integral representation of the Bessel function [3]. Now $2 J_{1}(x) / x$ equals 1 at $x=0$ and falls to 0.9 at $x=0.911$ Thus the condition on $e$ is

$$
e<\frac{0.911}{2 \pi \sigma R}
$$

which for our stated tolerance (5) gives $e<1.5 \mu$ radians. This must be respected during initial alignment of the instrument and held during the motion of the table.


QUALITY OF THE TABLE MOTION


Rotation about
$x$ axis: Initial motion is in the plane (ROLL) OF THE MIRROR $\rightarrow$ SMALL EFFECT

Y AXIS: ANGLE BETWEEN INTERFERING (PITCH) BEAMS IS FOR PITCH $\triangle P$ $8 \triangle P \cos \theta \sin \theta$
$\therefore \triangle P<10^{-6}$ RAD FOR BEAT ANGLE $<1.5 \mu$
Z AXIS: CANCELS TO FIRST ORDER
(YAW) BECAUSE OF DOUBLE REFLECTION (COMPARE PENTAPRISM)

## SUMMARY OF TOLERANCES

## ITEM

Incoming beam:
Angle
Width
Relative tilt of interfering wavefronts
Mirror surfaces:
Slope
Sphericity
Beamsplitter surfaces:
Slope
Sphericity
Moving table:
Pitch
Roll
Yaw

TOLERANCE
$\pm 2.2$ mradian
2 mm (full width)
$1.5 \mu$ radians
$\pm 0.5 \mu$ radian ( 1.0 peak to valley) Radius $>4.6 \mathrm{~km}$
$\pm 1.0 \mu$ radian ( 2.0 peak to valley)
Radius $>2.3 \mathrm{~km}$
$\pm 1.0 \mu$ radian
large
large

SAMPLING CONSIDERATIONS


$$
y(f(x))=F(f)
$$

$$
y\left[f(x) \|\left(\frac{x}{\tau}\right)\right]=F(f) *|\tau| \|(f \tau)
$$


$10 \times$ undersampled

Mestricted band
 OK!

MOMMMDMMYMMMMM.

SAMPLING THEOREMS


Theorem I:
A function $F(t)$ which is bandwidth-limited within a range $2 W$ centered on zero is fully defined by its values $F\left(t_{n}\right)$ at an infinite series of points $t_{n}$ where $n$ is an integer and

$$
t_{n}=\frac{n}{2 W}
$$

and

$$
F(t)=\sum_{n=-\infty}^{n=+\infty} F\left(t_{n}\right) \operatorname{sinc}\left[2 W\left(t-t_{n}\right)\right]
$$

where $\operatorname{sinc}(x)$ is defined as $\sin (\pi x) / \pi x$.
Theorem II:
A function $F(t)$ which is bandwidth-limited within ranges $W$ centered on $f_{0}$ and $-f_{0}$ is fully defined by its values $F\left(t_{n}\right)$ at an infinite series of points $t_{n}$ where $n$ is an integer and

$$
t_{n}=\frac{n}{W}
$$

and

$$
\begin{aligned}
F(t) & =\sum_{n=-\infty}^{n=+\infty} \operatorname{sinc}\left[W\left(t-t_{n}\right)\right]\left\{F\left(t_{n}\right) \cos \left[f_{0}\left(t-t_{n}\right)\right]+\hat{F}\left(t_{n}\right) \sin \left[f_{0}\left(t-t_{n}\right)\right]\right\} \\
& =\sum_{n=-\infty}^{n=+\infty} \operatorname{sinc}\left[W\left(t-t_{n}\right)\right] \sqrt{F\left(t_{n}\right)^{2}+\hat{F}\left(t_{n}\right)^{2}} \cos \left[f_{0}\left(t-t_{n}\right)-\phi_{n}\right] \\
\phi_{n} & =\tan ^{-1}\left(\frac{\hat{F}\left(t_{n}\right)}{F\left(t_{n}\right)}\right)
\end{aligned}
$$

where $\hat{F}(t)$ is the Hilbert transform of $F(t)$.
the complex envelope function


$$
\begin{gathered}
\text { Analytic } \\
\text { signal }
\end{gathered} \hat{R}(\tau)=e^{2 \pi i f_{0} \tau} g(\tau) \longleftarrow \begin{gathered}
\text { complex } \\
\text { envelope }
\end{gathered}
$$

Measured autocorrelation function

$$
\begin{aligned}
& R(\tau)=\sqrt{g_{R}(\tau)^{2}+g_{I}(\tau)^{2}} \cos \left(2 \pi f_{0} \tau+\phi(\tau)\right) \\
& \phi(\tau)=\tan ^{-1} g_{I} / g_{R} \\
& \text { Modulated }
\end{aligned}
$$ carrier wave



## Gaussian Distribution

@65.35 eV, Sigma=0.05 eV,50 $\mu \mathrm{eV}$ Point Density With He Resonance Absorptions, $10 \%$ absorption $2 n+$ series, peaks $9+$ to $60+$


# SUMMARY OF MAIN ISSUES 

## OPTICAL COMPONENT ALIGNMENT

BEAM SPLITTER<br>MOTION QUALITY<br>MOTION DRIVER<br>DETECTOR: SHOT-NOISE LIMITED?

# Some Technical Issues in Implementing the ALS Fourier Transform Spectrometer 

## Zahid Hussain

Lawrence Berkeley Laboratory

## VUV/SOFT X-RAY INTERFEROMETER (ENERGY RANGE $=\mathbf{3 0 - 1 2 0} \mathbf{e V}$ )

- BEAMLINE DESIGN (BL 9.3.2)
- MECHANICAL MOVING STAGE
flexure hinges (M H)
- DRIVING MOTOR

INCHWORM ( 2 Cm TOTAL TRAVEL) WITH ADDITIONAL HIGH RESOLUTION PZT ( $12 \mu \mathrm{~m}$ TRAVEL WITH A RESOLUTION OF BETTER THAN $10 \AA$ )

- INDEXING
mitutoyo laser holoscale linear encoder
RESOLUTION $=10 \mathrm{~nm}$
INTERFEROMETER (HP OR ZYGO)
RESOLUTION $=1.25 \mathrm{~nm}$
- BEAM SPLITTER (GRADING)
$25 \mu \mathrm{~m}$ REFLECTING AND TRANSMITTED WIDTH THICKNESS $=0.5-1.0 \mathrm{~mm}$
- MIRROR

DIMENSION = 5"x1"x1"
FLATNESS < $1 \mu \mathrm{~m}$
ROUGHNESS < $5 \AA$ (RMS)

- DETECTOR

SI BASED VUV/SOFT X-RAY PHOTODIODE

- SIGNAL CHARACTERISTICS (EM)
- MEASURING SCHEME LOCK-IN METHODS (EM)
- DATA ANALYSIS

FT TECHNIQUES (EM)

## The figure below shows the layout for Beamline 9.3.2.






## HYSTERESIS AND CNNEAKITY

PIEZOELECTRIC Devices


CINGARIAY
$\geq 1-2 \%$



INDEXING OF MOTION

1. Laser holoscale linear encoder

TWO BEAM InTERFEROMETER (MIGAGL SUN- TYpE) USES MOCOGRAPHC DIFFRACTION GRATINC (2000 \% /
High a Resolution $=10 \mathrm{~mm}$ ( $100 \dot{A}$ )
Presently not una compatible


FIGURE 4. SCALE ALIGNMENT I


WEED In sha AOJUSTAE To Align.

| SCALE VERTICAL POSITION | 1 mach from the moraine bess $\pm 150$ inch |
| :--- | :---: |
| PITCH | $\pm 12$ are min |
| ROLL | $\pm 25$ are min |
| YAW | $\pm 12$ arc min |

TABLE 4. POSITIONAL DEVIATION SPECIFICATION
2. It P un z.y co INTERFEROTESER

Resolution: 1.25 nm
UAV Comprtirs.if


$$
\begin{aligned}
& \Rightarrow P 2 T-8: \\
& \text { EXTENSIONA }=0-12 \mu \mathrm{~m} \\
& \text { FOR }=0-100 \mathrm{~N} \text { VOLT } 5 \\
& \text { CANEARITY }-2 \%
\end{aligned}
$$

Hammert tee RST: $x^{64} 308(1992)$


Fig. 1 Inchworm motor operation

UNCCAMA 3


Time
ULTRA LOW NOISE
DRIVE SIGNAL

- inchinorm 3 Pze segions
- O-S00Vocss NoISE CEVEL $\leq 2 m V$ RMs (<0.02t

$$
\Rightarrow \begin{aligned}
& \text { STEP SIZE } \$ 0.6 \mathrm{~A}^{\circ}(16 \mathrm{BIT} \mathrm{BACI} \\
& \text { VARIARLE }
\end{aligned}
$$

JERKINC OF VARIABLE GAIN Q-200
IWHWORM AVOIDEO BY APPLYRACG RAMPING VOLTA TO CLAMPS INSTEROOFON/ OFF.

- THAEE DISTINCS O-SOOVOLTS WUVEFARMA RES. To curimon clearence conpenisciran ar fixen Potentare ( $\neq 0$ ).
- CONTROLCED REVERSE METIEN (~.O5 Mm) WHEN BOTH:



Fig. 5 Inchworm Motion Profile at a Clamp Change

BURLEIGH ARIS-10S
INGTWORA WITH. 12 um travel Pt RESOLUTION $=0.5 \mathrm{~A}^{\circ}$



DETECTOR
Silicon Photodiode (HIGELY SUITABLE IN THE 30-120 eV RANG,
(Anti refgeting.
Passivatinc
CAYER)

a) Si-np-Diode

- high QuAntum efficiency

$$
\simeq \frac{E \text { (Photon) }}{3.8} \text { e-h pain }
$$

- HIGH STAB/C/TY UP to $2 \times 10^{14} \mathrm{Mhotar} / \mathrm{am}^{2}$
- UHV COMPRTIBL/JY
- Active arga $\simeq 100 \mathrm{~mm}^{2}$


# Fourier Transform Soft X-Ray Spectroscopy (FT-SX) 

E.J. Moler<br>Lawrence Berkeley Laboratory

# Fourier Transform Soft X-Ray Spectroscopy (FT-SX) <br> E. J. Moler 

Workshop- June 25, 1993

## OUTLINE

- Expected Signal Characteristics
- Fundamental Requirements for Absorption Spectroscopy in the 65 eV Region (He N=2 double excitation series \& more)
- Data Collection \& Analysis
- Signal Collection Scheme


# Fundamental Requirements 

## for $\mathrm{He} \mathrm{N}=2$ Double Excitation Series

 $\sim 65.5 \mathrm{eV}$
## Sampling Rate/Energy Range

- "Beat" Envelope Max. Frequency

$$
\begin{aligned}
& \Delta \mathrm{E}=0.17 \mathrm{eV}(\mathrm{n}=9+\text { to } \mathrm{IP} 2)=> \\
& \lambda=1.24 \mathrm{eV} \cdot \mu \mathrm{~m} / 0.17 \mathrm{eV}=7.3 \mu \mathrm{~m}
\end{aligned}
$$

- Nyquist Sampling Rate $7.3 \mu \mathrm{~m} / 2=3.6 \mu \mathrm{~m}$


## Sampling Range/Resolving Power

- 1 cm travel =>

$$
\begin{aligned}
\text { Res. } & =1.24 \mathrm{eV} \cdot \mu \mathrm{~m} /(2 * 10,000 \mu \mathrm{~m}) \\
& =65 \mu \mathrm{eV}
\end{aligned}
$$

- $\mathrm{E} / \Delta \mathrm{E}=65 \mu \mathrm{eV} / 65 \mathrm{eV}=1$ million !

Maybe can double using mirror symmetry
Resolving Power $\quad \mathrm{n}_{\text {max }}$ Observable
1,000,000 $\quad \sim 71$ ( 21 current max̀)
750,000
500,000 65 56

- Min \# Data Points $=10,000 \mu \mathrm{~m} / 3.6$ $=2778$


## Positioning Accuracy and Resolution

- Absolute Positioning Accuracy

For envelope "peak" w/in $1 \%=>$ accuracy $\sim \lambda / 22=7.6 \mu \mathrm{~m} / 22=345 \mathrm{~nm}$

- Positioning Precision finding average freq. "peak" within $1 \%$
$\Rightarrow \quad 19 \mathrm{~nm} / 22=8.6 \AA$


## Data Collection and Analysis

- Measure Envelope Amplitude,
- Use known "average" frequency as set by monochromator band pass,
- Fourier Transform

Question: What are uncertainties introduced by assuming an average frequency which may be incorrect by e.g. $0.15 \%$

## Signal Collection Scheme

- Low signal/background ratio implies lock-in technique,
- Noise levels cannot be known in advance, but can be estimated.
- 5500 points in 6 hrs $\sim 4$ secs/point - acquire position, - "count"

Gaussian Distribution
$@ 65 \mathrm{eV}$, Sigma=1.0 eV
2 meV Point Density, Normalized


> Gaussian Distribution $@ 65 \mathrm{eV}$, Sigma $=1.0 \mathrm{eV}$ 2meV Point Density, Normalized With Sharp Absorption
> @65 eV, 2 meV Wide (1 channel)



Gaussian Distribution<br>$@ 65 \mathrm{eV}$, Sigma $=1.0 \mathrm{eV}$<br>2 meV Point Density, Normalized<br>With Sharp Absorption<br>$@ 65 \mathrm{eV}, 2 \mathrm{meV}$ Wide (1 channel)




## FT-SX Mirror Positioning and Signal Detection <br> Eddie Moler June, 1993

This note describes the important parameters and requirements for a high resolution ( $>300,000$ ) photoabsorption measurement of the He double excitation resonances $a t=65 \mathrm{eV}$ using the Fourier Transform - Soft X-ray (FT-SX) spectrometer. A scheme for signal detection and measurement is then proposed which will address the significant problems of signal/noise and signal/background ratios, accuracy and precision of the mirror positioning system, and time limitations for acquiring the full interferogram.

## Parameters and Requirements

Two parameters of fundamental importance in FT spectroscopy is the necessary sampling rate (points per unit distance) and range (total path-length-difference introduced) to achieve a given resolution and energy range. These parameters are dictated by the energies and energy differences of the expected spectral features. For interferometry in the X-ray region, the practical aspects of achieving the required accuracy and precision in introducing the path-length-differences and dealing with the expected signal characteristics are also critical in determining the resolution and energy range of the instrument. In this note, I consider the requirements for measuring the helium double excitations below the $\mathrm{N}=2$ ionization threshold.

## Sampling Rate / Energy Range

The wavelength of light at the $\mathrm{N}=2$ ionization threshold for helium, 65.4 eV , is $\approx$ 19 nm . This is the carrier wave of the absorption interferogram whose envelope we wish to measure. We deliberately limit the bandwidth of the light source so that only the envelope of the carrier wave need be measured. There are also advantages in the signal/ background ratios when limiting the band width. Figure 1 shows the Fano resonance profile for $N=2$, peaks $n=9+$ to $60+$. Note that the intensities of the peaks should all be the same, but in sampling a continuous curve discretely leads to "missing" the peak position. This does not affect the qualitative features of the simulation. Constraints presented by computer memory and computation time prevents a higher resolution simulation. Figure 2 shows the source gaussian and its expected interferogram. Figures 3,4 , and 5 show the interferogram of the source with a $10 \%$ peak Fano absorption profile with ranges of 15 to 100,500 , and $1000 \mu \mathrm{~m}$ path length differences, respectively. The envelope consists of the beat frequencies in the absorption lines which can be described by $\cos [(a-b) x]$ where " a " and " b " are the frequencies of two absorption lines. This relationship may be used to determine the minimum expected "envelope wavelength" and thus the minimum sampling rate as dictated by the Nyquist theorem. I choose the $n=9+$ peak as the first peak of interest because it is within the bandwidth of a 100 meV gaussian source peak centered at 65.35 eV , which has significant intensity at the IP2 threshold ( 65.40 eV ). The $\mathrm{n}=9+$ absorption line (in $\mathrm{N}=2$ ) is approximately 0.17 eV below the IP2 ionization threshold. The higher " $n$ " peaks' energies converge to the ionization threshold. Thus, 0.17 eV is the maximum spacing between the $9+$ peak and any other peaks higher in energy. The "wavelength" of the shortest envelope wave is then,

$$
\lambda=1.24 \mathrm{eV} \cdot \mu \mathrm{~m} / 0.17 \mathrm{eV}=7.3 \mu \mathrm{~m}
$$

Applying the Nyquist theorem gives a sampling rate of,

$$
\Delta x_{\max }=3.6 \mu \mathrm{~m}
$$

## Positioning Accuracy and Precision

To obtain the envelope amplitude peak within $1 \%$, one would like a positioning accuracy of $\pm 1 / 44$ wavelength, or $1 / 22$ of the beat wave $\lambda$. This corresponds to an accuracy of 332 nm for the $\mathrm{n}=9+$ to IP2 threshold. To include peaks out to the $\mathrm{n}=2+$ (@ $\sim 65.0 \mathrm{eV}$ ) would require a sampling rate that is a factor of 30 higher ( $5.2 \mathrm{eV} / .17 \mathrm{eV}$ ) and thus would require a positioning accuracy of 11 nm . Relaxing the envelope amplitude determination to within $3 \%$ requires an accuracy of $\pm 1 / 26$ wavelength, or 561 nm and 18.7 nm for $\mathrm{n}=9+$ and $2+$, respectively. There is the additional problem of the precision of the mirror positioning because the envelope amplitude must be measured across the carrier wave peak. This puts our precision requirements at $1 / 22$ of 19 nm or .86 nm .

## Sampling Range / Resolving Power

The energy resolution is determined by the maximum path length difference introduced. A design goal of a resolving power on the order of 1 million was taken as an ideal limit. The currently proposed design allows for a path-length-difference of 6.7 mm (see M. Howells, design note 1-28-93). This gives an energy resolution of,

$$
\Delta \mathrm{E}=1.24 \mathrm{eV} \cdot \mu \mathrm{~m} /(2 \cdot 6.7 \mathrm{e}+3 \mu \mathrm{~m})=92.5 \mu \mathrm{eV}
$$

and a resolving power of,

$$
\mathrm{E} / \Delta \mathrm{E}=65.4 \mathrm{eV} /(92.5 \mathrm{e}-6 \mathrm{eV})=700,000
$$

In principle, the resolving power could be doubled by making use of the mirror symmetry of the interferogram about the zero path-length-difference (ZPD) position, giving a resolution of 1.4 million (!), provided that the ZPD position was at one end of the travel. Based on the tabulations of resolving power and the number of peaks observable in Domke, Shirley, Kaindl, et al. (PRL march 11,1991, p 1306) and the fact that the peak widths go down as $1 / \mathrm{n}^{3}$ I can estimate the number of peaks for $\mathrm{N}=2$ we could expect to see with various resolving powers.
Using,

| $\mathrm{n}_{\text {max }} \approx(0.360 * \text { resolving power })^{1 / 3}$, |  |
| :--- | :--- |
|  |  |
| Resolving Power nmax observed <br> 350,000 50 <br> 500,000 56 <br> 750,000 65 <br> $1,000,000$ 71 |  |

A travel of 6.7 mm , with a sampling rate of $3.6 \mu \mathrm{~m}$, means acquiring $\sim 2000$ data points. To include peaks out to the $\mathrm{n}=2+$ (@ $\sim 65.0 \mathrm{eV}$ ) would require 60000 data points at the same resolution.

## Requirements Summary

For $\mathrm{N}=2$ double excitations of $\mathrm{He}^{+}$, considering very high resolution, including peaks $\mathrm{n}=2+$ to IP2 or $\mathrm{n}=9+$ to IP2,

Total Travel
Sampling Rate
Absolute Positioning Accuracy Positioning Resolution
Total Data Points Measured
6.7 mm
.12-3.6 $\mu \mathrm{m}$
$11-332 \mathrm{~nm}$
0.86 nm

2000-60,000

## The Proposed Mirror Positioning and Signal Detection Scheme

The stringent requirements on the mirror positioning and drive system, along with the extremely small signal/background ratios of the absorption spectra require substantial deviations in design and measurement technique from previous interferometers. Because the signal detection scheme and the mirror drive mechanisms are inherently intertwined, they must be considered together. As we will see, there are ways of taking advantage of these relationships.

The proposed positioning and detection scheme utilizes a modulation of the mirror positions and a lock-in amplifier to extract the resulting amplitude and phase of the time varying signal from the photo-detector. The modulation frequency must be selected to minimize the noise content of the signal while still matching the response characteristics of the photo detector and subsequent amplifiers. In addition to greatly increasing the signal/noise ratio, a problem made apparent by the simulations in figure 5 , the phase of the signal can be used as a very precise position monitor. This will be described below. The reader is urged to read the attached analysis of the lock-in technique and expected outputs.

The following sections will address the methods of meeting the requirements inherent in obtaining a high resolution Fourier transform spectrum in the soft X-ray region.

## Signal/Noise Ratio Improvement

## Noise Sources

The critical aspect of measuring the interferogram signal is the uncertainty associated with each data point. The noise associated with the signal is the source of this uncertainty. The primary sources of noise are:
a) johnson noise, associated with thermal motions of electrons in a resistor,
b) shot noise, associated with the motion of the discreet electrical charges,
c) flicker or $1 / \mathrm{f}$ noise, resulting from variations in the electrical characteristics of materials which are proportional to the DC current flowing through them, and
d) interference, from electrical and mechanical pickup of nearby sources of em radiation,
e) inaccuracy in the signal determining parameters, e.g. mirror positions.

Only the first three, the signal noise, will be considered here. The others will be addressed elsewhere in this note.

The frequency spectra of each of these three distributions is interesting. The johnson and shot noise are "white noise", i.e. they have equal noise power at each frequency (up to some very high limit, of course). The $1 / \mathrm{f}$ noise has equal power per decade, it is sloped on a log scale and has approximately a $1 / \mathrm{f}$ distribution. Below 100 Hz , the $1 / f$ noise dominates over the others except at certain frequencies where the interference from nearby sources can have a very "spiky" nature. The interference signals are typically from the line noise, having frequencies of 60 Hz and the first few harmonics. These signals are particularly important to avoid and filter.

## Band-width Reduction

The method of dealing with these uncertainties in practice can be all placed under the strategy of "band-width narrowing". The simplest of band-width narrowing techniques is signal integration. Basically, the longer you count, the better your signal/noise ratio because while the signal grows with counts, the noise grows with $\sqrt{ }$ counts. Counting for a time $t$ means reducing the band-width $\Delta f$ to $1 / t$. The band-width begins at zero frequency, thus the most intense portion of the noise spectrum accompanies the signal for even very long counting times. Ideally, one would want to 1) shift the signal of interest up in frequency away from the $1 / \mathrm{f}$ and interference noise, and 2) impose a band-width that is centered on the signal and thus excludes all of the noise in the signal except for a very small contribution that is "beneath" the signal.

The Lock-in Technique
The lock-in technique is a sophisticated form of band-width limiting. The lock-in amplifier multiplies the incoming signal with a reference signal and passes the result through a low pass filter. This results in a rejection of very large portions of the noise spectrum without integrating for impractically long times, mainly by avoiding the lower frequency noise, where most of the noise power is. The band pass is determined by the time constant in the low pass filter, $\Delta \mathrm{f}=1 / 2 \pi \mathrm{RC}$ and the time for the filter to get within $99.3 \%$ of its final value is 5RC. Thus, the expected noise characteristics and the required accuracy of the signal determines the desired time constant and the "acquisition" time for one data point. A selectable time-constant range of 1 ms to 100 s is common in commercial lock-in amplifiers. In addition, the phase of the signal relative to the reference can be measured quite accurately.

## Signal Collection

The proposed method to acquire one data point is as follows (assuming one begins within 1 wave of the desired position. How to get there is described later):

- Impose a triangular modulation on the mirror position via the linear piezo actuator. The displacement of the piezo is assumed for now to be known exactly and set to $1 / 4 \lambda$. The correct phase factor in the lock-in is also assumed to be known. The modulation signal is also the reference signal for the lock-in amplifier,
- Using a lock-in amplifier in 2 f mode, move the mirrors to where the output of the lock-in is zero,
- Using a lock-in in 1f mode, wait 5 RC and measure the output signal. This signal is within $0.7 \%$ of the final output value. The positioning accuracy also places the output within $1 \%$ of the true maximum (see mirror positioning discussion, below). This method is far superior to the proposal to integrate the signal at several points across the wave to find the peak. In addition to the signal/noise ratio improvement, it also has the added benefit of allowing rapid determination of the carrier wave peak position by using the zero crossing of the 2 f mode lock-in amp as described in the mirror positioning section.

Finding the correct values for the phase and peak-to-peak displacement involve maximizing the lock-in output by searching the phase-displacement-position parameter space. This need only be done once unless the voltage/expansion characteristics of the linear piezo actuator change drastically. It may be necessary to avoid large expansions of the piezo to prevent hysterisis. The search can proceed rather quickly if one is judicious in selection of the search method. The reader is referred to the output surfaces in the back of the lock-in analysis attachment.

## Mirror Positioning

The requirements of length of travel and accuracy of positioning have been solved in the past, for IR and visible FT spectroscopy, by using a continuous drive lead-screw or gearing mechanisms. The relatively long wavelengths of visible and infra-red light are easily handled with a precision machined screw. However, the short wavelengths of Xrays demand accuracy and resolution in positioning that are not amenable to current machining technology. Thus, we have selected piezo-electric "inchworm" motors to drive our translation stage. These are readily available as they are the same drives used in STM for allowing the metal tip to approach the sample. Still, the position measurement is critical and is addressed below.


#### Abstract

Absolute Accuracy By absolute accuracy, I mean how closely to a desired absolute position can the mirror be placed. The current solution to this is to use a Mitutoyo holoscale linear encoder fixed to the translation stage of the interferometer. The resolution of the encoder is claimed to be 10 nm and the linearity is $\qquad$ For the currently proposed translation stage, 10 nm travel corresponds to -7 nm of path length difference. This easily meets the accuracy requirements of 332 nm for the $\mathrm{N}=2$ resonances starting with $\mathrm{n}=9+$. For including peaks down to $n=2+$ the required accuracy still is sufficient. The consequence of the encoder linearity errors on the measured spectrum will be to introduce an uncertainty in the energy calibration of the spectrum of the same magnitude. The inchworm motor drives are capable of 4 nm steps, thus allowing the desired encoder position to be achieved.


## Positioning Resolution

Resolution refers to the smallest amount of motion we can move the mirror by reliably. The resolution is important because we wish to measure the amplitude of the peak of the carrier wave with a wavelength of 19 nm . The linear encoder gets us to within $1 / 2$ of a wavelength of the desired position. To allow high resolution positioning of the mirrors, we will use a piezo actuator with very good linear expansion characteristics. The above mentioned inchworm motor can clamp and hold it's position while the piezo crystal is used for high resolution motion. With and expansion of $12 \mathrm{~nm} /$ Volt, a stability of sub-angstrom position is achievable. In addition, the position modulations will be easily implemented with high precision with a standard laboratory wave form generator.

The signal output from the lock-in amplifier is extremely sensitive to the average position of the mirrors, as seen from the lock-in "output surfaces" in the attached analysis
of the lock-in technique. I proposed that we use the zero crossing of the output of the lockin in 2 f mode to find the exact position of the carrier wave with very high precision. The slope of the output with position is highest at the zero crossing, thus providing the most precision in maintaining that position. At the zero crossing in 2 f mode, the 1 f mode output is the amplitude of the carrier wave. This is a direct consequence of the fact that the $2 f$ output is the derivative of the 1 f signal. A lock-in output at $0.0 \pm 3.5 \%$ of the maximum output amplitude results in a (average X0) position within $\pm \lambda / 44$ or $4.3 \AA$. This meets the precision criteria quite well and I believe is realistically possible. It is also possible to use this system in a closed-loop positioning mode, maintaining the position despite creep in the piezo actuators real position.

## The Data Acquisition Algorithm

The question of how to acquire the entire interferogram depends on the number of data points and the time scale of acquiring one data point. There are two possible methods, the continuos-pickoff and the step-creep-sit methods. A schematic of the data acquisition system is shown in figure 6.

## The Continuos-Pickoff method

The basic idea here is to slowly scan the mirror position and when there is a zerocrossing in the $2 f$ lock-in read the output of the 1 f lock-in amplifier. Of course, there must be breaks in the scan every $10 \mu \mathrm{~m}$ as the end of the piezo travel is reached. The linear encoder can allow repositioning within $1 / 2$ a wave, so this should not be critical. The main concern with this method is the trade-off between scanning rate and the low-pass filter time constant. A larger time constant gives a better accuracy of the output, but also limits the rate at which the amplifier can adapt to changing signals. For a scan of 7 mm to be done in 6 hrs determines a scan rate of $324 \mathrm{~nm} / \mathrm{sec}$ or 1 wave/ 61 msecs. If we wish to find the peak amplitude within $1 \%$ we can average the signal as it passes over the top $2 \%$ of the peak. This corresponds to $1 / 15$ of a wave and thus sets the time constant of the low pass filter to

$$
\begin{aligned}
& \lambda(15 * 5 \mathrm{RC})=\text { scan rate }, \\
& \mathrm{RC}=\lambda(75 * \text { scan rate })=0.82 \mathrm{msecs}
\end{aligned}
$$

which give a band width of

$$
\Delta \mathrm{f}=1 / 2 \pi \mathrm{RC}=203 \mathrm{~Hz}
$$

This is not acceptable, so this method does not seem feasible in this "pure" continuous form for the high resolution measurements. This method could have advantages where the required resolution is less by a factor of 50 or more, particularly if the signal is not bandlimited as it is for the He absorption experiment. Of course, the noise power per unit root band-width must always be taken into account in determining an acceptable time constant. It should be noted that a time constant of 637 msecs gives a band width of 1 Hz .

This method has the advantage of avoiding the uncertainties in energy position
associated with the properties of the linear encoder. This may not be critical, though, anyway. In addition, this "fringe-counting" method may be very useful in measuring the linearity and resolution of the encoder as well as the piezo actuator. If the linearity of the encoder is known, this can be accounted for. The calibration and hysterisis measurement of the piezo actuator is also useful information to have.

## The Step-Creep-Sit Method

By taking advantage of the band-limited light source, we do not have to measure every peak (positive and negative) amplitude, but need only sample the envelope, which substantially reduces the required sampling rate. The acquisition algorithm here, then, would be to take a large step using the inchworm motor, and then creeping to the 2 f zerocrossover to take the signal measurement by waiting 5 RC . If we wanted to measure 4000 data points over 6 hrs, this allows 5.4 secs/point to find and measure it. This should give very accurate results. Assuming that the peak position could be found in 1.5 secs, the allowable time constant of $4 / 5$ gives a band width of 0.2 Hz , probably more than enough. Conversely, if we wish to have a band-width limit of $1 \mathrm{~Hz} \rightarrow \mathrm{RC}=.64$ secs, the entire high resolution interferogram would take under 4.5 hrs . This seems reasonable. Depending on the noise characteristics of the signal, larger band-widths may be usable, allowing more data points to be collected in the reasonable time frame of $6 \mathrm{hrs} .60,000$ data points would mean .36 secs/point to find the peak and make the measurement. This may be very difficult to do with high accuracy in the measurements.

It should be noted that while positioning using the carrier wave as a reference is necessary and desirable, the exact frequency of the carrier wave is only known to within certain limits, since it is the weighted average of the frequency of each absorption line. This is where the narrow band-width of the source is particularly important. For 100 meV FWHM at 65.5 eV , the uncertainty in the possible frequency of the carrier wave is .1/65.5 $=.15 \%$. This is not too bad, as that is then the uncertainty in the energy calibration of the transformed spectrum. For a 5.00 eV FWHM, the uncertainty is $7.6 \%$. Some prior knowledge of the peak spacing and widths can be used to reduce the uncertainty in this case, though. The linearity of the linear encoder can also affect this uncertainty if the error in a single step is greater than the wavelength of the carrier wave. For a step size of 3.6 um and a carrier wave of 20 nm a linearity of $0.5 \%$ or better is required to get to the exact wave we want. For measuring the $\mathrm{n}=9+$ and above peaks, the positioning accuracy required is 332 nm . This is a linearity of better than $9 \%$, which is far worse than the encoder's claimed value. In general, one would like to have a linearity better than $1 / 22$ of twice the sampling rate to measure an envelope peak amplitude within $1 \%$ of the "true" amplitude.

## Conclusion

The very high resolution measurement of the He double excitation resonances are feasible using the proposed positioning and measurement scheme. The lock-in amplifiers' outputs provides a high signal/noise ratio in measuring the amplitude of the signal while the phase information allows very precise positioning of the mirrors, with real-time feedback if necessary. The data collection time is reasonable when making use of the band-width limited source to reduce the sampling rate and allowing a longer signal averaging of the lock-in output.

Fano Resonance Simulation $\mathrm{N}=2+, \mathrm{n}=9-60,50 \mu \mathrm{eV} /$ chan 65.15 eV to 65.55 eV Range



Some issues still left to consider (wrt mirror positioning and signal detection) are:

- Detector selection: we must keep in mind the time response characteristics of both the detector and any amplifiers subsequent to it necessary for the modulation technique to work and the noise characteristics which in part determine the required low-pass filter time constants, thus the acquisition time per data point,
- Minimizing the external noise interference by use of short, low noise cables, etc.,

Gaussian Distribution

## @65.35 eV, Sigma $=0.05 \mathrm{eV}, 60 \mu \mathrm{eV}$ Point Density




## Gaussian Distribution

@ 65.35 eV , Sigma= $0.05 \mathrm{eV}, 50 \mu \mathrm{eV}$ Point Density
With He Resonance Absorptions, $10 \%$ absorption $2 \mathrm{n}+$ series, peaks $9+$ to $60+$


# Gaussian Distribution 

 @ 65.35 eV , Sigma= $=0.05 \mathrm{eV}, 50 \mu \mathrm{eV}$ Point Density With He Resonance Absorptions, $10 \%$ absorption $2 \mathrm{n}+$ series, peaks $9+$ to $60+$



First, the modulation signal and interferogram signal will be considered. Then, the resulting modulated interferogram signal and lock-in output will be analyzed.

## The Modulation Signal

We modulate the mirror position with a triangle function which varies from +1 to -1 over $t=1$. The time and frequency units are arbitrary.

$$
\operatorname{Tri}(f, t):=1-4 \cdot f \cdot \mathrm{if}\left(\bmod \left(t, \frac{1}{f}\right)<\frac{1}{2 \cdot f}, \bmod \left(t, \frac{1}{2 \cdot f}\right), \frac{1}{2 \cdot f}-\bmod \left(t, \frac{1}{2 \cdot f}\right)\right)
$$

For example, $f:=1 \quad t:=0, .01 . .2$


## The Interferometer Signal

The interferometer signal as a function of path length displacement is a small cosine like function on a large background. The cosine-like function is the carrier wave and we are interested in the amplitude of the carrier wave across one peak. As an example,

$$
I_{0}:=1 \quad x:=-2,-1.99 \ldots 2 \quad A:=1
$$

$$
I_{s}(x):=A \cdot \cos (2 \cdot \pi \cdot x)+I_{0}
$$



The amplitude A is what we are interested in ultimately extracting. One should note that the signal/background ratio in the real system will be typically $<0.1 \%$.
The signal is AC coupled to the electronics and thus the time-averaged signal is subtracted out. This means that if the mirrors are stationary, only transient noise will be recorded with time. If the mirrors are moving in an oscillatory mode, the time averaged signal across the oscillation amplitude (delta-x) will drop out.

## The Modulated Interferometer Signal

We next explore the effect of applying the modulation to the interferometer position to get a time varying output from the photo-detector. There are two parameters of interest here, the average X position of the mirrors, X 0 , and the peak-to-peak maximum displacement induced by the modulation, D. We can define the position as a function of time by,

$$
X(D, X 0, T):=X 0+\frac{D}{2} \cdot \operatorname{Tr}(f, T)
$$

We assume that $\mathrm{f}:=1$ for the following.
The time varying output of the detector can now be expressed as a function of time, position, and displacement as,

$$
\begin{aligned}
& 10(D, X 0):=\int_{0}^{\frac{1}{f}} I_{s}(X(D, X 0, T)) d T \\
& I_{\bmod }(D, X 0, T):=I_{s}(X(D, X 0, T))-I O(D, X 0)
\end{aligned}
$$

Where 10 is the DC baseline of the detector signal over which the oscillation takes place. To understand where the time varying signal comes from, refer to the picture of the interferometer signal as a function of " X " below. If X 0 , the average position of the mirrors, is centered at the $1 / 4$ period point, and the total displacement, D is $+1 / 8$, then the time varying signal will oscillate back and forth between the points marked D/2 and -D/2.

D := 25.
$\mathrm{X} 0:=0.25$
$\mathrm{T}:=0, .05 . .2$



Increasing the peak to peak displacement of the modulation to exactly $1 / 2$ of a wave gives a perfect cosinusoidal signal output with time.

D := . 5
$\mathrm{X} 0:=0.25$
$\mathrm{T}:=0, .05 . .2$


Shifting X0 over to center on the top of the carrier wave peak gives a time varying output that is twice the modulation frequency as it traces back and forth over the "hump" for each period of the modulating signal.

$$
\text { D := . } 5
$$

$\mathrm{X} 0:=0.0$
$\mathrm{T}:=0, .05 . .2$



The Lock-in Technique and Output
The lock-in amplifier multiplies a reference cosine-wave, I-ref, and the AC coupled signal, I-s, and gives as an output the time-averaged product. Typically, the reference cosine-wave is locked with great precision to the periodic modulation wave imposed upon the experiment. A phase shift between the modulation signal and the reference wave can also be introduced with great accuracy. The signal wave is AC coupled to a high gain, low noise AC amplifier and several different filters before multiplication. The lock-in technique can be extremely sensitive to small signals and can reject very large signals that are not of the frequency of interest, thus greatly enhancing the signal/background and signal/noise ratios.

We can write the output of the lock-in amplifier as the time average of the product of the phase-shifted reference cosine-wave and the modulated input signal,

$$
O(\mathrm{ff}, \mathrm{nf}, \mathrm{phi}, \mathrm{D}, \mathrm{XO}):=\frac{\int_{0}^{\mathrm{nf}} \cos (2 \cdot \pi \cdot \mathrm{ff} \cdot \mathrm{~T}+\mathrm{phi}) \cdot \mathrm{I}_{\bmod }(\mathrm{D}, \mathrm{X} 0, \mathrm{~T}) \mathrm{dT}}{\mathrm{nf}}
$$

where ff is the reference frequency, nf is the integration limit, and phi is the phase shift of the reference relative to the modulation signal after adjusting for the phase delays of the detector amplifiers, piezo amplifiers, and any other intervening electronics. It is assumed here that any frequencies close to but not exactly ff will be properly averaged after nf periods of the reference frequency. For all calculations and examples below, ff will be set to f , the modulation frequency, since this is the point of introducing the modulation in the first place, to use the lock-in amp to extract the signal intensity. It is useful to note that

$$
\mathrm{O}=\mathrm{A}^{*} \sin (\mathrm{phi}) / 2
$$

for I-mod $=A^{*} \cos \left(2^{*} \pi^{*} f^{*} T\right)$. Thus, the output is proportional to the amplitude of the peak and the $\sin$ of the phase angle between the two waves.

It is interesting to see the lock-in output as a function of relative phase angle phi for the optimum case of an exact cosine signal from the modulated interferometer signal, i.e. a displacement of $1 / 2$ a wave (peak to peak) and an average position $1 / 4$ of a wave from the top of the "hump".
$D:=.5 \quad \mathrm{X} 0:=0.25 \quad \mathrm{~T}:=0, .05 . .2 \quad$ phi $:=0, .5 .2 \cdot \pi$


As expected, the output looks like $\sin (\mathrm{phi})$.

It is more interesting to observe the lock-in output as a function of average position, X 0 , since this is how it is proposed that the precise positioning of X0 is done. Here we assume ideal phase adjustment and displacement.
D := . 5
$\mathrm{X} 0:=0, .1 . .1$
$\mathrm{T}:=0$
phi $:=\pi$


Not surprisingly, the X 0 also produces a $\sin \left(2^{*} \pi^{*} \mathrm{~d}\right)$ output in the lock-in, where d is the fraction of a wavelength of the carrier wave.

If the lock-in reference wave phase is shifted 90 degrees from optimum, the output is zero.
D := . 5
$\mathrm{X} 0:=0, .1 . \mathrm{I}$
$\mathrm{T}:=0$
phi $:=\frac{\pi}{2}$


With the hope of finding an algorithm for precise positioning of the mirrors on the carrier wave, below is shown the lock-in output as a function of reference wave phase shift, phi $=0 . .2 \pi$, and center position, $\mathrm{X} 0=0 . .1$ wavelengths.

$$
\begin{aligned}
& N:=10 i:=0 . . N \quad j:=0 \ldots N \quad x_{i}:=\frac{1}{N} \cdot i \quad p_{j}:=2 \cdot \frac{\pi}{N} \cdot j \\
& x 0 \_p h i_{(i, j)}:=O\left(f, \frac{3}{f}, p_{j}, D, x_{i}\right)
\end{aligned}
$$


x0_phi

There are four nodal lines on this "output surface" where the output is zero. Two are along the constant lines $\mathrm{X} 0=0$ and $\mathrm{X} 0=0.5$, corresponding to sitting at the extrema of the carrier wave. The other two are along lines of constant phi, at phi $=\pi / 2$ and $\mathrm{phi}=3 \pi / 2$. There are also four lines of maximum fluctuation, $X 0=0.25,0.75$, and phi $=0, \pi$.

Next consider the lock-in output surface again vs. X 0 and phi, but with doubling the reference frequency relative to the modulation frequency

$$
x 0 \_p h i \_2 f_{(i, j)}:=O\left(2 \cdot f, \frac{3}{f}, p_{j}, D, x_{i}\right)
$$



Are there nodal lines on this surface?
D := . 5
$\mathrm{X} 0:=0, .1 . .1$
$\mathrm{T}:=0$
phi $:=\frac{\pi}{2}$


Yes, there are nodal lines along the constants $\mathrm{X} 0=0.25,0.75$, and $\mathrm{phi}=\pi / 2,3 \pi / 2$.

The four lines of maximum amplitude are $\mathrm{X} 0=0,0.5$, and $\mathrm{phi}=0, \pi$. It is useful to recall that using the 2 f reference frequency in the lock-in gives the derivative of the If output. Thus, the 2 f surface is still harmonic, but shifted by 90 degrees from the 1 f surface, along each axis. This means that where there is a peak in the If surface, there is maximum slope in the $2 f$, and vice versa. This will contribute greatly to the positioning precision and signal detection scheme

Next we consider the lock-in output surface as a function of position, X0, and displacement, D . We assume optimum phase for maximum output signal at $\mathrm{D}=1 / 2$.

$$
\begin{aligned}
& d_{j}:=\frac{2.0}{N} \cdot j \\
& x 0 \_D_{-} f_{(i, j)}:=O\left(f, \frac{3}{f}, \text { phi }, d_{j}, x_{i}\right)
\end{aligned}
$$


x0_D_1f

Also, look at output surface for $2 f$ lock-in reference mode, for X 0 and D

$$
x 0 \_D \_2 f_{(i, j)}:=O\left(2 \cdot f, \frac{3}{f}, p h i, d_{j}, x_{i}\right)
$$


x0_D_2f

# Application of Hard X-Ray Interferometry 

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The ANL/APS Effort in
Hard X-Ray Fourier Transform Techniques
1: Scientific Applications:
Fourier transform spectroscopy
Fourier transform in aging of surfaces and interfaces
Real-time spectroscopy
Real-time in aging of surfaces and interfaces

2: Fourier transform spectrometers:
Amplitude-division
wavefrant-division

Basic principle of x-ray reflectivity technique

Incident beam
Reflected beam


Reflected intensity is dependent on the interference of the amplitudes reflected from the interfaces (two here).



Fig. 3. Reflectivity of $\mathrm{Cu}-\mathrm{on}-\mathrm{Si}$ electrode at various potentials in borate buffer solution (pH 8.4). A, B, C, D correspond to potentials indicated in cyclic voltammogram of Fig. 2.


Cu


Fig. 4. Schematic of multi-layer model for Cu-on-Si electrode (not to scale). The oxide film has been represented as $\mathrm{Cu}_{2} \mathrm{O}$.

Table I. Parameters Derived from Least Squares Fit to Experimental Data.

| $E(V)$ | $\mathrm{d}_{\mathrm{Cu}}(\mathrm{A})$ | $\mathrm{d}_{\mathrm{Cu}_{2} \mathrm{O}}(\mathrm{A})$ | $\rho \mathrm{Cu}_{2} \mathrm{O}(\mathrm{g} / \mathrm{cc})$ | $\sigma_{c}\left(\begin{array}{l}\text { ( }\end{array}\right)$ | $\sigma_{\mathrm{Cu}_{2}}{ }^{\mathrm{o}} \mathrm{Cu}$ <br> (Å) | $\sigma_{\mathrm{Cu}_{2} \mathrm{O}} /{ }_{\mathrm{sol}}$ <br> (A) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| -0.12 | 268 | 24 | 6 | 17 | 8.3 | 3.4 |
| -0.8 | 284 | -- | -- | -- | -- |  |
| +0.4 | 250 | 26 | 5.5 | 26 | 9.4 | 2.2 |
| -0.8 | 275 | -- | -- | -- | -- | -- |




different frequencies. Reinforcement occurs whenever $\left|\nu_{\mathbf{z}}-\nu_{\mathbf{1}}\right| \tau$ is an even integer, then for a limited range of $\boldsymbol{r}$ both cosines oscillate together between $\pm 1$. giving a $y$ that also oscillates between $\pm 1$. Cancellation occurs whenever $\left|\nu_{2}-\nu_{1}\right|$; is an odd integer and is complete if $P_{1}=P_{z}$; otherwise the fringes are still present but with reduced strength.

The interference fringes in Figs. 6.7-6.9 coninue periodically for all values of the retardation time $\pi$. This behavior is unreal and is a property of the discrete nature of the distribution functions that we have used thus far.


Fig. 69

Mup of lowZ mtl,Be mafiedy 3:58:31 PM 4/6/92




FIG. 2. Beam-path geometry of the Michelson interferometer for $x$ rays and thermal neutrons. $S$ : splitter, $M$ : mirror, $A$ : analyzer components of a LLL interferometer generating Laue-case waves by Bragg transmission. $B_{1}, B_{2}$ : grooved crystals generating Bragg-case waves by surface Bragg refiection.


FIG. S. Spectrum measured with the new interferometer for the copper $K \alpha_{1} K \alpha_{2}$ doublet. Clearly visible are the nodes occurring due to the slightly different wavelengths. The approximately 630 orders of interference appearing as fast oscillations in the spectrum cannot be resolved in this representation (see Fig. 6).

Spatially Resolved X-Ray Microspectroscopy:
rnicroprobe + Real time Fousier trousfonr spectrometer.


Fig. 2. Schematic illustration of the amplitude-division Fourier transform interferometer to be developed. This interferometer consists of a skew symmetry LLL interferometer and a phase shifter. The LLL interferometer consists of a beam splitter S, two transmission mirrors/crystals M1 and M2, and an analyzer A. The relative phase difference between the two interfering beams split by $S$ is obtained by adjusting the thickness of the phase shifter. Real-time Fourier transform spectroscopy or Fourier transform imaging of surfaces and interfaces may be obtained by using a single wedge rotated 90 degrees from that shown above. A position sensitive detector is required to record the intensity distribution behind the analyzer crystal A.


Fig. 3 Calculated phase change $\eta$ introduced to $x$-rays when they travel through a slab of material of thickness equal to the amplitude linear absorption length of the material. Calculated results for several low-Z materials are presented here.


Fig. 1 Schmatic diagram of a wavefront-division Fourier transform $x$-ray interferometer. A spatially coherent x-ray beam is incident on and physically split into two beams at mirror $M_{1}$. Each of the two beams is reflected by a two-mirror optics. When the six mirrors are properly arranged and aligned, the two beams combine into one after the mirror M6: A variable phase delay of one beam relative to the other can be introduced by moving one of the mirror sets along the direction normal to the beamsplitter. While the spatial coherence of either beam is reserved, the two beams are recombined after a linear zone plate and the resultant power of the interference of the two beams is recorded as a function of the phase delay

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