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Microscope-based Profilometer

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The Design, Performance, and Application of an Atomic-Force Microscope-based Profilometer

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ABSTRACT

Rayleigh-Taylor instabilities during implosions of inertially confined fusion (ICF) capsules affect capsule performance. During acceleration, surface imperfections grow and can, if large enough, lead to an asymmetric implosion or even shell breakup. For this reason, characterizing the topography of target capsules is extremely important. We have developed a profilometer based on an atomic force microscope combined with a precision rotary air bearing. Averaged 1D surface height power spectra obtained with this instrument are converted to 2D mode spectra, which are used as input to hydrodynamic simulations. We describe the design of the system and its performance in terms of runout and repeatability. We also discuss the simulation of these measurements and the statistics involved in averaging 1D power spectra. Finally, we show the application of this measurement technique to capsules whose surfaces have been modified by laser ablation, resulting in a well-defined surface topography. This special case provides an excellent test for the system, since the expected results are exactly calculable.

I. INTRODUCTION

Hydrodynamic instabilities during implosions of inertially confined fusion (ICF) capsules are expected to play a dominant role in determining overall capsule performance [1]. The ablation front is Rayleigh-Taylor (RT) unstable due to hot low-density plasma blow-off pushing against and accelerating the denser, cooler shell. During this acceleration, surface imperfections grow at the ablation front and can, if large enough, lead to an asymmetric implosion or even shell breakup. The growing imperfections also feed through and imprint on the inner surface of the shell. During the deceleration phase of the implosion the roughened inner surface also becomes

hydrodynamically unstable. Further RT growth degrades the final symmetry of the implosion and creates mix at the pusher-fuel interface, potentially decreasing burn efficiency or preventing ignition. Unfortunately, high-gain capsule designs require shaped drive pulses and high aspect ratios (ratio of radius to wall thickness) to maximize the hydrodynamic efficiency of the implosion. These designs—with thin capsule walls, an extended acceleration phase, and steep density gradients at the ablation front—create a particularly conducive environment for hydrodynamic instabilities [2].

In light of the critical role these hydrodynamic instabilities play in ICF, considerable effort has been expended on manufacturing capsules with very smooth surfaces. Optimizing processing techniques requires the ability to measure the surface finish of a capsule at the nanometer level. Another area of significant effort has been the theoretical and experimental programs focused on understanding hydrodynamic instabilities in regimes relevant to implosions. A number of experiments on the Nova laser have measured RT growth of known perturbations on ablatively accelerated foils [3-5]. The LASNEX code [6] has been used to simulate these experiments and has given good agreement. While the planar experiments have been quite useful, the ultimate goal is to accurately simulate RT growth in a convergent geometry and determine its effect on capsule performance. Performing the relevant experiments depends on the ability to characterize the initial roughness of the imploded capsule.

The amount by which capsule surface perturbations are amplified during the implosion is dependent on the ratio of the capsule circumference to the wavelength of the perturbation. This ratio is called the mode number. Because of this dependence on mode number, it is natural to describe the surface in terms of a mode spectrum. The transformation from surface height into a frequency representation is directly analogous to conventional Fourier analysis, except that the basis set used is the spherical harmonic functions $Y_{lm}(\theta, \varphi)$. Expressed as an equation, $Z(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l R_{lm} Y_{lm}(\theta, \varphi)$, where

$Z(\theta, \phi)$ represents the height of the surface as a function of position. Ultimately, the desired quantity is a power spectrum, i.e., the square of the mode amplitude as a function of mode number: $P_{2D}(l) = (4\pi)^{-1} \sum_{m=-l}^l |R_{lm}|^2$. This is the quantity used to characterize the capsule surface for input to LASNEX.

II. MOTIVATION

In practice, it is very difficult to measure $Z(\theta, \phi)$ over the entire surface of a sphere with the required accuracy. Two alternatives have been pursued. The first is to measure a two-dimensional patch on the surface, with the assumption that it is representative of the entire sphere. The second is to measure a number of 1D traces around the sphere, which can be used to calculate P_{2D} . With both techniques, we use an atomic force microscope (AFM) to non-destructively measure the surface topography. However, the length scales over which information is gathered are very different in the two cases. When measuring a patch on a sphere, the maximum size of an image can be affected by the curvature of the surface. For large spheres ($> \sim 1$ mm diam), it is set by the lateral travel limit of the AFM tip (~ 100 μm). For smaller spheres, the vertical range of the AFM (~ 4 μm) limits the image size. The largest image we can obtain from a 0.5-mm-diam (Nova scale) capsule is ~ 60 μm on a side. For a typical 512×512 image on such a capsule, in principle this provides information on modes 25, 50, ... up to 12,500. In practice, image distortion makes measurements of the lowest modes rather inaccurate. By contrast, in collecting a 1D trace, the AFM tip remains static laterally while the sphere is rotated beneath it, thus providing information on all modes up to half the sampling interval. Calculations indicate that for Nova scale capsules, the largest RT growth will occur between modes 10 and 30. Patch images are therefore unsuitable for collecting the data necessary for hydrodynamic instability experiments. It was this fact that originally drove the development of an apparatus for collecting 1D profiles.

There are a number of issues to consider in the characterization of a 2D surface with 1D measurement. Because one trace represents a very small sample of the total surface,

even the collection of many traces from a particular sample will not yield a decent measurement of $Z(\theta, \phi)$. This precludes any direct calculation of the R_{lm} . However, a 2D surface can be characterized by an "average" 1D power spectrum $P_{1D}(n)$; that is, the spectrum toward which an average of many 1D spectra (as calculated from traces) will converge. This average 1D spectrum can be readily converted to the desired 2D power spectrum (or the other way) [7]:

$$P_{1D}(n) = \sum_{l=n, n+2, \dots} P_{2D}(l) \frac{(l+n-1)!!(l-n-1)!!}{(l+n)!!(l-n)!!}, \text{ and} \quad (1)$$

$$P_{2D}(l) = -(2l+1) \sum_{n=l, l+2, \dots} P_{1D}(n) \frac{n(n+l-2)!!(n-l-3)!!}{(n-l)!!(n+l+1)!!}. \quad (2)$$

The issue then becomes one of determining how well one knows $P_{1D}(n)$. The statistics involved are fairly clear, and are discussed in some detail below. However, in applying these statistics to a real measurement, the assumption is made that the surface is reasonably isotropic, at least in the sense that the local topography "looks" similar regardless of position. There is always the possibility that a large localized defect could pass undetected. Such a defect could actually dominate $P_{1D}(n)$ on an otherwise smooth capsule. The extent to which this is a problem depends on the application of the measurement. For example, a bump several μm in diameter on a Nova-scale capsule will generate significant spectral power in all modes below a few hundred, but would probably have little effect on capsule performance.

III. APPARATUS

A side view of the apparatus is shown in Fig. 1. The principle mechanical components are a precision air bearing (Professional Instruments model 4R) and a stand-alone multi-mode AFM (Digital Instruments NanoScope III). The bearing, which is mounted in a cast iron frame, has a rotary encoder and a capillary-sealed vacuum feedthrough attached to the spindle. The rotary encoder has 1800 line pairs, providing a maximum resolution of 0.05° . A two axis tilt stage is mounted on top of the spindle, and to that is attached a vacuum chuck that holds the sample. This is a relatively compact

and convenient method for centering a sample on the rotation axis of the bearing. The spindle is driven by a small DC motor via a pulley. Since the rotational speed (5 rpm maximum) and torque requirements are very modest, practically no tension is required in the belt, so the spindle is not measurably deflected by this drive arrangement. The cast iron stand sits on an optical table, underneath a small Super Invar breadboard which has a hole cut in the center. The vacuum chuck and tilt stage extend through this hole. The AFM is attached to a 3-axis translation stage which is mounted on the breadboard. The horizontal (x and y) axes are manually driven, while the z axis is adjusted using a computer-controlled, closed-loop actuator. Not shown on the breadboard are an additional 3-axis stage and a small CCD camera, which are used during sample transfers. A hand-held vacuum chuck, which is used to pick up the samples, is clipped to the translation stage. With the magnified view provided by the camera, the sample can be gently and precisely transferred to the air bearing vacuum chuck.

The hardware and software used for data acquisition are based on a Macintosh Quadra 650 equipped with an I/O board and a GPIB board from National Instruments. The AFM controller provides the feedback circuit necessary to maintain constant tip deflection, which it accomplishes by varying the voltage applied to a piezoelectric tube to which the tip is attached. Since the tip is not normally scanned across the surface (except to center the tip on the sample equator), the imaging capabilities of the AFM hardware and software are usually not needed. The piezo program voltage, which is proportional to the surface height at the tip, is sent through an anti-aliasing filter to a 16-bit D/A converter. For every 0.1° of bearing rotation, the controller for the rotary encoder sends a trigger pulse to the converter, which initiates a series of conversions (typically 100, but adjustable in software). The average of these numbers represents the surface height at that angular position. The data are displayed as a plot of surface height (relative to the zero of the AFM piezo) versus angle. Drift during a measurement is

compensated to first order by drawing a line through the first and last points and subtracting it from the trace (the drift is typically well under 20 nm). The traces shown in this paper have all had mode 1 removed. Mode 1 primarily comes from the sample being mounted off-center.

After a sample has been mounted on the vacuum chuck, a measurement begins with the bearing stationary while the AFM tip is brought into contact with the sample surface and the feedback circuit is engaged. The runout is then minimized, and the tip is centered on the capsule. The system is now set up for a measurement. Three parallel traces are normally taken: one at the equator, and two others 20 μm on either side. Each trace consists of 3600 points, with each point representing an average of up to 100 voltage measurements. For a full characterization, this procedure is performed for three approximately orthogonal orientations of the capsule on the vacuum chuck, for a total of nine traces. Figure 2 shows examples of traces from typical samples. Fig. 2a shows a trace taken from a precision silicon nitride ball bearing. This is a relatively rough, but extremely spherical, sample. The small mode 2 component represents the dominant contribution from the synchronous error motion of the airbearing spindle. Fig. 2b shows a trace from a Ti-doped hollow polystyrene shell made at LLNL [8]. As is often the case with these samples, the surface is quite smooth, but the asphericity is very pronounced. Figure 3 shows the power spectra derived from these data. Each curve represents an average of the power spectra calculated from the individual traces.

IV. PERFORMANCE

There are several potential sources of random error in these measurements. These include asynchronous deviations in the motion of the air bearing, vibration of the AFM, thermal drifts, or electrical pick-up anywhere prior to the A/D converter. Although work is ongoing to identify the individual magnitudes of these contributions, there are some data regarding the total random noise. By repeatedly measuring the same trace on a very smooth capsule, some idea of the reproducibility can be obtained. This is not a

perfect technique, since drift in the position of the AFM tip over the course of the measurements will cause the tip to encounter slightly different topography each time around. Nevertheless, it is unlikely to yield an underestimate of the error. We present the data as power spectra, obtained by subtracting two successive traces from each other, computing the FFT of the remainder, dividing by $\sqrt{2}$, and calculating the power spectrum. Figure 4 shows the average of four such measurements. The origin of this noise is unknown. Static measurements, in which the AFM tip is engaged on a flat surface and the output is digitized at the same frequency as when measuring a ball, indicate that electrical noise represents less than 10% of this error. However, comparison with fig. 3 illustrates that this noise is not a significant problem in the measurement of actual samples.

The principal source of systematic error is synchronous error motion, or runout, of the air bearing spindle; i.e., wobble motion that repeats each time around. If one could profile a perfectly spherical sample, the synchronous error could be obtained by simply averaging successive traces (to eliminate random noise). Unfortunately, the accuracy of the bearing is such that the runout is of the same order as the topography of a precision ball. The traces must therefore be measured in such a way as to permit the bearing error to be deconvoluted from the topography of the sample. Briefly, this is accomplished by measuring a trace, or set of traces, on a capsule, rotating it with respect to the vacuum chuck (while maintaining the same polar orientation), and measuring it again. Since the capsule topography will be the same, but shifted in phase, while the synchronous runout will not, these data allow the runout to be isolated. Figure 5 shows the results of measuring the runout using a Si_3N_4 ball bearing. Ten traces were measured and averaged together, the ball was rotated by 105° , and ten more traces were measured. Fig. 5a shows the extracted runout, while fig. 5b gives the power spectrum derived from averaging several similar measurements. The spikes on the runout trace are an artifact arising from the fact that the second set of traces do not exactly follow the first due to

slight errors in remounting the sphere. For this reason, only the lowest modes in the power spectrum are meaningful. The spectrum is zeroed at mode 7 because that mode is nearly synchronous with 105°, and cannot therefore be measured. Comparison of the power spectrum in fig 5b with the noise spectrum in fig. 4 suggests that only the dominant mode 2 component will consistently exceed the noise.

V. STATISTICAL ANALYSIS

The most straightforward way to determine the uncertainty in the measurement of a particular 1D mode is to take a large number of traces, compute their power spectra, and calculate the statistics for the mode of interest. It is not practical to measure a sufficient number of traces on a real capsule to perform this analysis, so we have written a computer program that generates great circle traces of user-specified model spherical surfaces. This allows us to collect hundreds of traces, so decent statistical distributions can be obtained. To accommodate special types of surface topography, there are actually two different implementations of the program. In outline, they work the same way: first, a model spherical surface is generated by calculating a set of R_{lm} coefficients. Simulated traces are generated by computing the θ, ϕ coordinates of 256 equally-spaced points around a great circle of the surface, then evaluating $\sum_{l,m} R_{lm} Y_{lm}(\theta, \phi)$ at each point. The orientation of the trace is normally chosen at random. The two versions differ in how the R_{lm} are calculated. There are generally two types of surfaces that need to be specified: ones that have a random topography, as would normally be seen on an unmodified surface, and ones that have a defined pattern impressed on them.

Generation of a random surface starts with a 2D power spectrum. Using the definition of the mode spectrum as $P_{2D}(l) = (4\pi)^{-1}(2l+1)\langle |R_{lm}|^2 \rangle$, the R_{lm} are chosen to be consistent in a statistical way with this relation. Specifically, each R_{lm} is generated by assigning a random number to $\text{Re}(R_{lm})$ and $\text{Im}(R_{lm})$, where the random numbers come from a Gaussian distribution with a variance of $2\pi(2l+1)^{-1}P_{2D}(l)$. Note that this does not result in a surface with exactly the same 2D mode spectrum, since

$(4\pi)^{-1} \sum_l |R_{lm}|^2$ is not forced to equal the initial $P_{2D}(l)$. The lowest mode numbers will tend to deviate the most, while the higher mode numbers will agree very closely. For the applications studied here, the differences are unimportant.

Currently, patterned surfaces are created using an excimer laser to ablate quasi-Gaussian pits in the surface of polymer capsules [9]. This experimental procedure is duplicated on the computer in a way that closely parallels the calculation of Fourier coefficients. First, a function is derived that describes the shape of the pit. This is usually either a 2D Gaussian or an empirical fit to the measured profile of a pit. Next, the area over which the function is significantly non-zero is subdivided into as many as 97 square cells and the average value H_i of the function in each of these cells is calculated. This array, along with the grid defined by the positions of the cells, is used to describe an individual pit. For each pit position, the program superimposes the grid on the surface of a sphere and calculates θ_i and ϕ_i for the center of each cell. These coordinates are used to compute values for $Y_{lm}(\theta, \phi)$. The contribution to $\int d\Omega Z(\theta, \phi) Y_{lm}^*(\theta, \phi)$ from the pit at this position is approximated by $\sum_i H_i Y_{lm}^*(\theta_i, \phi_i) \delta\Omega$, where $\delta\Omega$ is the area of each cell. This procedure is repeated for every pit position and the results are summed to give the particular R_{lm} . The entire sequence must be performed for each coefficient. At present, both versions generate the R_{lm} for $l=1$ to 100, $m=0$ to l ($R_{l,-m} = (-1)^m R_{lm}^*$).

Once the R_{lm} are determined, the generation of the traces is straightforward. A random number generator is used to create a set of θ, ϕ coordinates. These are used to define the orientation of each of the desired traces. To avoid accuracy problems in the routine that calculates the coordinates of the points around the trace, θ values in the range of $\pi/2 \pm .002$ are excluded. For each trace, the coordinates of 256 equally-spaced points are generated.

VI. RESULTS OF CALCULATIONS

Two different surfaces with nearly identical 2D mode spectra were generated. The first was a perfect sphere with 200 randomly placed, 1 μm deep Gaussian pits. The second was a randomly generated surface, as described above. The input 2D spectrum was the one calculated for the 200 pit surface. Figure 6 shows a comparison between the actual 2D spectra. The spectrum for the random surface deviates slightly from the spectrum used to generate it, but the RMS roughness is the same to within less than 1.5%. In both cases, 300 randomly oriented traces were calculated.

The averaged and "correct" 1D spectra (as calculated by transforming the 2D spectrum) for the patterned surface are shown in fig. 7, along with the standard deviation of the 300 individual measurements of each mode. As expected, averaging power spectra from different traces reproduces the correct result. The measurement of a single mode, however, varies considerably from trace to trace. In fact, the standard deviation approximately equals the mean, as would be expected for the measurement of a random signal. Histogram analysis shows that the data are consistent with an exponential probability distribution. This result can easily be generalized to the typical measurement in which multiple power spectra are averaged together. The general distribution $P(l_{\text{avg}})$ for the value of a mode l obtained by averaging n power spectra is

$$P(l_{\text{avg}}) = \frac{(an)^n l_{\text{avg}}^{n-1}}{(n-1)!} e^{-anl_{\text{avg}}} \quad (3)$$

where $1/a$ is the mean and $1/(a\sqrt{n})$ is the standard deviation. As n increases, this distribution becomes Gaussian-like.

To verify that the results obtained for a surface covered with pits were not unique, we performed the same calculation for the randomly rough surface described above and shown in fig. 6. The results are quite similar to those shown for the previous surface.

VII. APPLICATION TO ABLATED CAPSULES

As discussed in the motivation section, $P_{2D}(l)$ cannot usually be directly evaluated. However, when we ablate capsules, we are effectively defining $Z(\theta, \phi)$, since the

underlying topography of the ball can usually be neglected in the mode range of interest. Measuring laser-ablated capsules thus provides an opportunity to verify that our results are consistent with the "correct" 1D spectrum, since we can calculate P_{2D} in this case. Figure 8 shows some typical results for two capsules, each with the same random pattern of 200 pits but with different pit depths. The pit profile used in each calculation was a least-squares fit to a profilometer trace of one of the calibration pits. There is only a relatively minor difference between spectra generated with the best-fit profile and those using a Gaussian profile. Between modes 4 and 60, the measured spectra are in good agreement with the calculations. Below mode 4, the spectrum from the capsule with 0.3 μm pits shows the influence of low-mode capsule distortion. Above mode 60, the underlying topography of the capsules dominates the measured spectra.

VIII. CONCLUSION

The profilometer described in this paper has proven to be an effective tool for characterizing the topography of ICF target capsules, especially at long wavelengths (low mode numbers). Capsule distortions at low modes (~ 30) are particularly important for determining the severity of Rayleigh-Taylor instabilities during indirectly-driven implosions of Nova-scale capsules. By measuring capsules with a defined surface geometry, we have demonstrate that the measured 1D power spectra are in good agreement with the calculated values.

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FIGURE CAPTIONS

FIG 1. A schematic diagram of the apparatus.

FIG 2. Typical examples of traces from (a) a precision Si₃N₄ ball bearing and (b) a Ti-doped polystyrene mandrel.

FIG 3. Power spectra calculated from the data in fig. 2. Each curve represents an average calculated using 9 traces from three different capsule orientations (see text).

FIG 4. Power spectrum of the random noise, as measured by subtracting successive, nominally identical traces. The curve is an average of 4 such difference traces.

FIG 5. (a) An average of four measurements of the synchronous error motion of the air-bearing spindle. The high frequency noise is not associated with the air bearing. (b) The averaged power spectra from the four measurements.

FIG. 6. The calculated 2D power spectrum of a sphere with 200 75- μm -diam randomly-placed Gaussian pits, and the power spectrum of a random surface generated to have a similar spectrum (see text).

FIG. 7 The results of calculating 300 randomly-oriented traces on the sphere with pits from fig. 6. The correct 1D spectrum is derived from transforming the calculated 2D spectrum.

FIG. 8. A comparison between data and calculation for two capsules with the same 200-pit pattern but different depths. The data are an average of the power spectra of 9 traces, as in fig. 3. An empirical fit to a measured pit profile, rather than a Gaussian, was used in the calculation. The inset show a photograph of an actual ablated capsule.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig 5.

Fig. 6

Fig. 7

Fig. 8

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