Tailoring tunnel magnetoresistance by ultrathin Cr and Co interlayers: A first-principles investigation of Fe/MgO/Fe junctions

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We report on systematic ab-initio investigations of Co and Cr interlayers embedded in Fe(001)/MgO/Fe(001) magnetic tunnel junctions, focusing on the changes of the electronic structure and the transport properties with interlayer thickness. The results of spin-dependent ballistic transport calculations reveal options to specifically manipulate the tunnel magnetoresistance ratio. The resistance area products and the tunnel magnetoresistance ratios show a monotonous trend with distinct oscillations as a function of the Cr thickness. These modulations are directly addressed and interpreted by means of magnetic structures in the Cr films and by complex band structure effects. The characteristics for embedded Co interlayers are considerably influenced by interface resonances which are analyzed by the local electronic structure.

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I. INTRODUCTION

During the last years magnetoresistive effects — in particular the tunnel magnetoresistance (TMR) effect[1,2] — became increasingly important for the fast developing field of spintronic devices[3,4]. The first industrial applicable TMR contacts have been built using crystalline MgO insulators which are epitaxially grown on as well as coated with iron electrodes[5,6]. Fe/MgO/Fe magnetic tunnel junctions (MTJs) have been extensively investigated to elucidate the mismatch between theoretically predicted[7,8] and the at least one order of magnitude smaller measured[9,10] TMR ratios. It turned out that the disparity can be attributed to differences between idealized (in theory) and real (in experiment) samples. More sophisticated theories which include imperfections, like interface disorder[11–17] or roughness effects[18], were able to close the gap between experiment and theory and highlight the importance of perfect interfaces.

Although other tunnel junctions, like CoFeB/MgO/CoFeB MTJs with their high TMR ratios[19], were put into the focus of attention, Fe/MgO/Fe MTJs are still intensely studied. Besides the emerging field of spin-torque effects[20], research is ongoing in search of other ways to increase the TMR ratio further. Instead of improving the interface quality an alternative means is found in the specific manipulation of the spin-dependent conductances by embedding ultrathin interlayers[21,22].

The insertion of a single layer-wise antiferromagnetic (LAFM) Cr interlayer results into even-odd oscillations of the TMR ratio as a function of the Cr thickness[23,24]. In this paper we report on a first-principles study of these transport characteristics. We discuss the origin of these modulations with the apparent 2 ML-wavelength as well.

Additionally, an analysis of the electronic transport results for Co interlayers at both Fe/MgO interfaces is presented. These investigations were motivated by previous ab-initio calculations[25] which predicted larger TMR ratios for MgO tunnel junctions with bcc Co(001) leads instead of Fe(001) electrodes. Due to the fact that Co grows epitaxially only up to a few monolayers on bcc substrates, a question arises whether ultrathin Co interlayers could be alternatively used to obtain an enhancement of the TMR ratios in Fe/MgO/Fe MTJs. To answer this question we computed the conductances and TMR ratios for small Co interlayer thicknesses and analyzed the results by means of the electronic structures.

II. THEORETICAL BACKGROUND

Our computational approach is divided into two steps. Firstly, the electronic structures of the MTJs are calculated from first principles. Secondly, the electronic transport properties are computed, using the potentials obtained in the first step.

The electronic structure is determined self-consistently within the framework of density-functional theory (DFT) using a scalar-relativistic screened Korringa-Kohn-Rostoker (KKR) Green function technique[26,27]. The spherical site potentials were treated in the atomic sphere approximation (ASA) using the local spin density approximation (LSDA) for the exchange-correlation potential[28]. Throughout this work a parameterization following Vosko, Wilk, and Nusair[29] was used.

Since structural information of Fe/MgO/Fe MTJs with embedded ultrathin Cr and Co spacers are not reported so far, we resort to a geometry of planar Fe(001)/MgO/Fe(001) junctions which has been determined experimentally by surface x-ray diffraction