SF-P007

Magnetic and electronic properties of Co/MgO/Co magnetic tunnel junction system: First-principles calculations

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Magnetic tunnel junctions (MTJs) with crystalline insulating barrier have attracted many interests because of high tunneling magnetoresistance (TMR) ratio. Since TMR is a phenomenon that resistance of a device changes depending on the directions of the magnetic moments of both ferromagnetic (FM) layers, non-collinear calculation which can alter the direction of magnetic moment of each atom is necessary. In this study, a MTJ system which consists of bcc Co FM layer and rocksalt MgO insulating barrier has been investigated with either parallel (P) and anti-parallel (AP) states of bottom (polarizer) and upper (analyzer) electrodes. The first-principles calculations were conducted with Vienna *ab-initio* simulation package code using projector augmented wave method with generalized gradient approximation scheme. Spin polarization (SP) results revealed to show high SP at both FM layers in P state (~91%). Co bottom layers also represented high SP values in AP state, but Co upper layers showed relatively low SP values compared to those in P state, even negative ones. Thus, it is concluded that fluctuation in sign of SP is the major reason for TMR phenomenon of MTJs.

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Surface complexes formed in the interactions of SO_2 with ice surfaces

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We studied the interactions of SO_2 gas with ice surfaces at temperature of 80-140K. Crystalline water-ice films were prepared in either a neutral or basic condition, and SO_2 was adsorbed on to the ice films. Hydroxide ions were added onto the film surfaces by the hydrolysis of Na atoms. Cs^+ reactive ion scattering (RIS) and low energy sputtering (LES) techniques were used to scrutinize the chemical species present at the surfaces, in conjunction with temperature-programmed desorption (TPD) to monitor the desorbing species. We detected both neutral (SO_2 and DSO_2) and anionic species (OD^-, SO_2^-, DSO_2^-, and DSO_3^-)present on the surfaces by RIS and LES experiments, respectively. These species may represent the surface complexes formed at initial stages of the dissolution and hydrolysis of SO_2 gas in an ice film.