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A cellular automata simulation of atomic layer etching

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ABSTRACT

A two-dimensional, cellular automata model for atomic layer etching (ALE) is presented and used to predict the etch rate and the evolution of the roughness of various surfaces as a function of the efficiencies or probabilities of the adsorption and removal steps in the ALE process. The atoms of the material to be etched are initially placed in a two-dimensional array several layers thick. The etch follows the two step process of ALE. First, the initial reaction step (e.g., Cl reacting with Si) is assumed to occur at 100% efficiency activating the exposed, surface atoms; that is, all exposed atoms react with the etching gas. The second reaction step (e.g., Ar ion bombardment or sputtering) occurs with efficiencies that are assumed to vary depending on the exposure of the surface atoms relative to their neighbors and on the strength of bombardment. For sufficiently high bombardment or sputtering, atoms below the activated surface atoms can also be removed, which gives etch rates greater than one layer per ALE cycle. The bounds on the efficiencies of the second removal step are extracted from experimental measurements and fully detailed molecular dynamics simulations from the literature. A trade-off is observed between etch rate and surface roughness as the Ar ion bombardment is increased.

Keywords: Atomic layer etching, cellular automata, simulation

1. INTRODUCTION

Nanoscale device fabrication increasingly requires near atomic-scale precision[1-5]. Advanced lithography, deposition and etching methods are being developed to meet these requirements. Atomic layer etching (ALE) is currently the method expected to achieve the desired precision for critical dimensions (CDs) and variations in CDs in the future[6-7]. ALE achieves this by ideally removing one surface layer of a selected material at a time.

ALE is a two-step process, and its fundamental mechanism can be illustrated by considering the etching of silicon[6, 8]. In the first step, the silicon surface is exposed to chlorine gas. At a sufficiently high pressure and time, the surface atoms of silicon are chlorinated. Very little chlorine penetrates beyond the first layer, and the process is practically self-limiting. In the second step, the chlorinated surface is bombarded with Ar^+ ions to facilitate the removal of the $SiCl_x$ from the top level. The two steps comprise an etch cycle that is repeated to reach the desired levels of etch.

Rapid cycling of the gases in the two-step ALE process is a challenge to ensure sufficiently high throughput in the process[5-6]. Increases in the power of the plasma can accelerate the second step but at potential cost to etching beyond the top layer of the material. Simulations can provide insight into the trade-offs between increased etch rate and surface roughness as a result of increased power.

Molecular dynamics and coupled plasma simulations with cellular automata have been used to explore ALE[9-12]. Here we present a simpler cellular automata method where the probabilities of removing atoms are based on experimental measurements in the literature. These probabilities vary with the power applied to the plasma in the second step and the coordination of the exposed atom relative to other atoms on the surface. The resulting surface become rough with etching, with roughnesses up to 2.5 atomic layers. The roughness evolves slowly, requiring many etch cycles to reach

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steady state. A correlation is found between the layers etched per cycle and the roughness of the surface. The layers etched per cycle and the roughness are found to be related to the probabilities of removal of atoms.

2. METHODOLOGY

2.1 Model

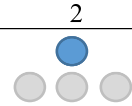
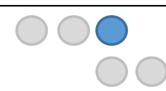
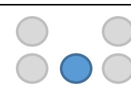
We create a two-dimensional cellular automata simulation to understand the evolution of etch rate and surface roughness for ALE. The system consists initially of an array of atoms placed in a square pattern over a rectangular grid. The particles are arranged on the surface to form a smooth, sinusoidal or square-wave profile. The latter two arrangements are meant to simulate surfaces that are initially rough. Once the positions of the atoms are specified the, the simulated etching process begins. Similar to atomic layer etching of silicon by chlorine and argon in a two-step process, the simulated behavior of the atoms on or near the surface follows two steps.

In step one, the surface atoms are activated by reaction with a gaseous species, such as chlorine on silicon. It is assumed that all atoms exposed on the surface are activated with a probability of 100%. This is reasonable for fast surface reactions and sufficiently long reaction times. In step two, the activated surface atoms are removed based on the second reaction. This second reaction is assumed to be similar to the removal of silicon activated by chlorine due to the impact of argon atoms in the plasma. In this second step the probability of desorption of the atom depends on the position of the activated atom relative to other atoms on the surface. In addition argon bombardment and sputtering effects can remove the atom underneath the surface atom. This also occurs at a probability that depends on the position of the atom in consideration. In general this secondary removal has a lower probability than the removal of the overlying activated atom. Also, the secondary removal can only occur once the overlying atom has been removed.

2.2 Computational Implementation

The computational implementation of this process is as follows. All the atoms exposed to the surface are activated in the first step of the ALE process. In the second step, probabilities of removal are assigned based on five possible atom configurations of the nearest and next nearest neighboring atoms (Table 1). An activated surface atom is removed if a random number drawn from a uniform distribution from zero to one is less than the probability of desorption for its configuration. Note that the atoms are assumed to be removed simultaneously based on the initial exposure of the surface atom in a given cycle. Removal of an atom during a cycle does not change the desorption probability of neighboring surface atoms. After some of the surface atoms are removed, their underlying atoms are removed with the probabilities listed in Table 1 due to energetics of the etching ions, such as Ar+ for silicon.

Table 1. Probabilities for the desorption of atoms (blue) depending on five types of of configurations of surrounding atoms (gray). Set 1 is the base case and assumes no bombardment or sputter that can remove underlying atoms.

	Configuration 1	Configuration 2	Configuration 3	Configuration 4	Configuration 5
Configurations					
Probabilities - Set 1 (no sputter)	85%	100%	92.5%	70%	72.5%
Probabilities - Set 2	100%	100%	100%	85%	93%
Sputter Probabilities - Set 2	15%	25%	20%	5%	10%
Probabilities - Set 3	100%	100%	100%	100%	100%
Sputter Probabilities - Set 3	25%	35%	30%	15%	20%

The probability of removing an atom is assumed to depend on its position with respect to neighboring atoms. In general, the more exposed or the fewer neighbors the surface atom has, the greater the probability of removal during the ALE cycle. Accordingly, the relative values of the configuration probabilities for each probability set are qualitatively reasonable. Moreover, the absolute values of the configuration probabilities are consistent with experimental observations of etch rates per ALE cycle. Ideal ALE removes one layer of atoms per cycle. The removal of atoms from the layer just underneath the surface layer due to the argon bombardment and sputtering enables etch rates greater than one layer per cycle, which is observed in experiments[8, 13].

Three sets of probabilities are considered here. Set 1 is a base case assuming no sputter where only surface atoms may be removed during a cycle. Sets 2 and 3 include the possibility of sputter to remove the atoms in the second layer. The probabilities for removal grow proceeding from Set 1 to Set 3. This increased probability, especially of the sputter, aims to capture the effects of increased power during the argon etch in ALE. The probabilities in Table 1 are based on experimental measurements[8, 13-14] and produce etch rates from about 0.8 to 1.2 layers per cycle.

The initial surfaces are flat, sinusoidal or a square wave. The latter two can have different amplitudes and wavelengths. During the course of the simulations, the average position of the surface is computed to determine the etch rate per cycle. The standard deviation of the positions of the surface atoms relative to the average position of the surface is computed to measure the surface roughness. Next the evolution of the position of the surface and its roughness are explored for the different sets of probabilities and initial surfaces.

3. RESULTS

Figure 1 illustrates the evolution of an initially flat surface as it is etched according to the Set 1 probabilities. Because the probability for removal of an atom in configuration 1 on the surface is less than 100%, the surface roughens as the etch proceeds. Fig. 1e illustrates the etch depth versus the cycle number. The etch rate from the slope of the data is constant and 0.87 layers per cycle. Fig. 1f shows the evolution of the standard deviation or roughness of the surface. It reaches a constant of about 0.7 layers in about 10-12 etch cycles.

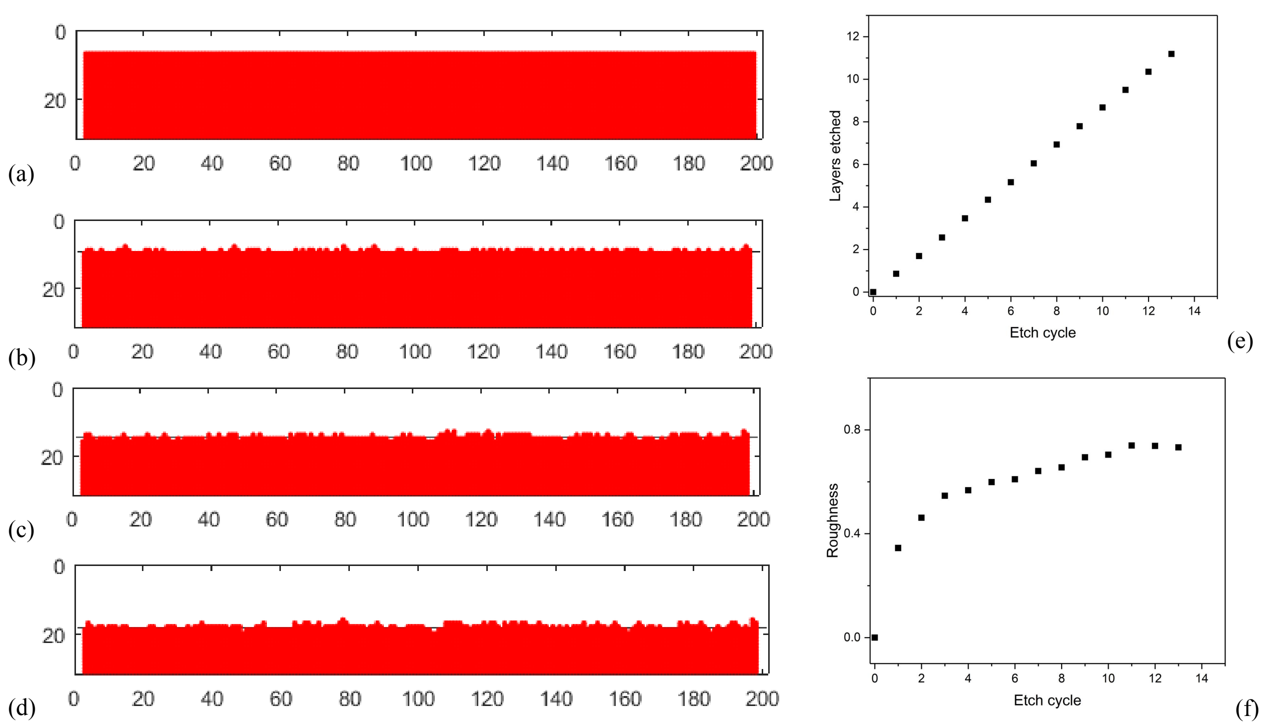


Figure 1. Evolution of an initially flat surface with Set 1 probabilities. Images of the surface at etch cycle (a) 0, (b) 4, (c) 10,and (d) 14. The layers etched (e) and the standard deviation or roughness of the surface (f) as a function of etch cycle.

Figure 2 illustrates the evolution of an originally flat surface according to the Set 2 and Set 3 probabilities. The surfaces are much rougher because of the additional removal due to sputter. The interface also etches more quickly at a rate of 1.14 and 1.27 layers per etch cycle for Set 2 and Set 3 probabilities, respectively. Again, the average etch rate is constant throughout the process as noted by the remarkably linear plots in Fig. 2g. A greater number of etch cycles is needed to achieve the steady state with sputter compared to without it. The roughnesses are about 1.1 and 1.45 for the Set 2 and Set 3 probabilities, respectively.

The effect of initial roughness is explored in simulations for surfaces with initially sinusoidal or square wave patterns as show in Fig. 3. The patterns of the initial roughness are degraded considerably after around 13 etch cycles. The periodicity of the pattern, however, is apparent even after 20 etch cycles. As will be shown later, it takes many more cycles for the etched surface to no longer reflect its starting configuration. The layers etched versus the etch cycles is the same for the sinusoidal and square wave surface for the probabilities of Set 2 as seen in Fig. 3g. The etch rate is 1.16 layers per etch cycle, which is the same as that for an initially flat interface. Indeed we find that the etch rate depends only the probability set and not on the initial configuration of the surface.

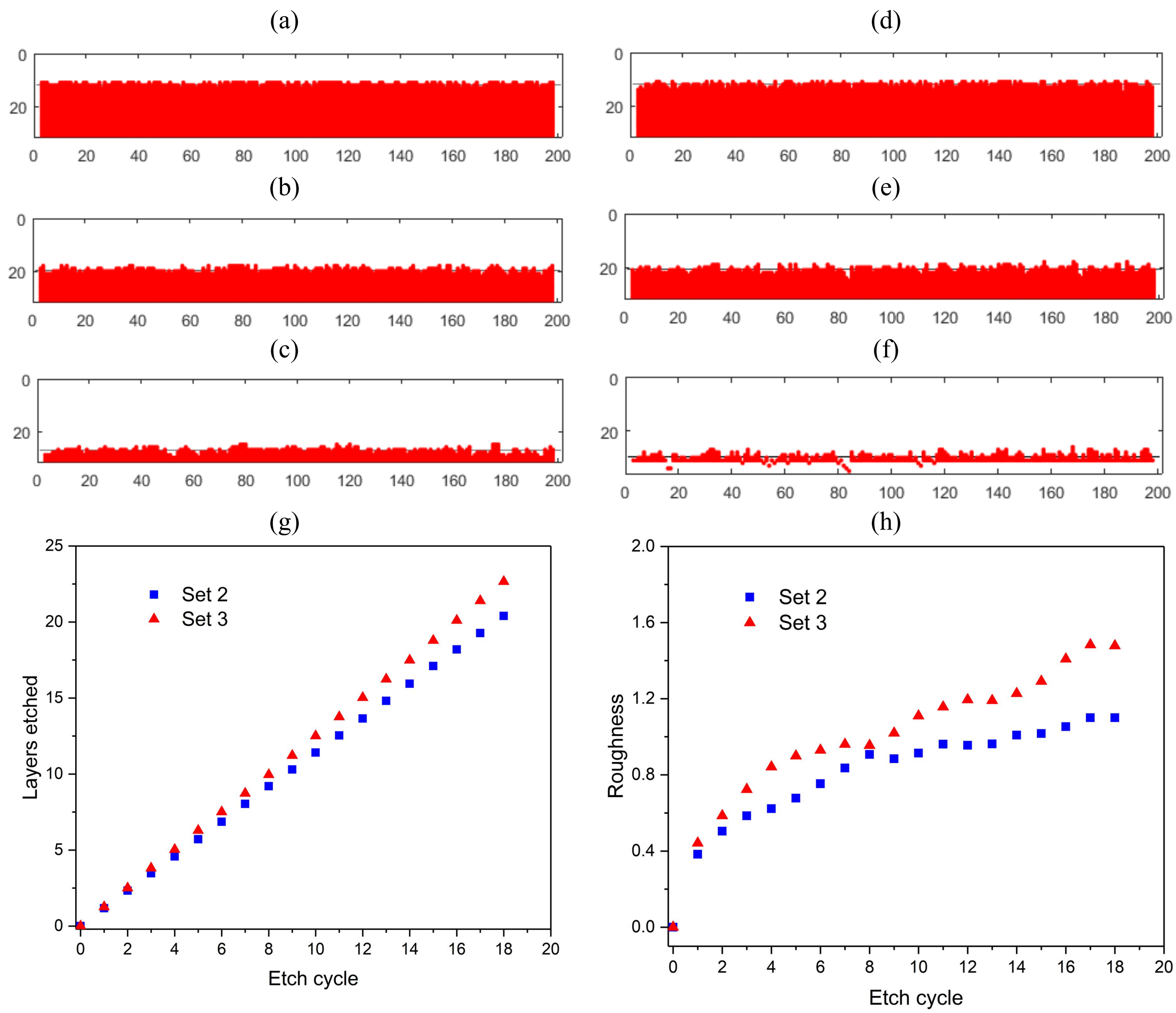


Figure 2. Evolution of an initially flat surface with Set 2 and Set 3 probabilities. Set 2 for etch cycles (a) 6, (b) 13, (c) 20 and Set 3 for etch cycles (d) 6, (e) 13, (f) 20. The layers etched (g) and the standard deviation or roughness of the surface (h).

The roughnesses in Fig. 3h for the sinusoidal and square wave surfaces decreases with the number of etch cycles, showing a smoothing from the initially non-flat surfaces. The rates of decrease of the roughness are about the same. They have not reached a steady-state even after 50 etch cycles.

The number cycles to reach a steady state roughness depends on the initial configuration of the surface and the probability set. Fig. 4 shows the evolution of roughnesses for initially flat and sinusoidal surfaces with probability Set 2. The initially flat surface roughens to steady state value of about 1.6 at around 50 etch cycles. The initially sinusoidal surface reaches a steady state value of the roughness of about 1.9 in about 150 cycles. This is because considerably more etch cycles are required for the roughness on the second surface to no longer show any remnants of its initial sinusoidal shape. In general the initially flat interface with probability Set 1 takes the least number of cycles (around 80) to reach a steady-state roughness and the initially square patterned surface with probability Set 3 takes the most number of cycles (around 200).

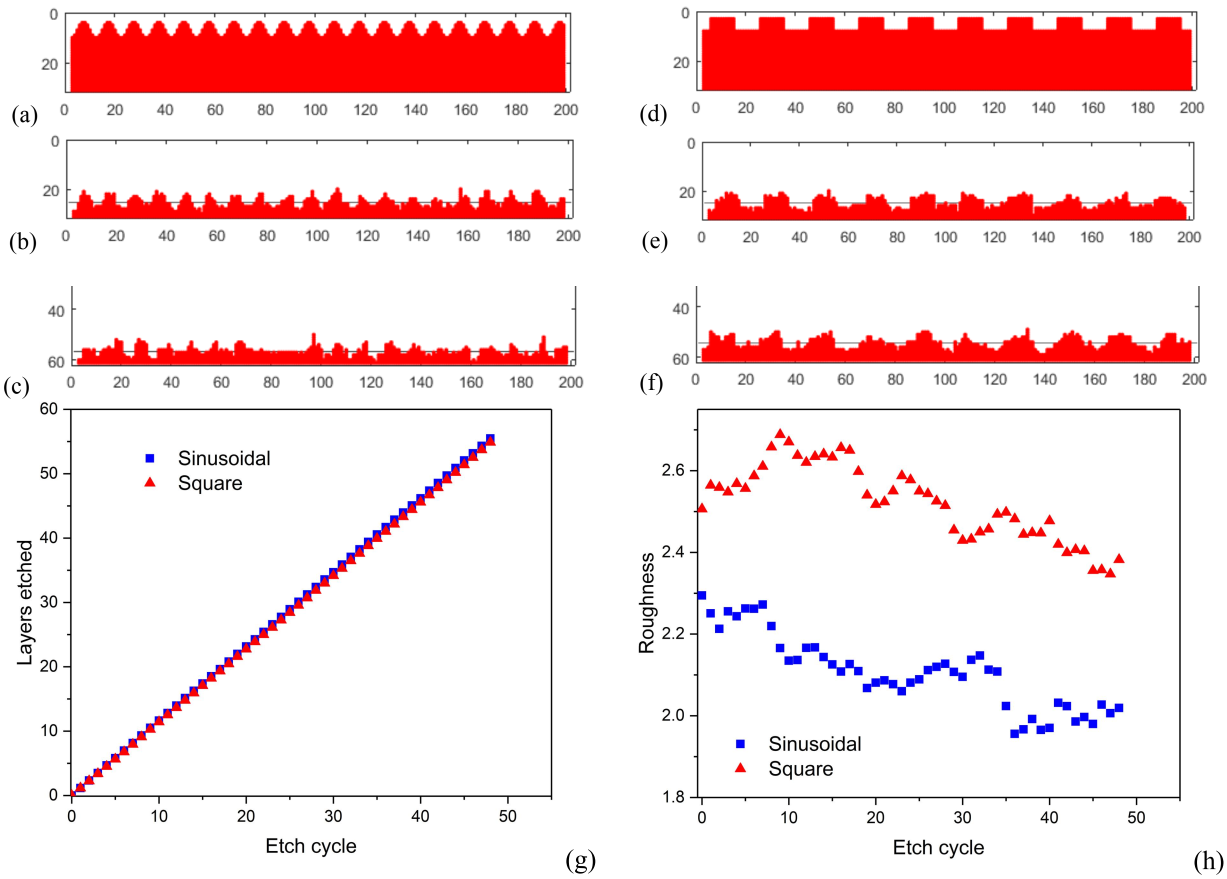


Figure 3. Evolution of initially sinusoidal and square wave surfaces with Set 2 probabilities. The amplitude and period for both are x and y, respectively. Initially sinusoidal surface for etch cycles (a) 0, (b) 18, (c) 45 (and initially square wave surface pattern for etch cycles (d) 0, (e) 18, (f) 45. The layers etched (g) and the roughness (h) is also presented.

4. DISCUSSION

The layers etched per cycle and the steady-state roughnesses for the three different probability sets and five different configurations are listed in Table 2. The layers etched per cycle or etch rates are independent of the initial configuration of the surface and increase with increasing etch probabilities. The etch rate for probability Set 1 of about 0.88 is close to the average of the probabilities of configurations 1-5 of Set 1 in Table 1, which is 0.84. The discrepancy is due to the fact that the lower probability configurations are sampled at slightly lower frequencies. Similarly, if the probabilities for each of the two rows for Set 2 are averaged and summed, the estimated etch rate is 1.11 close to the observed value of 1.16. The estimated layers etched for Set 3 is 1.25, very near the observed 1.28.

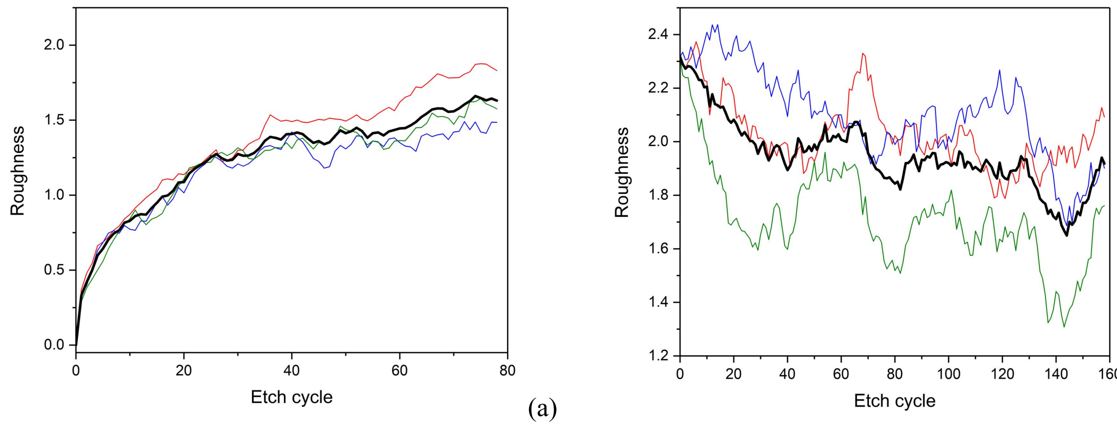


Figure 4. Evolution of the roughness for three different realizations of the etch on initially flat (a) and sinusoidal (b) surfaces for probability Set 2. The colored lines are the different realizations and the thicker black line is the average of the realizations.

The roughnesses are independent of the initial configurations of the surfaces and depend more strongly on the probability sets. There is greater roughness the greater the average sputter probabilities. The square patterned surface shows a greater roughness in general than the initially flat surface.

Table 2. Layers etched per cycle/roughness for different probability sets and initial configurations of the surface

Initial Surface	Probability Set 1	Probability Set 2	Probability Set 3
Flat	0.87 / 1.20	1.14 / 1.75	1.27 / 2.75
Sinusoidal	0.89 / 1.40	1.16 / 1.63	1.28 / 2.70
Square Wave	0.89 / 1.50	1.16 / 1.91	1.28 / 2.85

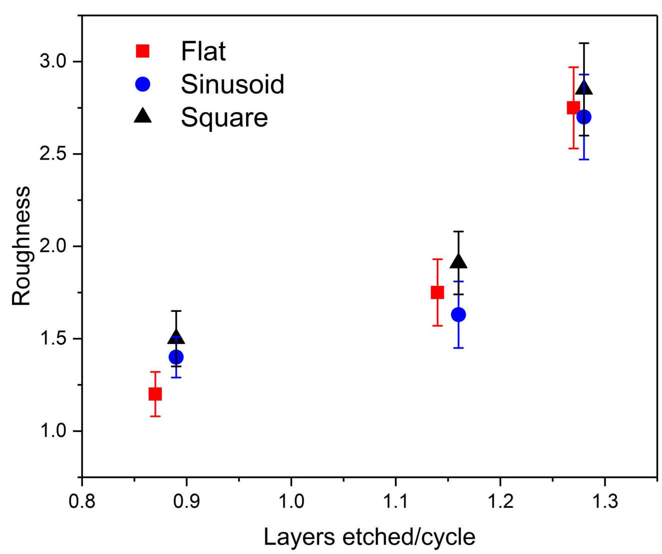


Figure 5. Standard deviation or roughness of surface versus the etch rate for initially flat, sinusoidal and square wave patterned surfaces. The error bars are based on averages of three realizations each for the roughness at steady-state for the specific initial surface and probability set.

There is a tradeoff between etch rate and roughness of the surface as seen in Fig. 5. Faster etch rates result in great roughness. This is because the sputter which increases the etch rate, but is less effective at removing atoms surrounded by more atoms. Because speed is a critical factor in the application of ALE, these results indicate that the tolerance for roughness will dictate the etch rate for the conditions explored here.

5. CONCLUSIONS

A cellular automata model has been presented to simulate atomic layer etching (ALE). The probability of removal of the atoms depends on their exposure to the surface. Increased power increases the probability of removal including removal of secondary layers due to sputter. The etch rate depends only on the probability sets used and not on the initial configurations of the surface, whether they be flat, sinusoidal or square patterned. The roughnesses are also independent of the initial configurations of the surface and increase with the increasing probabilities of removal of surface atoms and sputter probabilities. The roughness correlates strongly with the etch rate and so there is a trade-off between desirable higher etch rates and undesirable roughness. Smoother surfaces require lower plasma energies to minimize the sputter removal of additional layers of atoms.

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