Effect of Boron diffusion on Electronic and Magnetic Structures of CoFeB/Ta multilayers

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The perpendicular magnetization of materials is certainly one of the most important technologies in spintronics, and the atomistic understanding of it is a subject of great interest in condensed matter physics. Recently, the perpendicular magnetization of the MgO/CoFeB/Ta multilayer structure has attracted much attention as the structure is used for the magnetic layer of magnetic tunneling junction (MTJ) devices of spin-transfer torque magnetic random access memories (STT-MRAMs). In this study, we have investigated the electronic and magnetic structures of CoFeB/Ta and CoFe/TaB superlattices from first principles by using the density functional (DFT) method to investigate the effect of the B atom diffusion on the electronic and magnetic structures. Calculations clarified that the B atom diffuses from the CoFeB layer to the Ta layer, which energetically stabilizes the superlattice, and that the diffusion inverts the magnetization of the Ta layer, antiferromagnetically coupling the Ta layer with the CoFe layer. The results indicate that the B atom diffusion significantly affects the magnetization of the MgO/CoFeB/Ta structure. The magnetocrystalline anisotoropy of the superlattices is discussed in conjunction with the B atom diffusion effect on the superlattice magnetization.