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Optimization of plasma etch processes using evolutionary search methods with *in situ* diagnostics

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Abstract
This paper presents several approaches that have been used to control, optimize and characterize a low pressure (10–300 mTorr) plasma processing system. Methods such as contour following and differential evolution have been used to find contours of DC bias, total ion flux, ion energy flux, quadrupole mass spectrum (QMS) intensity ratios and line intensity ratios of the optical emission spectrum (OES) in argon and nitrogen plasmas.
A mapping for a 4 × 4 multi-dimensional parameter space is also presented, in which the relationship between four control parameters (power, pressure, mass flow rates of two supplied gases) and four measurement outputs (DC bias, ion flux, QMS ratios and OES line intensity ratios) is determined in a plasma etching process. The use of these methods significantly reduces the time needed to re-configure the processing system and will benefit transfer of processes between different systems. A similar approach has also been used to find quickly an optimum condition for directional etching of a silicon wafer.

1. Introduction and strategy

Although a huge complexity arises for the processing environment [1–3], low temperature plasmas have advantages in processing materials, which include enhanced chemical reactivity due to dissociation of molecules in the plasma as well as directionality due to bombardment with plasma ions accelerated through the space charge sheath. Each plasma process should be optimized based on its resultant characteristics, in etch processes, vertical and lateral etch rates, selectivity to any top mask and bottom stopper materials, damage, passivation residue, etc [4–6]. If such characteristics could be monitored *in situ* by a diagnostic method, it would be preferable because direct information on the desired characteristics could then be fed back into the plasma control system.

The effectiveness of commissioning and maintaining any manufacturing system is judged by the time needed to reach its optimum state and its ability to maintain a stable state. Also, the full value of plasma processing techniques will only be attained when it becomes possible to predict *a priori* the conditions and parameters required to optimize and control a particular process. Full exploitation of the advantages of plasmas in a manufacturing environment requires the ability to change the plasma parameters in a controlled and diagnosable way so that a system used for a particular process may be kept the same or economically and speedily changed for another.

Currently, most of the characteristics of plasma processing are obtained only by off-line surface characterization

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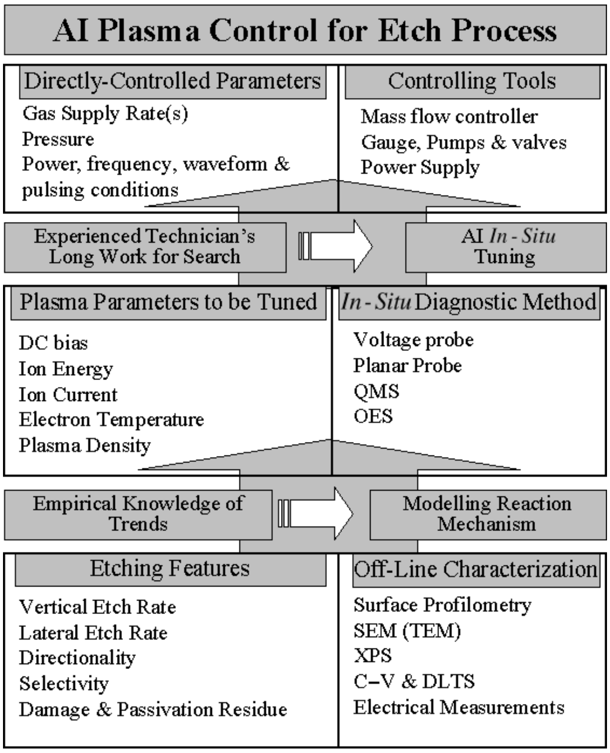

Figure 1. Control strategy for low temperature plasma processes.

techniques such as surface profilometry, scanning electron microscopy (SEM), transmission electron microscopy (TEM), x-ray photoelectron spectroscopy (XPS) and electrical measurements like capacitance–voltage (CV) measurements and deep level transient spectroscopy (DLTS). Obtaining these surface-specific parameters during plasma processing is far from trivial although real-time dielectric measurements using *in situ* ellipsometry and interference have been used [7, 8]. The relationship between the processing characteristics and the resultant surface characteristics is extremely complex, depending on physical and chemical laws. Important plasma parameters include DC bias, ion energy, ion current density, plasma density, electron temperature, chemical species and their densities, etc, which can be measured, respectively, by voltage probes, electrostatic planar probes, quadrupole mass spectrometry (QMS), optical emission spectroscopy (OES) and the like, installed together with interfacing electronics circuits to output derived quantities.

Our current strategy before developing each direct *in situ* monitoring method has been to use accumulated empirical knowledge or theoretical prediction in order to relate the process characteristics to the plasma parameters and then tune the direct input parameters of the plasma processing system so that the plasma parameters can be optimized (figure 1). This approach offers a powerful way of controlling and optimizing the complex plasma environment without some of the restrictions associated with traditional methods (e.g. time required, lack of flexibility and high costs).

Optimum solutions for plasma processing have been found using the genetic algorithm (GA) approach, in conjunction with neural network-based models of plasma behaviour [9]. We have previously demonstrated the advantages of artificial intelligence (AI) for controlling plasma processes, including the use of fuzzy logic for controlling DC bias, but process optimization was not attempted at that stage [10].

In this paper, we demonstrate an approach towards tuning four different plasma characteristics, namely DC bias, ion flux, QMS ratio and OES line intensity ratio, by using diagnostic techniques such as a surface embedded electrostatic planar probe, QMS and OES. Four input parameters (input power, total pressure and two mass flow rates) are controlled.

We also present methods such as contour-following (CF) and multi-dimensional methods to map the parameter space in terms of power, pressure and the flow rates of two supplied gases. These methods find contours for the ion flux, the DC bias, the ion energy flux, the QMS ratios of two chemical species and the OES line intensity ratios of two emission lines.

Powerful techniques that can tune the plasma processing system to the specified optimum in terms of single or multiple parameters such as DC bias, ion flux, ion energy flux, QMS ratio and OES intensity ratio are also presented in this work. The direct input parameters of power, pressure and two supplied gases are controlled for the optimization. Comparisons between two techniques are also given in which solutions are found globally and locally in a much quicker time than the time taken by a human operator.

We also demonstrate an application of this technique to directional etching of a silicon wafer, which is a difficult and complicated task, where our approach with empirical knowledge made it possible to determine quickly the optimum etching conditions.

2. Experimental system

A 13.56 MHz capacitively coupled RF plasma system was used (figure 2) in which two electrodes (grounded and powered) of 150 mm diameter were set 30 mm apart. The pumping system consists of a two stage high vacuum rotary pump and a turbo molecular pump with a pumping speed of 450 litre s^{-1}. Typical discharges were obtained in the pressure range of 10–300 mTorr (1–40 Pa), power range of 30–300 W, nitrogen flow rate range of 3–100 sccm, argon flow rate range of 10–70 sccm, oxygen flow rate range of 10–100 sccm and SF_6 flow rate range of 40–130 sccm. Measurements of pressure, power, gas flow rates, DC bias, ion flux, QMS ratios and OES line intensity ratios were passed to the controller. Settings for pressure, power and mass flow rates for up to two gases were passed from the controller to the system (extension to simultaneous control of additional gas lines is straightforward).

DC analogue signals proportional to the measured diagnostic intensities were fed to the A/D converter inputs of the data acquisition system and then transferred to the control system. The control system was equipped with our in-house software, DARBS (Distributed Algorithmic and Rule-Based Blackboard System), written in C++. This software is based on the blackboard model, an established AI approach that allows parallel or concurrent software modules to collaborate by writing to a shared area of memory known as the blackboard [11].

The gas discharge plasma acts as a nonlinear load to the RF generator. As a consequence, in response to the RF voltage

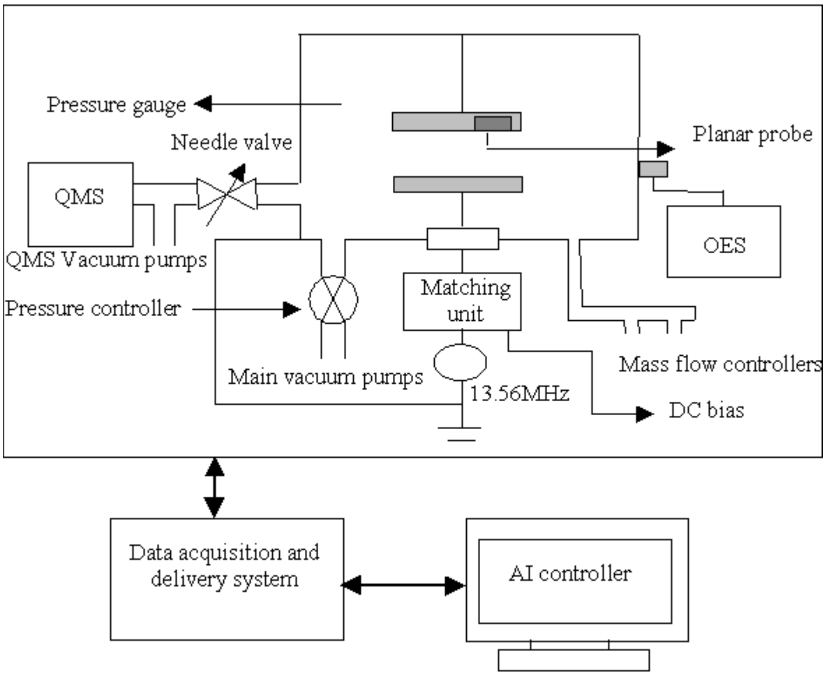

Figure 2. Computer-controlled RF plasma system with associated diagnostics.

supplied to the power electrode, a DC bias voltage refers to the modulus of the negative self-bias voltage and develops across the plasma sheath, reflecting the amplitude of the RF and the electrical circuit geometry of the discharge. The measured DC bias potential can be taken as a general indicator measure of the bombardment energy of positive ions accelerated to the processing surface (on the electrode).

An electrostatic planar probe, embedded into the ground electrode, was used to determine the total positive ion flux [12]. The probe is a large-area (38 mm^2) single-sided disc with a guard ring around it. The guard ring was maintained at the same potential as that of the central disc to remove edge effects. The probe was biased in the ion saturation regime, where the electron flux is small so that the signal could be taken as a direct measure of ion flux, reflecting the density of the plasma. The response of the probe in strongly electronegative media has been analysed [13]. The present arrangement for extracting positive ion currents remains satisfactory, provided the probe surface remains clean. In practice, several hours of operation in SF_6/O_2 mixtures have been achieved.

The product of the ion flux and the DC bias gives a measure of the ion energy flux through ion bombardment. The ion energy flux represents the amount of energy transferred from the plasma ions to the surface of the wafer per unit time and area. Therefore, this quantity has special importance to materials processing with plasmas. This combined measurement was used to directly control the plasma parameters in our control system.

QMS and OES systems were also integrated into the plasma control system. QMS was used to provide information on the relative concentrations of particular species in the system. The analogue outputs from the QMS controller were collected to obtain the partial pressure of specific species, selected by mass number. One of the benefits of this engineering approach is that we need high reproducibility more than absolute performance in our measurements. It is true that species other than ions are involved, but we monitor the ions because their behaviour is indicative of the state of the whole plasma.

OES provides rich, but highly convolved information about properties such as the densities of plasma species, electron–atom, atom–atom and ion–atom collisional effects and the energy distribution of species [14]. Our OES tool scans a range of wavelengths between 180 and 850 nm every 80 ms. OES line intensities at desired wavelengths were obtained as analogue DC voltages using digital delay generators and boxcar integrators. The ratio of two signal intensities was used to compensate for any inefficiency in the optics and drifts in the measurement intensity.

For N_2/Ar plasmas, N_2 (28 amu) and Ar (40 amu) were measured by the QMS, whereas the OES line intensity ratio of the emission at a characteristic nitrogen wavelength of 385 nm and one from argon at 750 nm was used to characterize the plasma light emission. For O_2/SF_6 plasmas, SF_3 (89 amu) and SiF_3 (85 amu) were measured by the QMS (figure 3(*a*)), whereas the OES line intensity ratio of the emission generated from O_2 (259.4 nm) and SF_6 (303.5 nm) were used to characterize the etching process (figure 3(*b*)).

Fluorine/oxygen based plasmas generated with O_2/SF_6 were used for demonstration of the etching performance as these gases have a lower handling risk than other possible chemistries. A patterned aluminium mask on silicon was used to demonstrate minimum mask erosion or dimension loss in the fluorine chemistry, making it easy to observe lateral etching. Etched features were examined by SEM, using secondary electron imaging, after processing.

Gas response times for a system like ours are a few seconds, whereas the electrical response times are considerably less. In this work the system response has been adequate.

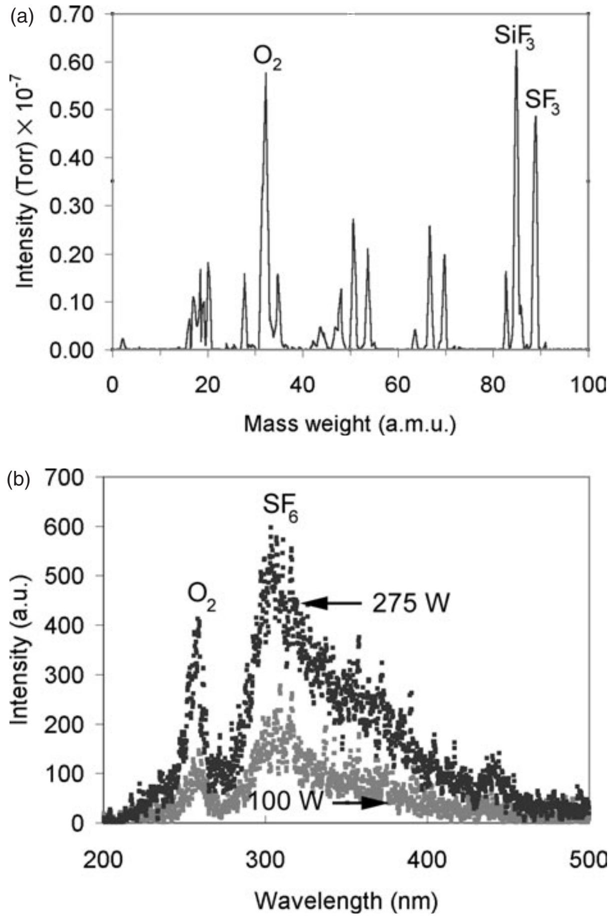

Figure 3. Typical spectra for O_2/SF_6 plasmas: (*a*) QMS, (*b*) OES.

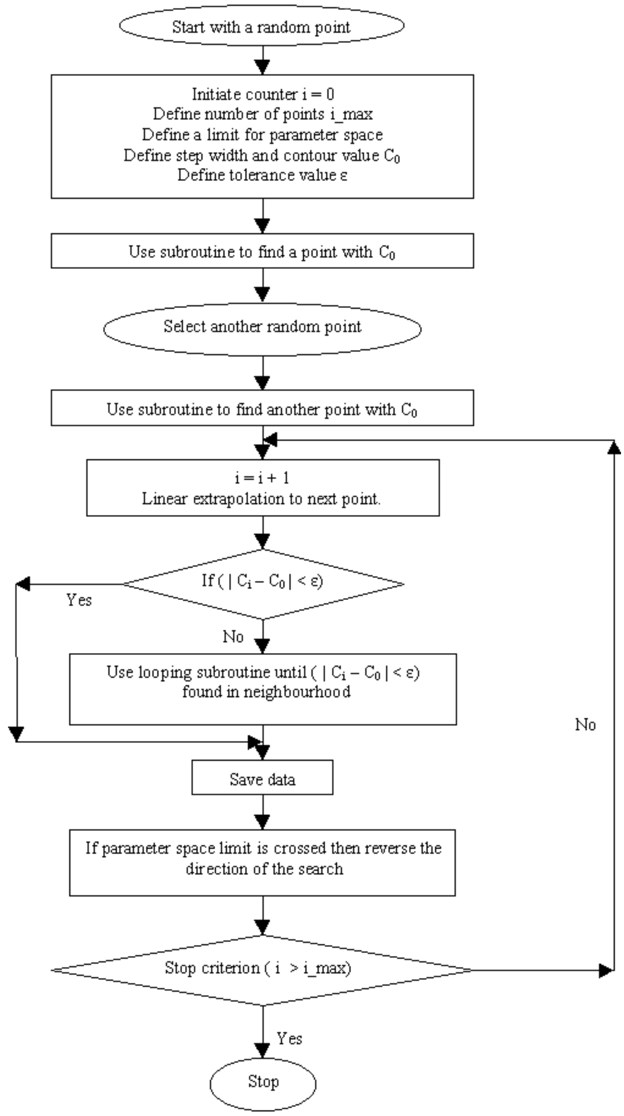

Figure 4. Flow chart of the CF method.

3. System mapping methods

The importance of controlling industrial processes based on plasma technology through the use of a diagnostic measurement system has increased over the last few years. This section presents two methods (CF and multi-dimensional methods) to map the parameter space in terms of power, pressure and the flow rates of two supplied gases. These methods are used to find contours for the ion flux, the DC bias, the ion energy flux, the QMS ratios of two chemical species and the OES line intensity ratios of two emission lines.

3.1. Contour following

The CF method was developed for finding all sets of plasma conditions that give a certain constant plasma parameter, i.e. the contour value, C_0. A point in the parameter space is initially chosen at random. A subroutine such as a gradient descent method is used to find a particular point value on the contour to be traced. To predict the location of another point near the contour, it is assumed that the line followed by the gradient descent is the steepest slope and is hence perpendicular to the contour at the point of intersection. The gradient descent algorithm is then used to locate the contour again, starting from an estimated point. Once two or more points have been located on the contour, then a linear extrapolation and the gradient descent method are used to estimate the next point on the contour. The criterion to accept a trial point as belonging to the contour is

$$|C_i - C_0| \leqslant \varepsilon \tag{1}$$

where C_i is the observed value at the trial point and ε is a pre-defined tolerance. Iteration is continued until the pre-defined number of points are obtained, during which the direction of search is reversed when the parameter space limit is crossed. The flow chart for this method is shown in figure 4.

Results of CF for DC bias, total ion flux, ion energy flux, QMS ratios and OES line intensity ratios in nitrogen and argon plasmas have been obtained and are shown in figure 5. These contours were followed between the limits of the parameter space in both directions. Since the settings and measurements of pressure, RF power and the mass flow rates of nitrogen and argon were passed from and returned to the controller, care was taken to ensure the tolerance was not too small [15].

The technique reveals significant dependences of the DC bias on power and pressure, the ion flux on power and pressure

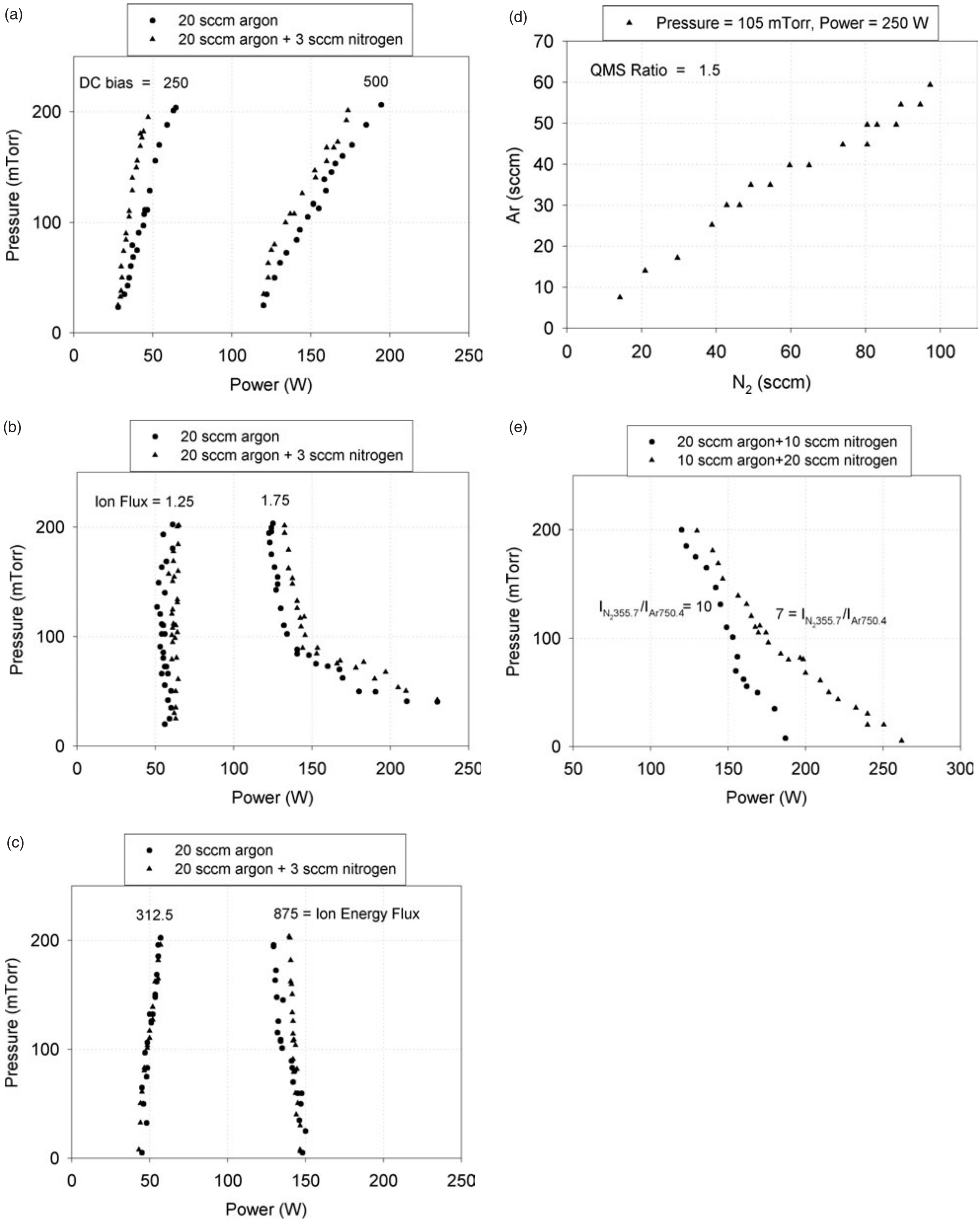

Figure 5. Contours for (*a*) DC bias (V); (*b*) ion flux (A m^{-2}); (*c*) ion energy flux (W m^{-2}); (*d*) QMS ratio and (*e*) OES line intensity ratios. The tolerance, ε, is $\pm 5\%$ of the required contour value.

in part, the ion energy flux on power, the QMS ratios on the flow rates of the two gases and slightly on the power and the OES line intensity ratios on power, pressure and the flow rates of the two gases.

The selection of an appropriate step width in the parameter space for the search was crucial to the performance of the CF method. If the step width is too small the method takes a long time to finish. If the step width is too large then the method

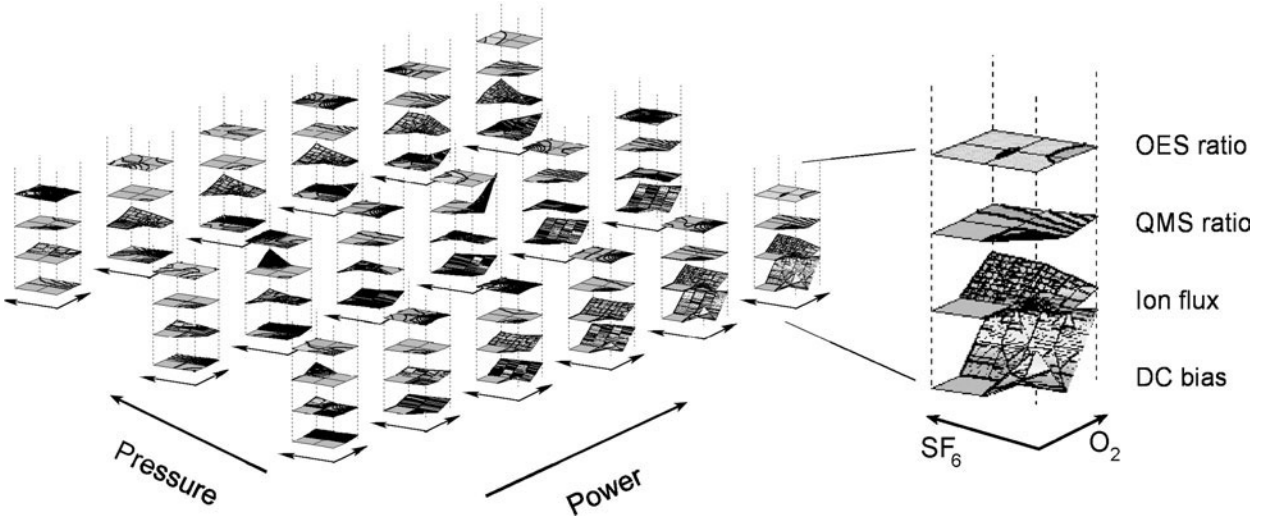

Figure 6. Parameter space display for an O_2/SF_6 plasma. Pressure, 100–300 mTorr; power, 25–300 W; oxygen flow rate, 0–100 sccm; SF_6 flow rate, 50–130 sccm. The signals obtained were 5–400 V DC bias, 0.2–2.5 A m^{-2} ion flux, 3–10 QMS ratio and 0.1–1.7 OES ratio.

takes a shorter time to finish but does not necessarily find the required number of points.

The time taken to determine these contours largely depended on the time taken to make a change to the plasma condition, to wait for it to stabilize and to measure the parameters. Nevertheless, the time taken to find 25 points on a contour was typically only between 10 and 30 min. The mapping of these parameters in this way is considerably easier than by manual (human) methods. There is considerable scope for automatic benchmarking of new systems or re-calibration of systems following maintenance and cleaning cycles using these methods, making the technique a valuable addition to an industrial process.

Hysteresis effects can be seen under certain conditions. Insufficient resolution of experimental measurements can give rise to the false appearance of hysteresis. The nature of our algorithms is such that hysteresis when it occurs would be apparent through data scatter, etc.

3.2. Multi-dimensional mapping

Plasma processes usually involve many parameters that are interrelated in a complicated manner. In order to determine the complex relationship between a number of these parameters, a multi-dimensional mapping method was introduced and applied to a 4×4 dimensional parameter space. The method is based on a simple technique using looping to search the space in terms of power, pressure and two supplied gases. Four output parameters (DC bias, ion flux QMS ratio and OES line intensity ratio) were then recorded. This method represented a fast and effective way of searching a multi-dimensional parameter space. A trial run displaying the mapping results of an O_2/SF_6 etching plasma is shown in figure 6.

The display consists of a subparameter space mapping for each diagnostic result, which is stacked and aligned along another subparameter space axis. In the case shown in figure 6, maps of the four output parameters (DC bias, ion flux, QMS ratio and OES line intensity ratio) are drawn as functions of O_2 and SF_6 content, stacked vertically and aligned as functions of power and pressure.

The time taken to obtain the results above was about 1 h, which is much shorter than that needed by a human operator. The advantages include the simplicity and flexibility of this method, which could be readily extended to encompass an increased number of dimensions or to another system with many more input/output parameters.

4. System searching methods

This section presents powerful techniques that can tune the plasma processing system to the specified optimum in terms of DC bias, ion flux, ion energy flux, QMS ratio and OES line intensity ratio. The direct input parameters of power, pressure and two supplied gases are controlled for the optimization.

4.1. Optimizing a single parameter

This subsection presents a method for searching the parameter space in terms of two input parameters, optimizing only a single output parameter, using the following definition of the fitness, F_i:

$$F_i = \frac{1}{1 + (|C_0 - C_i|/a_0)}, \qquad (2)$$

where C_0 is the target value of the output parameter, C_i is the measured value of the output parameter and a_0 is a constant for weighting.

Gradient descent is a simple method for finding the optimum, but it risks ending in a local optimum. An alternative method that is more likely to yield the global optimum is differential evolution (DE), in which a candidate solution x, referred to as an *individual*, is a real-number coded vector, which represents a set of plasma controlling parameters. Each iteration is referred to as a *generation* and a pool of candidate solutions is referred to as a *population* [16].

For each individual x in the current generation, DE generates a new trial individual x_t by adding a weighted

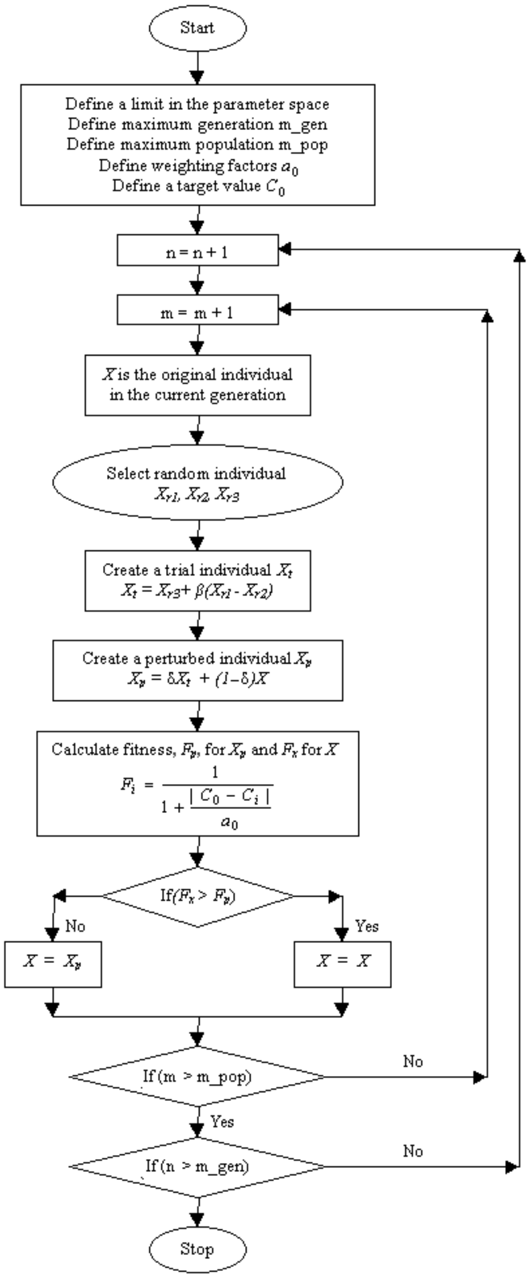

Figure 7. Flow chart of the DE method.

difference vector between two randomly selected individuals x_{r1} and x_{r2} to a third randomly selected individual x_{r3}. The resulting individual x_t is re-combined with the original x. A new individual vector x_p, called the perturbed vector, is thereby created, which consists partly of randomly selected components of x_t and the remaining components from x. This operation is called *crossover*.

The fitness of the perturbed vector x_p is then compared with the fitness of the original vector x. Only if the fitness of the perturbed vector is greater than the fitness of the original one is the perturbed vector copied into the population of the next generation. Otherwise the original vector is copied into the next generation. Figure 7 shows a flow chart of this method.

Results of the DE method applied to searching the specified values of DC bias and total ion flux in argon/nitrogen plasmas for a pressure range of 10–300 mTorr and power range of 10–300 W are shown in figure 8, where the target point is indicated by a solid triangle and all the evaluated candidate solutions are indicated by solid circles. The gas flow rates were set to 20 sccm of argon and 3 sccm of nitrogen. In other words, the optimization was evaluated only in terms of two input parameters. More specifically, this is a case of a one-to-two searching method. It can be seen that the candidate solutions scatter over the power and pressure parameter space, which confirms that DE explores the whole parameter space to seek the global optimum. While the DE is searching to obtain only the one best possible solution, figure 8 classifies all the solutions tried in the parameter space into interpolated surface maps with contours.

In these examples, the time used to search the whole parameter space by DE with a generation of 12 and a population of 15 was about 90 min, while CF takes 25 min to obtain a single contour. These characteristics would help one to choose a method, depending on the purpose of search and the nature of the parameter environment.

4.2. Optimizing multiple parameters

This subsection offers an overall system optimization method in terms of four input parameters (pressure, power and two gas flow rates), taking into account four output parameters by introducing a weighted tolerance, ΔS

$$\Delta S = \frac{|\mathrm{DC}_0 - \mathrm{DC}_i|}{a_1} + \frac{|\mathrm{IF}_0 - \mathrm{IF}_i|}{a_2} + \frac{|\mathrm{MR}_0 - \mathrm{MR}_i|}{a_3} + \frac{|\mathrm{LR}_0 - \mathrm{LR}_i|}{a_4} \quad (3)$$

and

$$F_i = \frac{1}{1 + \Delta S}, \quad (4)$$

where DC_0, IF_0, MR_0 and LR_0 are the target DC bias, ion flux, QMS ratio and OES line intensity ratio, respectively; DC_i, IF_i, MR_i and LR_i are their respective measured values; and a_1, a_2, a_3 and a_4 are constants for weighting each parameter. The values of these constants depend on the application intended. ΔS needs to be given a small nonzero target value.

Two techniques were examined for applying this method to a multi-parameter problem. One of these combines the CF method with equation (3). This obtains a set of solutions in the parameter space for a given tolerance for ΔS. An attempt was then made to choose the best solution out of this set. The other technique combines the DE method with equations (3) and (4). This can find the best possible solution in the parameter space.

Figure 9 compares the two methods of finding a specific point in the parameter space (pressure 10–250 mTorr, power 10–250 W, argon flow rate 10–30 sccm and nitrogen flow rate 5–30 sccm) for a DC bias of 452 V, ion flux 2.47 A m^{-2}, QMS ratio 0.25 nitrogen/argon and OES line intensity ratio 1.7 in nitrogen/argon plasma.

It is observed that the two techniques find the same optimum (power, 124 W; pressure, 78 mTorr; 5 sccm nitrogen; 20 sccm argon). However, the searched area in the method combined with CF is limited, so that there is a risk that the

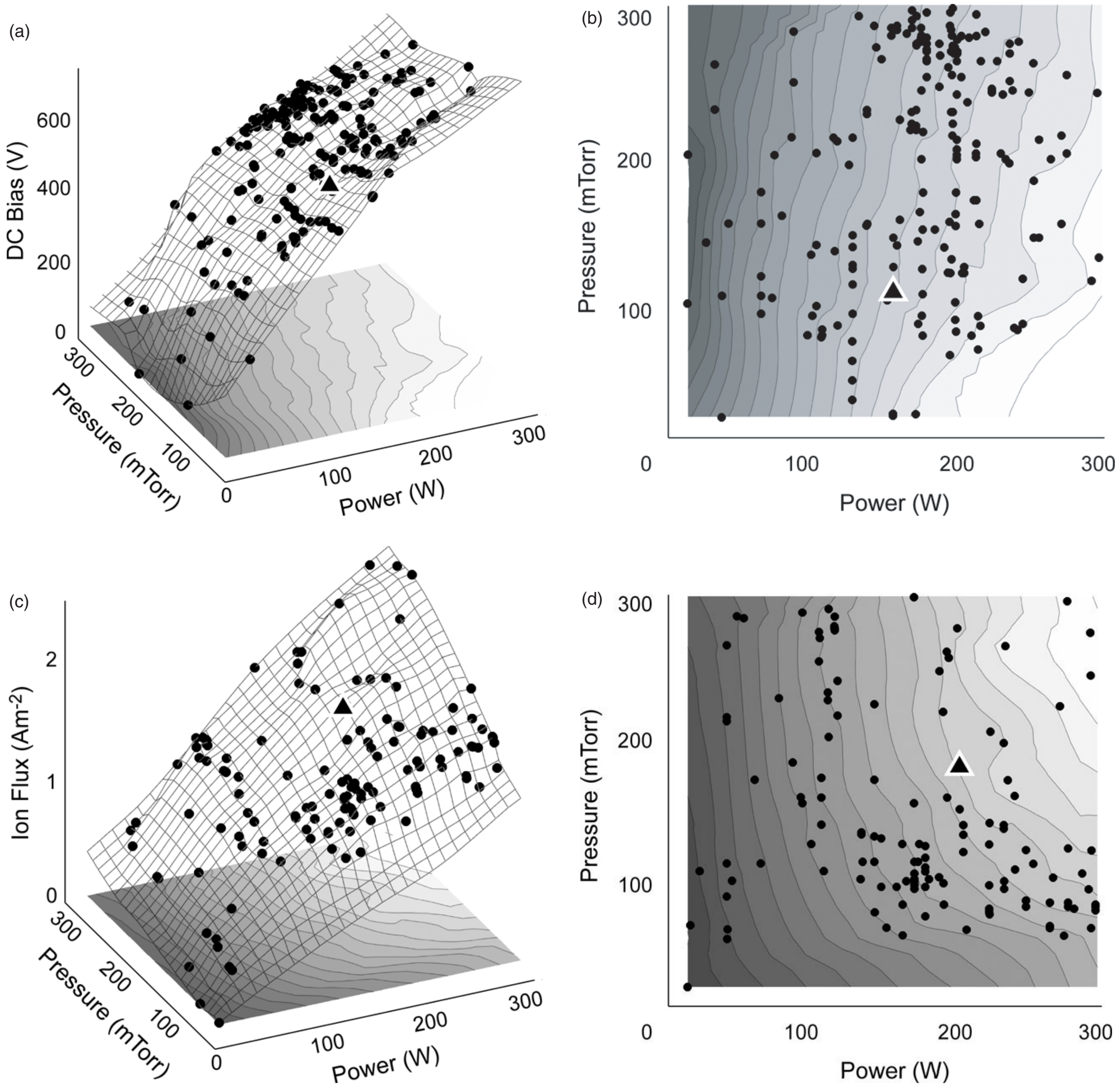

Figure 8. DE method searching for (*a*) and (*b*) DC bias = 500 V; and (*c*) and (*d*) ion flux = 1.7 A m^{-2} in Ar (20 sccm)/N_2 (3 sccm). Candidate solutions, ●; optimized solution, ▲.

method finds only the local optimum (figure 9(*a*)). In contrast, in the method combined with DE, the searched points scatter over the entire parameter space, which means that DE is more likely to yield the global optimum (figure 9(*b*)).The running time with CF was 50 min, shorter than the running time of 90 min with DE. This difference is due predominantly to the time taken to set the input parameters in our plasma system, unlike a pure mathematical system. In both methods, the required optimum was found more quickly and reliably than by a human operator.

5. Plasma etching control

In order to demonstrate the potential of our technique when applied to a real plasma process, silicon wafers masked with patterned aluminium have been etched with SF_6/O_2 plasmas. When silicon is etched vertically between the masked regions, the side walls exposed to the plasma may be subject to competition of lateral etching and sidewall deposition. Although certain plasma conditions may be suitable for etching at the bottom surface which is bombarded by energetic ions, they may also be suited to deposition at the side wall, with scarce bombardment.

The balance between etching and deposition is illustrated by the selectivity inversion in silicon film processes [17, 18]. Seeking out these regions of parameter space and then controlling a plasma within them poses a challenge, because finding an optimum condition is usually a difficult and complicated task, requiring an extended search of the parameter space. Our system made it possible to find an optimum in as few as 20 etch trials.

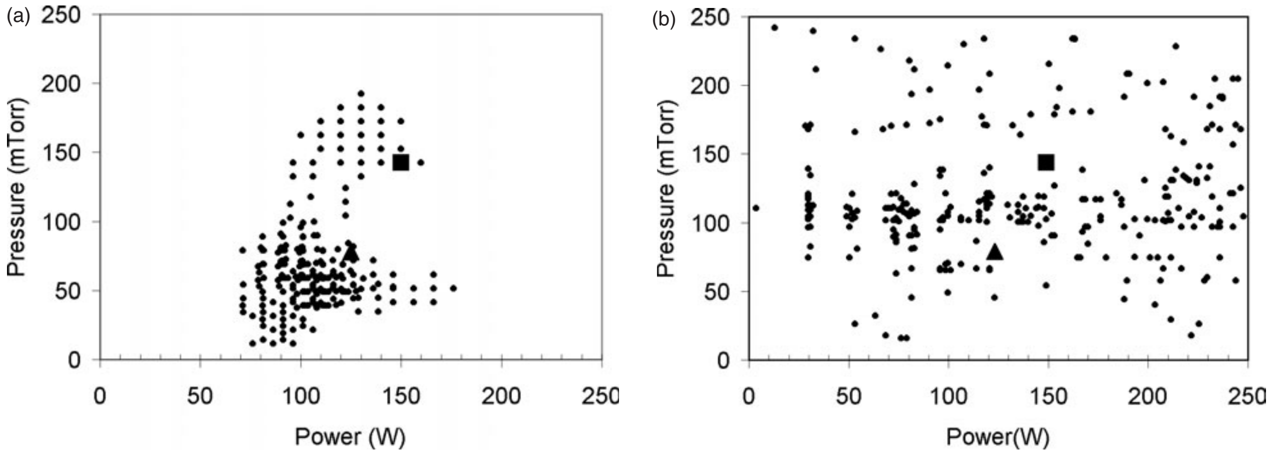

Figure 9. System optimum found by (*a*) CF method combined with equation (3); (*b*) DE method combined with equations (3) and (4) for DC bias 452 V, ion flux 2.47 A m^{-2}, QMS ratio 0.25 nitrogen/argon and OES line intensity ratio 1.7 nitrogen/argon. ● are search points, ■ are start points and ▲ are the identified optima (pressure 78 mTorr, power 124 W, 3 sccm nitrogen and 20 sccm argon).

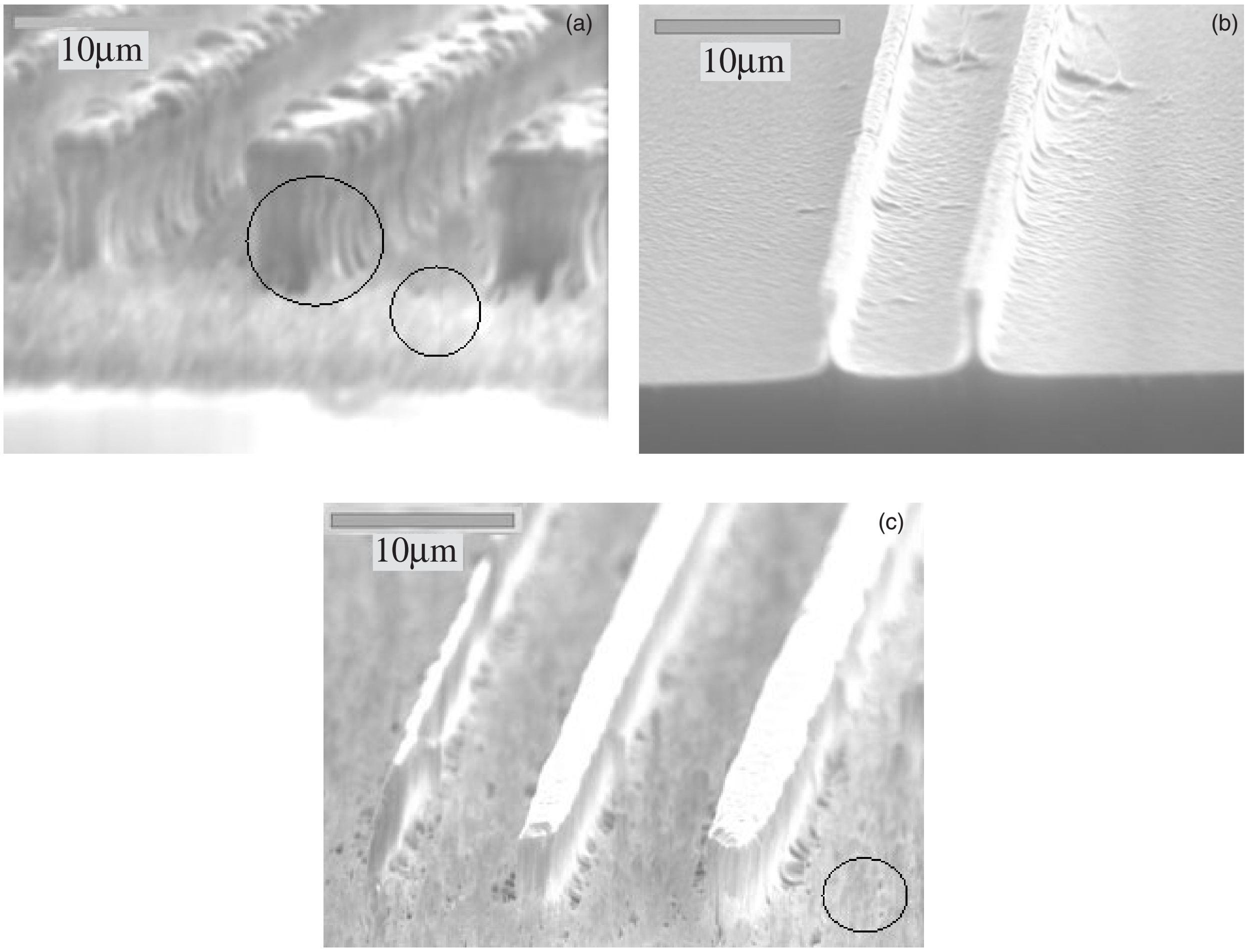

Figure 10. Electron micrographs of silicon etched for 20 min using a fluorine/oxygen based plasma: (*a*) continuous etching; (*b*) etching paused for 60 s after every 15 s; (*c*) etching paused for 180 s after every 15 s etching.

The etching characteristics of silicon that we aimed to achieve here were directionality with a considerable etch rate and smoothness of the etched surface. Since these characteristics are currently analysed only off-line after processing, the mapping results of plasma parameters described in figure 6 and empirical trends about etching (e.g. that a higher DC bias gives higher directionality) were used as knowledge bases for guiding the search strategy. Using these knowledge bases, we first chose several etch-condition candidates from the parameter space. The resultant etch features were evaluated by SEM and fed back to further searching for the optimum etching condition, again with the aid of the knowledge base. After 20 etch trials in total, a condition was found that gave an almost perfect vertical mesa in silicon.

Figure 10 shows SEM images of an etched silicon wafer using a SF_6/O_2 plasma away from and on the optimum condition. All three samples shown were etched at 100 mTorr and 275 W, with gas flows of 50 sccm oxygen and 50 sccm SF_6. The resultant plasma parameters were: DC bias 300 V, ion flux 1.2 A m^{-2}, QMS intensity ratio 3.33, OES line intensity ratio 1.43 and etch rate 0.4 $\mu m\,min^{-1}$ averaged over the etching time of 20 min. The three samples show the effects of different etch sequences (duty cycles), each with a total etch time of 20 min. In the optimum condition shown in figure 10(*b*), directional etching with a smooth surface was observed, whereas in the other off-optimized conditions shown in (*a*) and (*c*), an undercut (the large circle) or roughness (the small circle) was observed.

The pauses in the etching sequence may have caused a difference in the surface reaction temperature due to the lack of an effective cooling mechanism for the sample wafer in our current plasma system, so that removal of heat generated by plasma exposure takes a time comparable with that of the sequence time. Another possibility could be the effects of contamination, because our system is not ultra-high vacuum (UHV) compatible nor equipped with a load-lock for wafer introduction, where inhomogeneity through contamination on a micro-scale could cause temperature-dependent roughness. Even without such equipment for cooling and UHV, our approach has found a satisfactory etching condition as shown in figure 10(*b*). Although we have used empirical or physical and chemical knowledge bases for searching the etching condition in this study, future developments of *in situ* diagnostics could be readily installed into the system. The system is also advantageous in maintaining the optimum condition during processing in a complex parameter space despite drift in some of the process parameters.

6. Conclusions

New techniques have been developed for control and optimization of low temperature plasma processes, thereby avoiding wastage of materials and energy. The performance has been demonstrated by CF of the DC bias, total ion flux, ion energy flux, QMS ratios and OES line intensity ratios, as well as by a multi-dimensional mapping for 4 inputs $\times$ 4 outputs. The performance of CF and DE optimization algorithms has been compared in both the single and multiple parameter problems. The two techniques have shown a good agreement in characterizing a parameter space, but CF has searched more quickly within a narrower area of search space than DE. These methods have reduced significantly the time to re-configure the system and would benefit the transfer of processes between different systems. Our approach has also been used with empirical knowledge to find quickly an optimum condition for directional etching of silicon.

The strategy and novel methods developed here for parameter searching and control of plasmas are generic technologies that are applicable to a wide range of manufacturing industries. The plasma community will also benefit directly from application of these techniques to optimization and control of plasma processes. Plasma users can anticipate benefits such as improved quality control of plasma processing, improved plasma process reproducibility, the ability to quickly search for new plasma processing conditions and reducing running costs. Plasma equipment providers can also anticipate benefits such as quality assurance, flexibility to modify and customize a plasma system to meet specific needs and self-tuning with automatic determination of optimum operation conditions for the individual plasma processing equipment.

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