Supporting Information for

Different Etching Mechanisms of Diamond by Oxygen and Hydrogen Plasma: A Reactive Molecular Dynamics Study

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Etching results of the expanded simulation model

Simulations have been performed via expanding the model size of the original diamond (100) surface to $15.1 \times 20.2 \times 80.0$ Å under the continuous oxygen and hydrogen atoms etching with incident energies of 10 eV and 40 eV, and the other setting parameters have not been changed. The detailed results of the simulations are shown in Figure S1-S4.
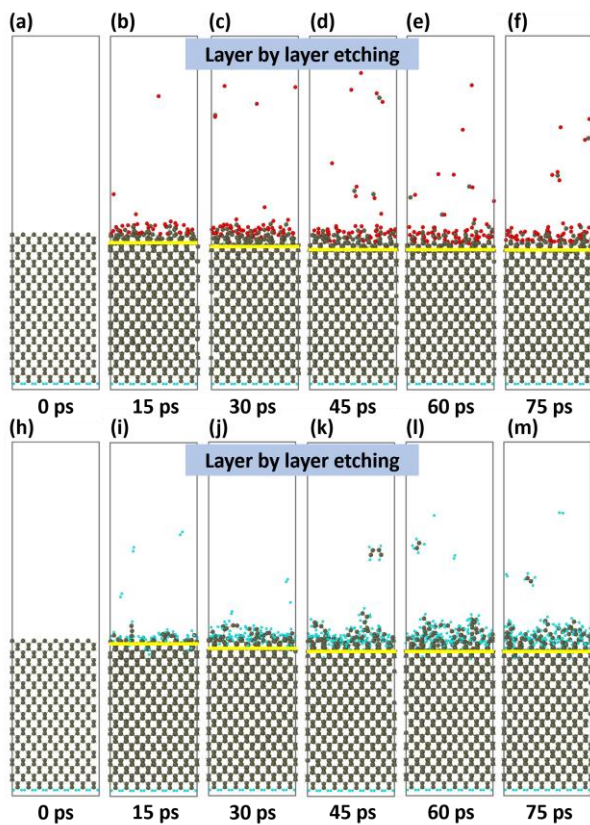

Figure S1. Snapshots of the diamond etching process by continuous irradiation of (a)-(f) oxygen and (h)-(m) hydrogen atoms with an incident energy of 10 eV. Dark grey, light blue, and red spheres indicate carbon, hydrogen, and oxygen atoms, respectively.
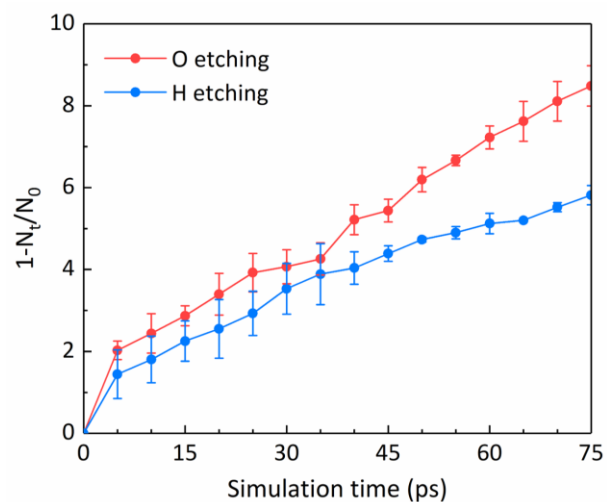
Figure S2. Time evolution of the loss rate of carbon atoms in diamond structure under the incident energy of 10 eV. The averaged data with the error bars for three simulation runs are shown.
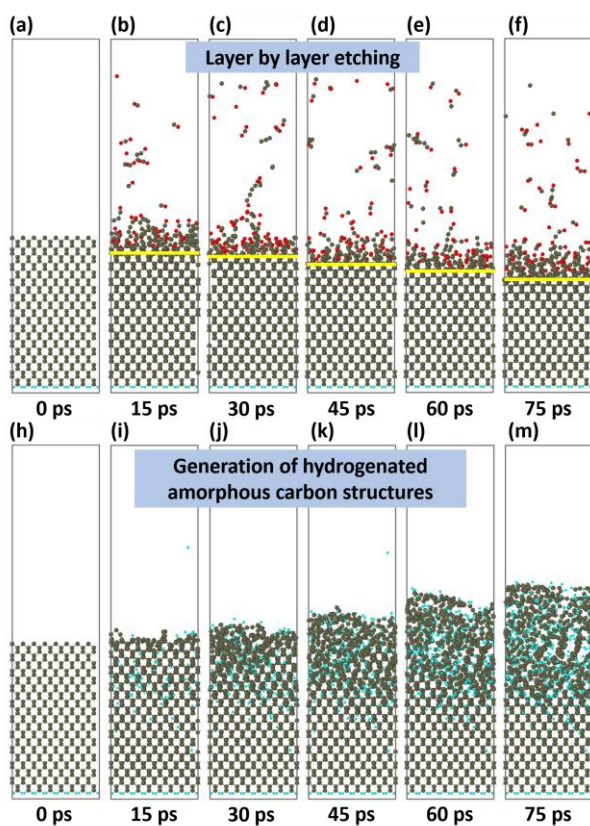
Figure S3. Snapshots of the diamond etching process by continuous irradiation of (a)-(f) oxygen and (h)-(m) hydrogen atoms with an incident energy of 40 eV. Dark grey, light blue, and red spheres indicate carbon, hydrogen, and oxygen atoms, respectively.
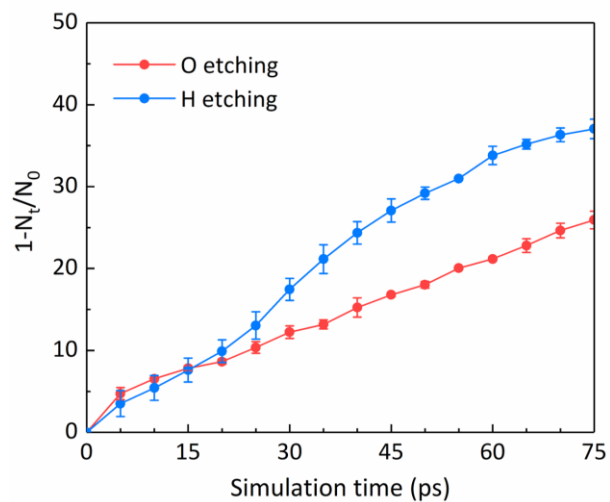

Figure S4. Time evolution of the loss rate of carbon atoms in diamond structure under the incident energy of 40 eV. The averaged data with the error bars for three simulation runs are shown.

The loss rate of carbon atoms in diamond structure at the end of simulation
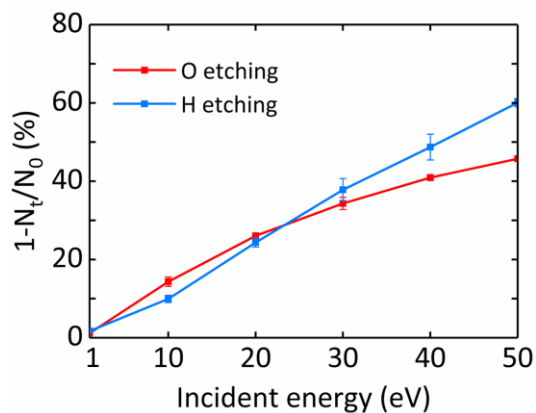

Figure S5. The loss rate of carbon atoms in diamond structure at the end of simulation as a function of different incident energies under oxygen and hydrogen plasma etching. The averaged data with the error bars for three simulation runs are shown.

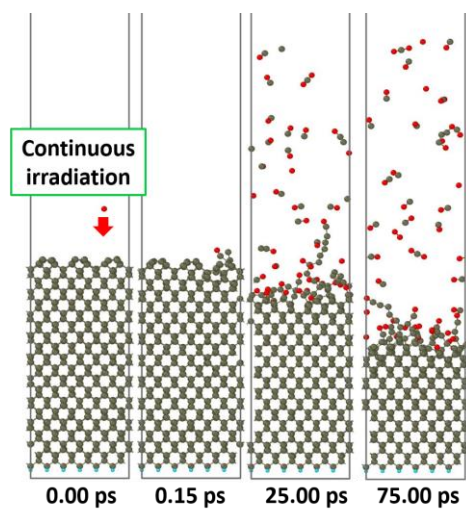**Snapshots of the diamond etching process by oxygen atoms**

Figure S6. Snapshots of the diamond etching process by oxygen atoms with an incident energy of 40 eV at t = (a) 0.0, (b) 0.15, (c)25.0, and (d) 75.0 ps. Dark grey and red spheres indicate carbon and oxygen atoms, respectively.