Ab-Initio Structural, Electronic and Transport Properties of $Fe_{1-x}Co_x/AlAs/Fe_{1-x}Co_x$ (001) Tunnel Junction

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The electronic structure of $Fe_{1-x}Co_x/AlAs/Fe_{1-x}Co_x$ (001) heterostructures are calculated by means of a self-consistent Green's function technique implemented in the framework of the tight-binding linear muffin-tin orbital method (TB-LMTO) in its atomic sphere approximation (ASA) and in conjunction with the coherent potential approximation (CPA) in order to describe the interdiffusion at the FeCo/AlAs interfaces. The conductance and the tunneling magnetorezistance ratio (TMR) are estimated in the current perpendicular to-the-plane geommetry (CPP) by means of the transmission matrix formulation of the Kubo-Landauer approach. The results show that at the FeCo/AlAs interfaces there is a net charge transfer from the FeCo magnetic slab to the AlAs semiconducting spacer resulting in a Schottky barrier. The magnetic behavior of interface Fe and/or Co atoms are dependent on the interface structure as well as on the semiconductor terminations. Thus, at the Fe/AlAs interface for Al termination the Fe magnetic moment increase over corresponding bulk value and for As termination it remains almost unchanged while at Co/AlAs interfaces, for both terminations, the Co magnetic moment is reduced. The TMR ratio is composition dependent and increase from 15% up to 60% with increasing Co concentration. Also, the TMR values are sensitive to the semiconducting spacer terminations.

9.7 cm

13.4 cm

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