Cyanide treatment to improve electrical characteristics of Si-based MOS diodes with an ultrathin oxide layer

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A reduction in the leakage current density flowing through ultrathin gate insulating layers of metal-oxide-semiconductor (MOS) diodes is necessary for the further increase in the number of components per IC chip. We have developed a method of decreasing the leakage current density of ultrathin silicon dioxide (SiO_2) layers by use of a simple chemical method. This method, we call "cyanide treatment", simply involves immersion of Si materials in KCN solutions followed by a rinse.

The leakage current density of <aluminum (Al)/SiO_2/Si(100)> MOS diodes with the 2.3 nm SiO_2 layer formed at 650 °C in wet-oxygen was relatively high. With the cyanide treatment, the leakage current density decreased to 1/3~1/8. 18-crown-6 molecules contained in the KCN solution effectively capture K^+ ions, and consequently the contamination of SiO_2/Si by K^+ ions is completely prevented. Capacitance-voltage measurements showed that the interface state density was decreased to less than 10 % by the cyanide treatment. We concluded that the decrease in the leakage current density resulted from the elimination of charge carrier flow paths via interface states.

Even when the MOS diodes with cyanide treatment were heated at 800 °C in nitrogen, interface states were not generated. This result shows that Si-CN bonds formed by the reaction of cyanide ions (CN^-) with Si dangling bonds are not ruptured at 800 °C. This thermal stability is important advantage of the cyanide treatment over hydrogen treatment where Si-H bonds are broken at 550~600 °C. It was also found that Si-CN bonds were not ruptured by prolonged irradiation of UV and visible light. Theoretical calculations using a density functional method showed that Si-CN bonds possessed a bond energy of 4.5 eV, more than 1 eV higher than the Si-H bond energy, which were the reason for the thermal and irradiation stability.

When the cyanide treatment was performed on polycrystalline Si-based MOS diodes, defect states in the depletion layer of poly-Si as well as interface states were passivated by CN^- ions, and consequently the leakage current density was decreased to a larger extent than that of the single crystalline Si-based MOS diodes.