How can first principles calculations give large contributions to industries?

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Recent technological problems especially in ULSI industries are intimately related to basic science, since each building block of ULSIs becomes nano-meter size. In such circumstance, first principles calculations are thought as a powerful tool to obtain useful knowledge of nano-structures and nano-materials that are crucial for the development of future technologies. However, there are few examples that first principles calculations really affect industries so far. This is due to the difference in the research attitudes between technological and scientific people: Technological people would like to develop high-performance devices timely according to commercial demands, whereas scientists would like to pursue deep science without considering markets. For instance, in order to contribute USLI technologies, we scientists have to take into account some unscientific factors: Among them, one of the most important factors is the research speed, since ULSI technologies need rapid progress based on ITRS road map. In this presentation, I show one recipe how first principles calculations can give large contribution to industries, by showing some examples which we have succeeded in contributing to ULSI technologies.

First, I show our new concept of interface physics that enegetics of interface reaction determines the Shottoky barrier height of metal/high-k dielectric interfaces, by using first principles calculations, model physics and experiments [1]. This new physical concept results in the big technological message that commonly used poly-Si gates should not be used with high-k gate dielectrics, leading to the world-wide change in the trend of ULSI technologies. Next, I show that this concept can naturally expand to another new concept of nano-interface: When the building block of interfaces becomes nano-scale, Shottoky barrier height of one interface can be governed by the energetics of the other interface as shown in Fig. 1 [2]. I also show that our designed photoemission experiments have clearly confirmed this concept [3].

Second, I show the atomistic mechanism of Si oxidation. Our first principles calculations clearly show that Si species should be emitted from the Si/SiO_2 interface toward SiO_2 region during thermal oxidation, since Si oxidation induces volume expansion due to the Si-O-Si bond formation [4]. Such knowledge is very important for recent ULSI technologies, since ULSI technologies require very thin SiO_2 dielectric films. To detect this phenomenon, we designed Rutherford backscattering (RBS) experiments, and have succeeded to detect Si emission from the Si/SiO_2 interface toward SiO_2 during Si thermal oxidation [5].

Moreover, I also show that “Shottoky limit” is not the real limit of Shottoky Barrier heights of metal/insulator interfaces by constructing a new physical concept, and this concept has also been confirmed by the experiments [6].

As described above, first principles calculations can really give large contributions to modern technologies by the proper and speedy collaboration with experiments and model physics.

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[1] K. Shiraishi, et al., Tech. Dig. 2004 VLSI Tech. p.108 (2004) ; Jpn. J. Appl. Phys. 43, L1413 (2004). [2] Y. Akasaka, et al. Jpn. J. Appl. Phys. 45, L1289(2006). [3] A. Ohta, et al., Extend Abstract, Int. Workshop Dielectric Thin Films, p.61 (2006). [4] H. Kageshima et al., Phys. Rev. Lett. 81 5936 (1998). [5] S. Hosoi et al., Nuc. Inst. & Method Phys. Res. Sec. B, 249, 390 (2006). [6] K. Shiraishi et al., Tech. Dig. 2005 Int. Electron Devices Meeting, p.43 (2005).

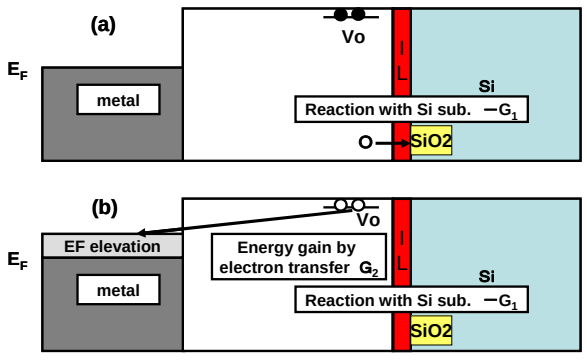

Fig.1: Schematic illustration of the mechanism of the Shottoky barrier formation of nano-scale metal/oxide/Si interface. (a) Interface reaction that generates O vacancy whose energy level is relatively high. (b) Subsequent electron transfer from a O vacancy level to a metal, leading to the elevation of metal Fermi level. As a result, Shottoky barrier height of nano-scale metal/oxide interface is governed by the energetics of the other interface reaction.