# Effects of RF-driven ion energy distribution on atomic layer etching of Si-based materials

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**Abstract:** Molecular dynamics simulations were performed to examine the influence of the radiofrequency (RF)-driven ion energy distribution function (IEDF) on the plasma-enhanced atomic layer etching (PE-ALE) of Si-based materials. The etching mechanisms, mixing layers, and resulting surface structures from the RF-driven IEDF will be compared with those obtained from monoenergetic Ar ions.

#### 1. Introduction

Plasma-enhanced atomic layer etching (PE-ALE) is a promising technique in the ongoing improvements of semiconductor manufacturing processes. The process alternates between surface modification and ion-induced desorption steps. In many plasma systems, the ion energy distribution function (IEDF) is non-uniform, indicating that ions impact surfaces at distinct energies. In this research, the RF-driven IEDF is used to understand its effects on the etching behavior of the PE-ALE process.

#### 2. Methods

A rectangular Si model system with an initial depth of 2.72 nm and dimensions of  $3.26 \times 3.26$  nm<sup>2</sup> was used to perform molecular dynamics (MD) simulations. The simulation followed Ref. [1], with the main difference of using RF-driven IEDF instead of monoenergetic Ar ions. The surface modification was done by exposing the Si surface to Cl ions, each with an incident energy of 20 eV. Subsequently, the modified surface was bombarded by Ar ions, each ion having an incident energy selected at random based on the IEDF from Ref. [2] and shown in Fig. 1.

## 3. Results and Discussion

Figure 2 (a) shows the atomic Si surface structure after the surface modification step. It is seen that Cl atoms tend to mix with the surface Si atoms. In Fig. 2(b), the atomic structure is taken after Ar ion bombardment with an ion dose of  $4.71 \times 10^{16}$  cm<sup>-2</sup>. From the IEDF, the average ion energy is about 50 eV. It is seen that most of the Cl atoms were removed from the surface, where some penetrated into the bulk. Also, the surface layer became amorphous after being bombarded with Ar ions.

To understand the effects of the RF-driven IEDF on the PE-ALE process, the etching mechanisms and surface structures after several PE-ALE cycles will be compared to the results obtained from using monoenergetic Ar ions.

### 4. Conclusion

MD simulations were performed to understand the effects of the RF-driven IEDF on the PE-ALE of Si-based materials. The differences in etching mechanisms and surface structures due to ion characteristics between monoenergetic Ar ions and Ar ions with an RF-driven IEDF will be compared.

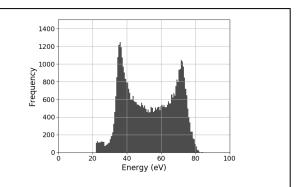
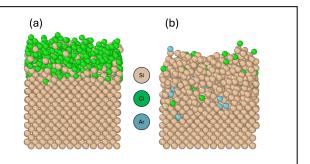


Fig. 1. IEDF sampling used for Ar ion bombardment with an average ion energy of 50 eV.



**Fig. 2**. (a) Atomic structures taken after the surface modification step, and (b) the resulting surface structure after Ar ion bombardment with an ion dose of  $4.71 \times 10^{16}$  cm<sup>-2</sup>.

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#### References

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