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Quantum chemical investigation for Chemical dry etching by flowing NF_3into H_2 down flow plasma TOSHIO HAYASHI, KENJI ISHIKAWA, MAKOTO SEKINE, MASARU HORI, AKIHIRO KONO, Nagoya University, KOUKOU SUU, ULVAC Inc. — The molecular orbital calculations were carried out in order to clarify the reaction schemes of the chemical dry etching using H_2 down flow plasma and NF_3 flowing. It was found that not only HF formation but also F atom generation takes place. And this F atom generation mechanism is very important to realize the highly selective SiO_2 etching process. Probably F formation is suppressed under the three-body reaction regime and the higher gas flow rate of H_2 than that of NF_3. So, careful control of the pressure is a key factor. The examined reaction schemes do not only take place in the vapor phase but also in the condensed phase on the wafer surface. As a result, complex $(NH_4)_2SiF_6$ is formed on the SiO_2 surface, and SiO_2 film is removed. This complex molecule is decomposed by elevating the wafer temperature to produce SiF_4 and the white powder based on NH_3-HF, which may be composed mainly by stratified $n(NH_4F)_3$ with C_3 symmetry axis. Increasing the wafer temperature moreover, up to 500 K, this white powder also decomposes to HF+NH_3.

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