In-Situ UV Absorption CF_2 Sensor for Reactive Ion Etch Process Control

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ABSTRACT

In this article, we report the use of ultraviolet absorption spectroscopy for CF_2 detection in a large area parallel plate capacitively coupled reactive ion etching system and correlation of data from this and other plasma sensors to the etch rate of SiO_2 and a-Si in CF_4/CHF_3 plasmas. We present statistical models for estimation of a-Si etch rate in the operational regime in which the CF_2 concentration is in the range of $0.4 \sim 1.6$ volume % of total gas in the etch chamber. A small change in CF_2 concentration translates into quite a large variation in terms of SiO_2/a-Si etch selectivity, and this makes CF_2 concentration a useful variable in process control. We will show statistically that silicon etch rates can be very well estimated by using sensors for CF_2 and fluorine.

Keywords: Reactive Ion Etching, Process Control, CF_2 absorption sensor, statistical models

1. INTRODUCTION

It is commonly acknowledged that reactive ion etching (RIE) processes require empirical tuning on each etch tool to achieve desired wafer-level results and also require periodic adjustment to maintain high yields. Real-time feedback control could be used to reduce these problems provided that adequate plasma state sensors are available.[1–3]

Real-time RIE control requires simultaneous control of the chemical etch species, ion bombardment, and surface passivation mechanisms. Our previous work demonstrating the potential advantages of multi-varible feed control used only indicators of chemical species and ion bombardment.[1] In fluorocarbon-based processes, CF-polymer formation acts as the major surface passivation mechanism and has been shown to be related to the CF_2 concentration in the plasma. CF_2 is known to have absorption lines in ultraviolet range, and UV absorption spectroscopy is well suited to the RIE process both for its simplicity and non-perturbative nature.[4] We can also extract chamber wall state information from the CF_2 sensor,[5] which is a sensitive indicator of etch performance. Combined with already used techniques such as reflectometry and actinometry, UV absorption spectroscopy for CF_2 detection can be a very useful plasma state sensor intended for real-time RIE feedback control.

In this study, we show that UV absorption measurements of $[CF_2]$ can be combined with actinometric measurement of relative [F] to build statistical models for a-Si etch rates which are applicable to real-time feedback control. The plasma densities in this study are relatively low compared to other studies in the current literature,[4,5] but the CF_2 detection still can be achieved with simple system requirements.

2. EXPERIMENT

A diagram of the apparatus used in this experiment is shown schematically in Fig. 1. The research vehicle is a Plasmatherm Clusterlock 7000 capacitively coupled parallel plate reactor. This machine is designed for etching flat panel display devices. This reactor accomodates 350 mm by 400 mm substrates, on which a few wafers can be placed and simultaneously processed. The chamber is of rectangular shape and there are five observation ports on each side. The UV grade quartz observation port windows allow 80% transmission at near 250 nm wavelength. The distance between opposing windows is 78 cm, and the width of the rf-biased rectangular electrode (along the observation line) is 61 cm. This electrode is connected to a 13.56 MHz rf generator and impedance matching network.

The light source of this absorption spectroscopy is a 100 W high pressure mercury arc lamp. To compensate the possible light source intensity level drift, we adopted the double beam technique. The light from the lamp is

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coupled to the common end of a bifurcated optical fiber. The light coming out from the two split ends are collimated and mechanically chopped at different frequencies. One of them is directly coupled to a 0.5 m monochromater with 1200 grooves/mm grating, which provides reference level of the light source, while the other beam is directed to a window, travels across the chamber, bounces back off the concave mirror installed on the other side of the chamber, travels back to the original departure window, and then enters the monochromater and converts into electrical signal through photomultiplier tube. Even though the collimated probe beam has a certain degree of divergence, due to the refocusing effect by the concave mirror, the beam diameter is not larger than 3 cm at all times. The reference and probe signals are recovered by phase-sensitive lock-in amplifers synchronized with the optical chopper.

The gas mixture we use for the experiment is CF_4/CHF_3. The range of varing flow rate ratio is from CF_4 : CHF_3 = 1 : 3 up to CF_4 : CHF_3 = 3 : 1. Total gas flow is fixed, which validates the assumption that for a given operating gas pressure the residence time of the gas species in the chamber is constant. There is 5 volume % argon included in CF_4 gas feed for actinometry purposes. Emissions at 750.4 nm for Ar and at 703.7 nm for fluorine are measured and used to estimate relative concentration of fluorine.

For a highly polymerizing gas chemistry, it is often observed that polymerization on the windows reduces overall transmission light intensity even during the run, which makes it hard to distinguish the absorption by gas species in the chamber from the absorption by the coating polymer on the window. For etch rate measurement experiments, we checked the transmission level before and after the experiment and made sure that window absorption had reached steady state("seasoned"). After confirming the chamber is properly seasoned for our operating conditions, we etched *a*-Si and/or SiO_2 blanket wafers on 350 mm by 400 mm aluminum plate and collected etch rate information by SP microscopic reflectometry thin film thickness measurement after each run. We collected sensor data from CF_2 absorption sensor and actinometry during the run.

3. RESULTS AND DISCUSSION

First, we scanned the monochromator from 245 nm through 254 nm wavelength range and verified the CF_2 signature.[6,7] There are 3 major absorption peak in this wavelength range; 246 nm, 249 nm, and 252 nm, which have absorption cross-section of $2.46\times10^{-17}cm^2$, $2.91\times10^{-17}cm^2$, and $2.48\times10^{-17}cm^2$. Once the peak location is verified,

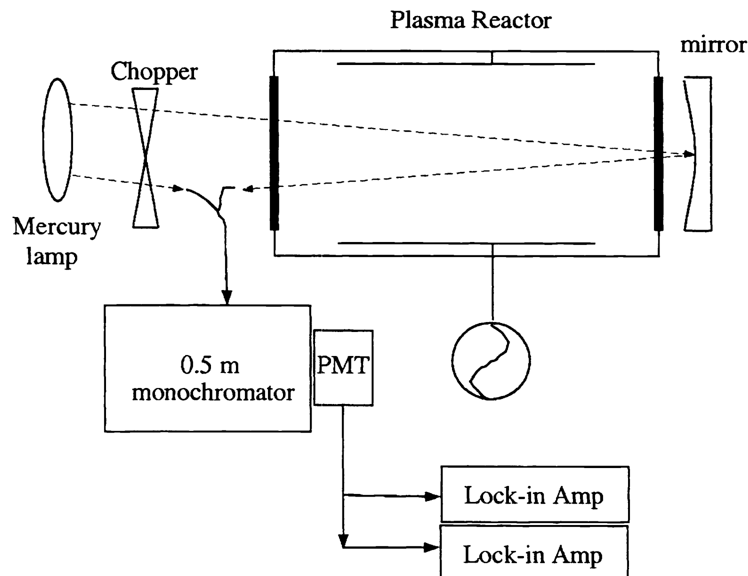

Figure 1. Schematic of the system used in this experiment.

we can fix the monochromator at that wavelength and measure the amount of absorption to get CF_2 density. The density of CF_2 (n) is calculated by the Beer-Lambert relationship,

$$n = \frac{1}{\sigma b} \ln \left(\frac{I_o}{I} \right), \tag{1}$$

where σ is the absorption cross-section of CF_2 at a given wavelength, b is the optical path length, and I and I_o are the transmitted probe beam intensity with and without the plasma on. This relationship assumes that the CF_2 molecules are uniformly distributed across a certain distance along the optical path. Since the beam diameter is small enough compared to the size of the chamber height and electrode dimensions, and the electrode area is less ion confining than inductively coupled high density plasma which confines more discharge in center magnetic bucket area, it is reasonable to assume that in our reactor CF_2 is distributed quite uniformly. With this assumption, the optical path length for this experiment is 156 cm (2 × distance between opposing windows), and this gives lower limit of the density.

Fig. 2 shows typical CF_2 absorption intensity observed at 252 nm wavelength as well as the percentage of the total gas under various operation conditions. Natural log of I_o/I is plotted against RF power for a few different pressures, which is proportional to $[CF_2]$. We see more absorption with increasing power and pressure as expected. But the partial pressure of CF_2 decreases as the total gas pressure goes up. With the values given above and Eq. 1, the CF_2 density in this plot is in the range of 2.6×10^{13} cm^{-3} $\sim$ 7.0×10^{13}cm^{-3}. For 40 mT total gas pressure, the volume % of CF_2 is from 1.9 % to 4.4 %, while it is only from 1.3 % to 2.2 % for 100 mT in the RF power range from 200 W to 1100 W.

Fig. 2 is the result when we use a conventional glass plate as a wafer carrying tray. We put a plate inside the chamber when the plasma is turned on even if wafers are not loaded, to prevent the ion bombardment damage to the powered electrode. But with this glass plate inside, the V_{bias} reading does not reflect an actual self-bias voltage maintained in the sheath in front of the wafers inside the chamber. We have noticed that glass plate V_{bias} reading varies significantly according to the degree of polymerization in the chamber during the etch process. The V_{bias} reading decreases while the chamber is being coated with polymer, and the reading increases when the coated polymer is being removed during chamber cleaning. This is because the coated polymer on the electrically floating glass plate functions as a capacitor connected to the V_{bias} reading circuit in series. While ion charged on the polymer

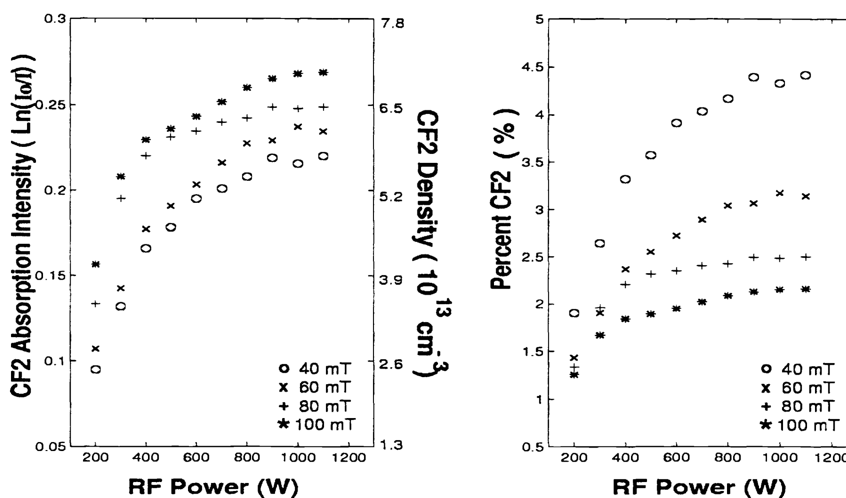

Figure 2. CF_2 densities and percentage of total gas in various operating conditions. CHF_3 plasma, 200 sccm gas flow, 252 nm absorption line.

film surface does not change drastically, increasing polymer thickness decreases the capacitance of the film, which in turn increases the voltage sustained by the polymer film capacitor. Therefore, voltage across the V_{bias} reading circuit reduces.

This phenomenon makes V_{bias} information provided by the Plasmatherm less useful when we try to correlate V_{bias} to ion flux. To get relevant V_{bias} information without placing another sensor in the chamber, we used a aluminum plate instead of glass, which provides direct electrical contact between electrode and plasma ambient. With this conducting plate in the chamber, V_{bias} reading stays constant during the run regardless of the degree of polymerization in our operational regime, and this gives a relevant information on dc self-bias in the plasma chamber. A typical set of experimental data is shown in Fig. 3. For the data presented in Fig. 3 and below, we used 249 nm absorption line. Wafers are etched for 3 minutes, and during this period sensor readings stay stable.

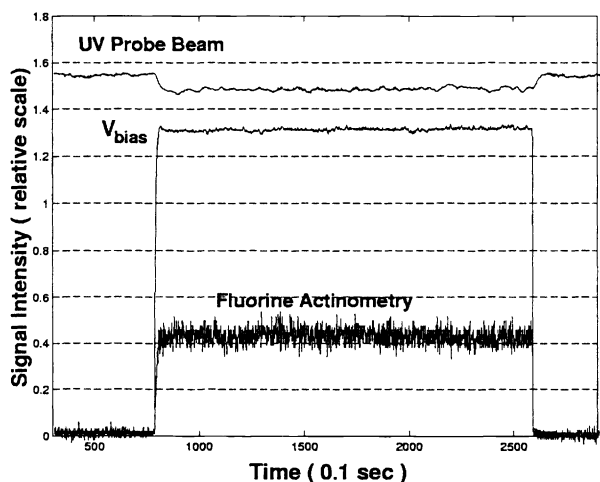

Figure 3. An example of raw data for a UV absorption experiment. The UV signal reduction when the plasma is on is about 3.8 %, which translates into 0.65% CF_2 in the total gas mixture. The pressure was 40 mT, the rf power was 200 W, and the CF_4/CHF_3 flow rate ratio was 3 : 1.

CF_2 is also a very sensitive indicator of etch selectivity between SiO_2 and a-Si. The etch rate change shown in Fig. 4 is measured under a fixed 40 mT, 500 W operation condition, while CF_4/CHF_3 flow rate ratio changes. When pressure and RF power are fixed, V_{bias} is also fixed. This is the etch condition where the etch rate change is limited by the fluorine concentration. As the CF_2 density increases, the SiO_2 etch rate slowly decreases but the a-Si etch rate quadratically decreases. In this set of experiments, CF_2 density varies from 1.2×10^{13} cm^{-3} to 1.8×10^{13} cm^{-3}, which corresponds to the range of 0.9 ~ 1.4 % of total gas. About 60% change in CF_2 sensor signal results in etch selectivity change by more than factor of 7.

We now try to extract statistical models from our data set to correlate the sensor information to the actual etch performance of the reactor . At a fixed pressure, by controlling RF Power and gas mixture we acquire information on CF_2 concentration, fluorine concentration, V_{bias} and silicon etch rate. A statistically obtained model is not unique, and the choice of a specific model to describe a given data set is up to the user's discretion, considering statistical reliability as well as physically meaningful relationship between variables and end result.

We collected a data set to analyze under the condition of a fixed pressure at 40 mT and a fixed total gas flow rate. The etched material is amorphous silicon blanket wafer grown by PECVD. Again, the gas flow ratio between CF_4 and CHF_3 varies from 1:3 to 3:1, and the RF power varies from 150 W up to 600 W. The selected operation set points are evenly spaced in this gas flow ratio and RF power range so that the statistical weight does not concentrate in a specific region of the data space. Total of 22 experiments were performed, and for each experiment, [CF_2], [F], V_{bias} as well as etch rate data were collected.

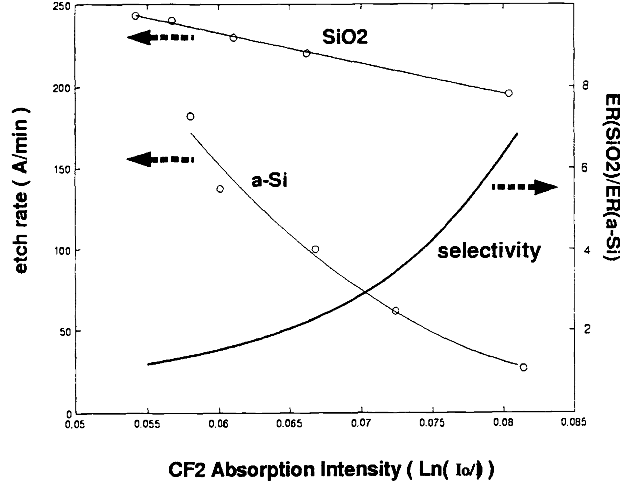

Figure 4. $[CF_2]$ dependence of the SiO_2/a-Si etch selectivity when V_{bias} is maintained constant.

We present six models to describe the data set :

$$\begin{aligned}
\text{model 1} : ER &= -0.796 + 1.079\,\text{CFR} + 0.814\,\text{Pw} \\
\text{model 2} : ER &= -0.971 + 1.108\,\text{CFR} + 0.992\,\text{V}_{bias} \\
\text{model 3} : ER &= -0.390 + 0.505\,\text{CFR} + 1.036\,[\text{F}] \\
\text{model 4} : ER &= -0.929 + 0.734\,\text{CFR} + 0.639\,[\text{F}]^2 + 1.764\,\text{V}_{bias} - 0.979\,\text{V}_{bias}^2 \\
\text{model 5} : ER &= -0.399 + 1.253\,[\text{F}] + 1.215\,[\text{CF}_2] - 1.369\,[\text{CF}_2]^2 \\
\text{model 6} : ER &= -0.891 + 0.481\,\text{CFR} + 0.991\,[\text{F}] + 1.820\,[\text{CF}_2] - 1.442\,[\text{CF}_2]^2
\end{aligned}$$

where ER is the etch rate of a-Si, Pw is the applied RF power of the set point, and CFR is the partial pressure fraction of CF_4 in CF_4/CHF_3 gas mixture, i.e. for $CF_4 : CHF_3 = 3 : 1$, CFR = 0.75, for $CF_4 : CHF_3 = 1 : 3$, CFR = 0.25, etc. Quantites in the bracket [ ] are the densities of the species of interest measured by UV absorption sensor and actinometry system.

These models are obtained by standard least squares model fitting.[8] All the varibles are normalized between 0 and 1 so that the coeffecient of each term represents the influence of the variable in etch rate estimation. The range of actual values for the variables is in Table 1.

Table 1. The range of variable values before normalization. $[CF_2]$ is in absorption intensity ($\ln(I_o/I)$), [F] is in arbitrary units.

	min	max
CFR	0.25	0.75
Pw	150 W	600 W
$[CF_2]$	0.0254	0.0939
[F]	0.1001	0.5558
V_{bias}	94.0 V	319.3 V
ER	20 Å/min	239 Å/min

Each model is the best performance model with each set of variables while keeping only meaningful order terms. Sometimes we can achieve infinitesimal amount of improvement in the overall least sqaure error by adding a number of higher order terms, but we have found variable terms with more than 3rd order do not play any statistically meaningful role in this particular estimation. A summary of fit table for these models is shown in Table 2. We can say that the model with smaller RMS_error and larger RS_Adj value is a better model. But this notion requires caution because we also have to take the physical reality into account.

With the gas pressure fixed at 40 mT, there are two degrees of freedom in setting the operation point: CF_4/CHF_3 gas ratio and RF power. We know qualitatively that the silicon etch rate gets higher for higher powers and higher CFR's, which are closely related to ion bomardment enhanced etch/echant formation and surface passivation inhibited etch behavior, respectively. Model 1 is an attempt to predict the etch rate by using only set point information, without any help from plasma state monitoring sensors. With RS_Adj = 0.866 and RMS_error = 0.096 (root mean square error, out of 0 to 1 scale), it certainly shows the etch rate trend we already know, but doesn't give us any new information let alone the accuracy the factory level process control requires.

In model 2, V_{bias} replaces Pw, and the fitting result gets better. This shows that even though V_{bias} is very much correlated to Pw(V_{bias} = 0.150 + 0.837 Pw, RS_Adj = 0.979, RMS_error = 0.03.), V_{bias} is a more directly related quantity to etch performance. V_{bias} can also be well estimated as a function of [F] and [CF_2] (V_{bias} = 0.010 + 0.688 [CF_2] + 0.631 [F], RS_Adj = 0.941, RMS_error = 0.0504).

The fitting quality experiences a boost when [F] replaces the position of V_{bias} in model 3. In this model, CFR reflects the degree of surface passivation inhibited etch behavior, and linear [F] term supports the established knowledge that chemical etching part of the Si etch rate is proportional to the fluorine density.[9] This shows that at least in this overall regime of operation set points, chemical etchant is more influential than ion bombardment enhancement etching.

It seems to be hard to point out any single individual physical etch mechanism from model 4. It is presented as a numerically best statistical model for our data set without the help of CF_2 sensor, regardless of physical meanings. We couldn't get anything better than this without CF_2 absorption sensor information. Model 4 serves as a baseline to show what benefit [CF_2] information can provide. It should be noted that absence in the formula does not mean the variable's irrelevance. Because of complex correlation between the variables, all models include effects from each variable to some extent. The task here is to find which set of variables represent the data set better and simpler.

In model 5, [CF_2] appears. The fitting performance of model 5 is slightly better than that of model 4, but the significance of this model is in that it achieves high correlation in etch rate estimation without the direct information of V_{bias}. We also put in V_{bias} as a variable, but with [CF_2] present, V_{bias} is eliminated in the fitting procedure. This model also explains the result shown in Fig. 4. Silicon etch rate quadratically decreases with [CF_2]. It linearly increases with [F]. Model 6 is the model 5 plus CFR. The result is the best of the six. Since CFR is always given as a set point parameter, the implementation of model 6 does not cost much more than model 5. By including a readily available parameter, we can limit the fitting space to more narrow and meaningful area.

Table 2. Fitting summary for etch rate estimation models. RS_Adj estimates the proportion of the variation in the response around the mean that can be attributed to terms in the model rather than to random error. To make it more comparable over models with different number of parameters, RS_Adj also uses the degrees of freedom in its computation. RS_Adj = 1 occurs when there is all-zero error perfect fit, while RS_Adj = 0 means that the fit predicts the response no better than the overall response mean. Mean response = 0.3324.

	RS_Adj	RMS_error
model 1	0.86586	0.09632
model 2	0.89582	0.08489
model 3	0.93827	0.06534
model 4	0.96749	0.04742
model 5	0.97296	0.04325
model 6	0.98234	0.03495

Fig. 5 is the comparison between actual a-Si etch rate from the experiments and predicted etch rate by model 6. All 22 points are shown. This is to show how well the statistical model predicts the etch rate. Fig. 6 includes contours for a few constant [F] values. A few contour lines ([F] = 0.1 ~ 0.45 (relative scale)) are shown. Model 5 and 6 indicates that for a constant [F], the silicon etch rate quadratically decreases as a function of $[CF_2]$.

4. CONCLUSION

UV absorption spectroscopy for CF_2 detection can be used in conjuction with fluorine actinometry to predict etch rates for a wide range of operation condition. In the set point regime used in this experiment, the silicon etch rate varies by more than a factor of 11, and etch selectivity between silicon and oxide varies by more than a factor of 8. A Small change of CF_2 density results in large variation in etch rate, and the phase sensitive lock-in detection scheme has a sufficient resolution to pick up this change in CF_2 density.

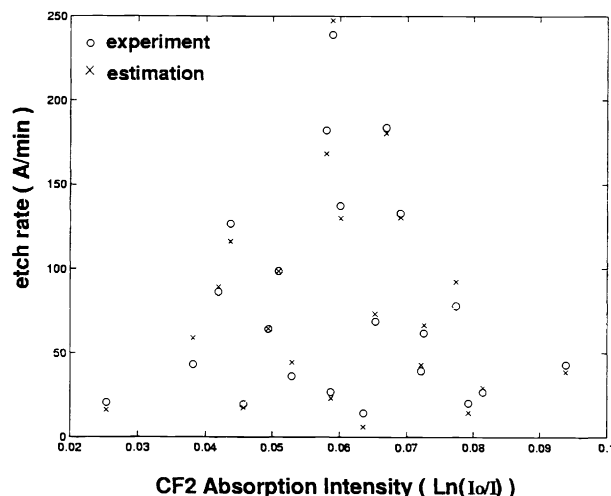

Figure 5. a-Si etch rate estimation by model 6.

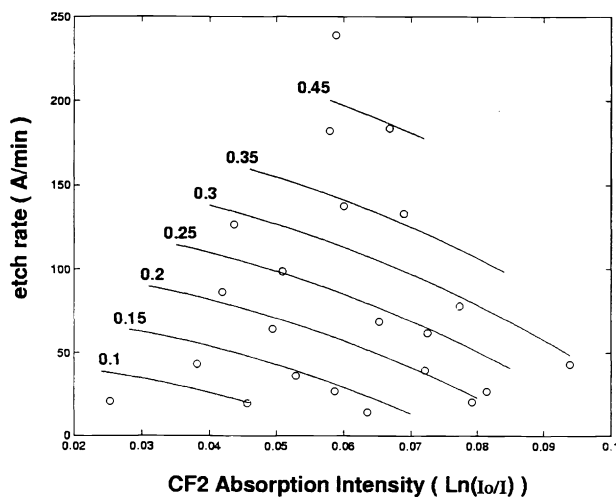

Figure 6. A Contour plot with [F] as a parameter. Experimental data points are denoted by small circles.

Even though ion bombardment enhacement, chemical echant and surface passivation mechanism are all important factor determining silicon etch rate, second order polynomial of [CF_2] can fill in the absence of dc self-bias information to a certain extent. Highly confident statistical etch rate estimation model showing less than 3.5 % root mean square error has been presented.

It requires further study to find what kind of information [CF_2] can give in more extreme coditions, where either physical or chemical etch mechanism is dominant.

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