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Magnetic and spin dependent transport properties of SrC/NaCl(CaS)/SrC (001) tunnel junctions

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Half metallic ferromagnetic (HMF) materials with metallic properties in only one spin direction and therefore having full spin polarization at the Fermi level are seen the most promising candidates for high performance spintronic device applications. Electronic structure calculations performed for SrC compound by using tight-binding linear muffin-tin orbital (TB-LMTO) method [1, 2] show, in agreement with previous predictions [3], that metastable rocksalt-type phase with an equilibrium lattice parameter a_{SrC}=5.57 Å has half metallic characteristics with a total magnetic moment of 2 m_B/f.u. and therefore is epitaxially compatible with both B1-type direct band gap NaCl (a_{NaCl}=5.64 Å) and G-X indirect band gap CaS (a_{CaS}=5.69 Å) barriers. Thus SrC/NaCl(CaS)/SrC (001) magnetic tunnel junctions (MTJs) represent feasible heterostructures for theoretical investigations as well as for potential technological applications.

Ground state electronic and magnetic properties of SrC/NaCl/SrC (001) and SrC/CaS/SrC (001) heterostructures are studied by using a first principles Green's function technique for surface and interfaces implemented within TB-LMTO formalism [2]. The spin dependent transport properties in the current-perpendicular-

to-plane (CPP) geometry are determined by means of the linear response of Kubo approach implemented within TB-LMTO formalism [4, 5]. Away from interfaces SrC layers have bulk-like HMF characteristics while at SrC/NaCl(CaS) (001) interfaces Sr and C atoms have magnetic moments little reduced compared with the corresponding bulk values. Small spin polarizations are induced on both Na(Ca) and Cl(S) interfacial sites. A ferromagnetic (FM) coupling is observed for NaCl based junctions while for CaS based ones it is antiferromagnetic (AFM). For both SrC/NaCl/SrC (001) and SrC/CaS/SrC (001) heterostructures the exchange couplings are small and decrease exponentially with the barriers thicknesses. In the FM state of the junctions the highest contributions to the total conductances are given by the minority spin electrons (Figs. 1a, 1b). All conductances decrease exponentially with the barrier thicknesses. The spin dependent transport properties are mostly determined by the electronic characteristics of interfacial SrC layers as well as by the complex band structures of the insulating (semiconducting) spacers. For CaS based magnetic tunnel junctions, tunnelling magnetoresistance ratio increases almost exponentially with the barrier thickness (Fig. 1c).