Large influence of capping layers on tunnel magnetoresistance in magnetic tunnel junctions

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Abstract: Since the discovery of tunnel magnetoresistance (TMR) in the Fe|Ge-oxide|Co trilayer structure, the TMR effect has become the significant principle of non-volatile magnetic random access memory (MRAM) and magnetic tunnel junction (MTJ) which is the basic element of MRAM. Thanks to rapid advances in growth technique of ultra-thin ferromagnetic films, CoFeB|MgO MTJs with high TMR ratio have been achieved as predicted by *ab initio* calculations. Recently, experiments have investigated the influence on TMR caused by capping layers, and drawn the conclusion that a higher TMR can be achieved in MTJs with W capping layers instead of Ta. To explore the essential influence caused by capping layers, we carry out *ab initio* calculations on TMR in the X(001)|CoFe(001)|MgO(001)|CoFe(001)|X(001) MTJ, where X represents the capping layer material which can be tungsten, tantalum or hafnium. We report TMR in different MTJs and demonstrate that tungsten is an ideal candidate for a giant TMR ratio. In order to explore transport properties in MTJs, the density of scattering states (DOSS) was investigated from the aspect of band symmetry. This work reports TMR and transport properties in MTJs with different capping layers, proves that tungsten is a proper capping layer material, which would benefit the design and optimization of MTJs.

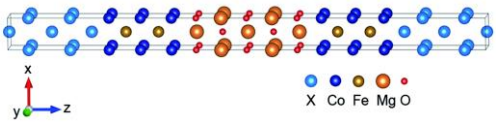

FIG. 1. Atomic structure of the X|CoFe|MgO|CoFe|X MTJ model, X represents the capping layer material W, Ta or Hf.

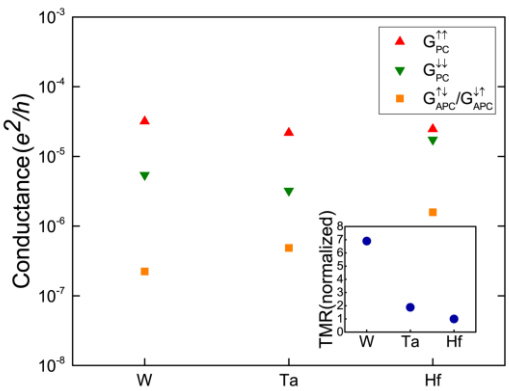

FIG. 2. Spin-resolved conductance in X-capped MTJs. Inset: TMR ratios of X-capped MTJs.

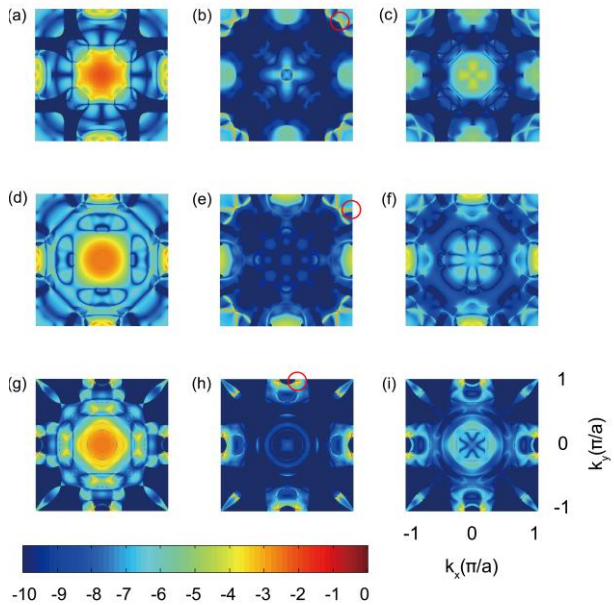

FIG. 3. Spin- and $\mathbf{k}_{\parallel}$-resolved transmission coefficients in Brillouin zone.