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Modeling molecules responsible for the sidewall protection during the chemical dry etching of silicon related materials using F_2+ NO_x $\rightarrow$ F + FNO_x SATOMI TAJIMA, TOSHIO HAYASHI, Nagoya Univ, KOJI YAMAKAWA, Katagiri Engineering Co., Ltd., MINORU SASAKI, Toyota Technological Institute, KENJI ISHIKAWA, MAKOTO SEKINE, MASARU HORI, Nagoya Univ, NAGOYA UNIV TEAM, KATAGIRI ENGINEERING CO., LTD. COLLABORATION, TOYOTA TECHNOLOGICAL INSTITUTE COLLABORATION — We have been investigating the chemical dry etching of Si related materials using the reaction of F_2+ NO_x (X = 1, 2) $\rightarrow$ F + FNO_x. In our previous study, we found that this chemical dry etching technique generated anisotropic etching profile when the substrate temperature was maintained at $<60^{\circ}$C. In this study, we evaluated the cause of the anisotropic etching by measuring the molecules present in the gas phase by Fourier Transform Infrared Spectroscopy (FTIR) followed by calculating the chemical bonding structure formed on the Si surface by density functional theory (DFT). First the reaction between SiF_4 and molecules generated by the reaction between F_2, NO_x, and adsorbed H_2O such as F_2, NO_x, FNO_x, H_2O, OH, and HF, measured by FTIR, were calculated by DFT to identify key molecules that can present in the gas phase. We found that the chemical reaction between SiF_4 and multiple FNO may play a key role to prevent the sidewall etching. The modeling at the surface reaction using DFT is in progress.

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