Spin dependent transport properties in MTJs having NaBr(AgBr) barriers

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Abstract

In present contribution the *electronic, magnetic and spin-polarized* transport properties of Fe/Na1-xAgxBr/NaBr/Na1-xAgxBr/Fe and Fe/AgBr/mNaBr/Fe magnetic tunnel junctions were studied by means of self-consistent atomistic first principles calculations. A model interface with Fe atoms sitting atop of Ag(Na) and Br positions has been considered. The ballistic electronic transport properties in the current-perpendicular-to plane (001) geometry and zero bias field were analyzed.

In the case of $Na_{1-x}Ag_xBr$/7NaBr/$Na_{1-x}Ag_xBr$ barriers, the conductances decrease in the composition range 0.2 = x = 0.8. High TMR ratios, of 10^3 % has been evidenced for the end series compositions.

The conductances decrease exponentially with the barrier thickness in case of Fe/AgBr/mNaBr/AgBr/Fe MTJ. The largest contribution to the FM conductance results from the spin-up electrons.

The $k_{||}$ resolved conductances of FM and AFM states are also analyzed.

Fe/Na(Ag)Br/Fe(001) (001) Multilayer Structure

Studied Systems:

/(semi-infinite) Fe (001)/nFe(001)/m(NaBr(AgBr, $Na_{1-x}Ag_xBr$, $Na_{1-x}Ag_xBr$/NaBr/$Na_{1-x}Ag_xBr$)/(n+1)Fe(001)/Fe (001) (semi-infinite)/

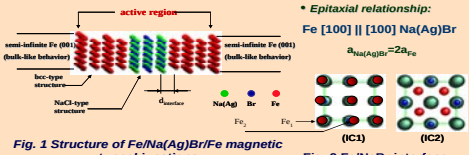

Fig. 1 Structure of Fe/Na(Ag)Br/Fe magnetic tunnel junctions

• Epitaxial relationship:

Fe [100] || [100] Na(Ag)Br

$a_{Na(Ag)Br}=2a_{Fe}$

Fig. 2 Fe/NaBr interface configurations

$d_{interface}=a_{Fe}$ in case of (IC1) interface configuration while for (IC2) interface configuration it is determined from ASA space filling requirements

Computational Details

Electronic Structure Calculations:

- Performed by means of a first principle Green's function technique for surfaces and interfaces, based on the tight-binding linear muffin-tin orbital method in the atomic sphere approximation (TB-LMTO-ASA) [4].
- The local spin density approximation (LSDA) was used for exchange correlation potential within Vosko-Wilk-Nusair parameterisation [5].
- The LMTO valence basis consists of s, p and d electrons and the input electronic configurations were taken as: Fe: core+3d^6 4s^2, Na: core+3s^1, Br: core+4p^5 and Ag: core+4d^{10} 5s^1, respectively.

$Na_{1-x}Ag_xBr$ barriers:

- Use of the coherent potential approximation (CPA) [4].

Spin dependent transport properties:

- The conductances through Fe/NaBr($Na_{1-x}Ag_xBr$, $Na_{1-x}Ag_x$/NaBr/$Na_{1-x}Ag_xBr$))/Fe MTJs are evaluated in the current-perpendicular-to-plane (CPP) geometry by means of the linear response of Kubo-Landauer approach implemented within TB-LMTO-CPA formalism and including vertex corrections [6, 7].
- 1024 in plane k-point grid is used for electronic structure calculations and $1.44\cdot10^4$ k-point grid is used for spin dependent transport calculations.

$$TMR = \frac{R_{AFM}}{R_{FM}} - 1 = \frac{G_{FM}}{G_{AFM}} - 1$$

Electronic structure of bulk NaBr and AgBr

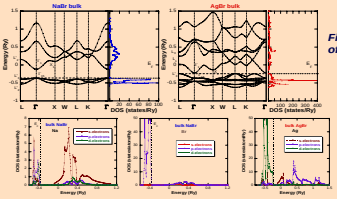

Fig.3 Band structures of bulk NaBr and AgBr

Fig.4 Partial DOS in NaBr and AgBr compounds

	a_{exp} (Å)	a_{calc} (Å)	E_g(exp) (eV)	E_g(calc.) (eV)
NaBr	5.97	5.68	7.1	3.65 (10 [1])
AgBr	5.64	5.58	2.68	0.2 (0.9 [2, 3])

Ground state electronic and magnetic properties

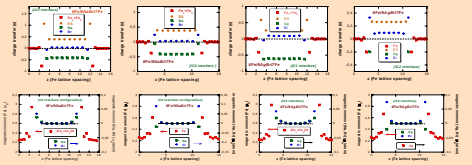

Fig. 5 Layer resolved charge transfer and magnetic moments for Fe/NaBr/Fe heterostructures

• Total energy calculations performed for Fe/NaBr/Fe heterostructures predict that (IC_1) interface geometry it is energetically more stable than (IC_2) one while for Fe/AgBr/Fe multilayer structures the IC_2 interfaces are energetically more favorable.

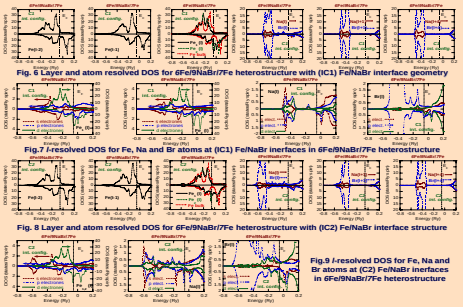

Fig. 6 Layer and atom resolved DOS for 6Fe/9NaBr/7Fe heterostructure with (IC1) Fe/NaBr interface geometry

Fig.7 l-resolved DOS for Fe, Na and Br atoms at (IC1) Fe/NaBr interfaces in 6Fe/9NaBr/7Fe heterostructure

Fig. 8 Layer and atom resolved DOS for 6Fe/9NaBr/7Fe heterostructure with (IC2) Fe/NaBr interface structure

Fig.9 l-resolved DOS for Fe, Na and Br atoms at (C2) Fe/NaBr interfaces in 6Fe/9NaBr/7Fe heterostructure

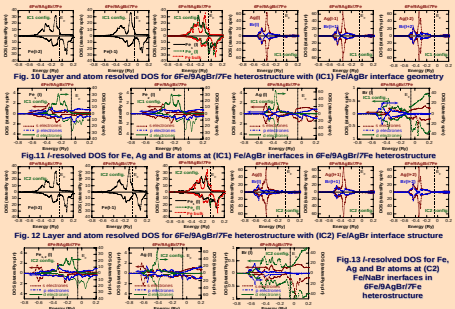

Fig. 10 Layer and atom resolved DOS for 6Fe/9AgBr/7Fe heterostructure with (IC1) Fe/AgBr interface geometry

Fig.11 l-resolved DOS for Fe, Ag and Br atoms at (IC1) Fe/AgBr interfaces in 6Fe/9AgBr/7Fe heterostructure

Fig. 12 Layer and atom resolved DOS for 6Fe/9AgBr/7Fe heterostructure with (IC2) Fe/AgBr interface structure

Fig.13 l-resolved DOS for Fe, Ag and Br atoms at (C2) Fe/NaBr interfaces in 6Fe/9AgBr/7Fe heterostructure

Exchange coupling in Fe/NaBr/Fe and Fe/AgBr/Fe heterostructures

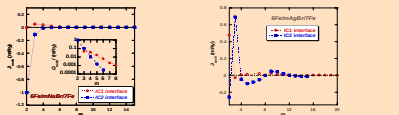

Fig. 14 The exchange coupling versus barrier thickness in Fe/NaBr/Fe and Fe/AgBr/Fe heterostructures for both (IC1) and (IC2) interface configurations

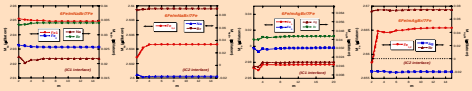

Fig. 15 Interfacial magnetic moments versus barrier thickness

Spin dependent transport properties of Fe/NaBr/Fe and Fe/AgBr/Fe MTJs

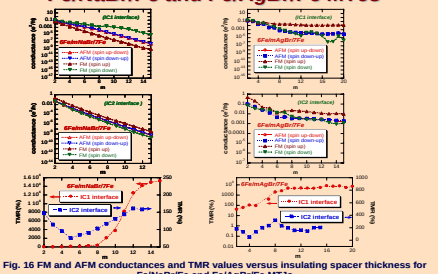

Fig. 16 FM and AFM conductances and TMR values versus insulating spacer thickness for Fe/NaBr/Fe and Fe/AgBr/Fe MTJs

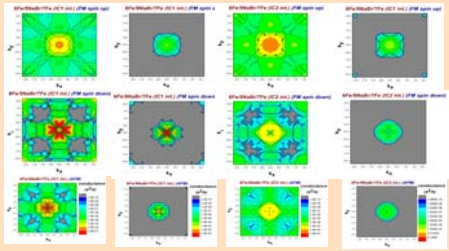

Fig. 17 k_z-resolved conductances of FM and AFM states for 6Fe/5NaBr/7Fe and 6Fe/9NaBr/7Fe MTJ for both (IC1) and (IC2) interface configurations

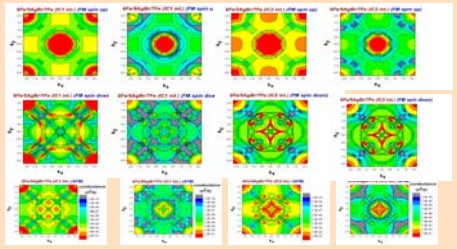

Fig. 18 k_z-resolved conductances of FM and AFM states for 6Fe/5AgBr/7Fe and 6Fe/9AgBr/7Fe MTJ for both (IC1) and (IC2) interface configurations

Spin dependent transport properties of $Fe/Na_{1-x}Ag_xBr/Fe$ MTJs

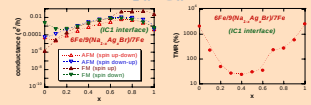

Fig. 19 FM and AFM conductances and TMR values versus composition in 6Fe/9($Na_{1-x}Ag_x$)Br/7Fe MTJs

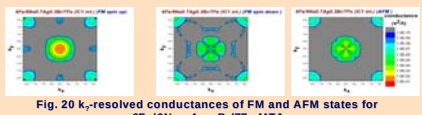

Fig. 20 k_z-resolved conductances of FM and AFM states for 6Fe/6$Na_{0.7}Ag_{0.3}$Br/7Fe MTJ

Spin dependent transport properties of $Fe/Na_{1-x}Ag_xBr/NaBr/Na_{1-x}Ag_xBr/Fe$ and Fe/AgBr/mNaBr/AgBr/Fe MTJs

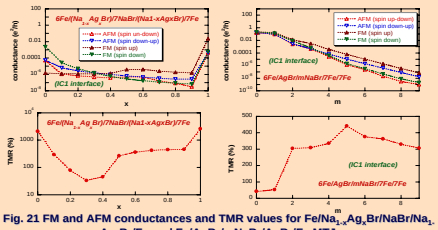

Fig. 21 FM and AFM conductances and TMR values for Fe/$Na_{1-x}Ag_xBr$/NaBr/$Na_{1-x}Ag_xBr$/Fe and Fe/AgBr/*m*NaBr/AgBr/Fe MTJs

Conclusions

- Electronic structure, magnetic and spin dependent transport properties of Fe/NaBr/Fe Fe/AgBr/Fe, Fe/$Na_{1-x}Ag_xBr$/Fe and Fe/$Na_{1-x}Ag_xBr$/NaBr/$Na_{1-x}Ag_xBr$/Fe heterostructures have been theoretically investigated.
- Formation of sharp Fe/NaBr and Fe/AgBr interfaces have been evidenced.
- Total energy calculations evidenced that Fe/NaBr interface configuration with Fe atoms sitting above Na and Br sites (IC_1) is energetically more stable than that with Fe atoms located above the hollow site between Na and Br ones (IC_2) while at Fe/AgBr interfaces the IC_2 interfacial geometry is more stable.
- Total energy calculations evidenced similar stable interface structures for other Fe/alkali halides and Fe/silver halides interfaces such as Fe/NaCl [8, 9], Fe/LiBr, Fe/AgCl [10].
- Due to the band offset of Na(Ag)Br relative to Fe ones, a small charge transfer is evidenced between Fe magnetic slab and Na(Ag)Br insulating spacers.
- The charge transfer is mainly localize at the interface layers. In the semiconducting (insulating) spacer the charge transfer is limited to the interfacial layer due to screening effects.
- For (IC_2) interface configuration the charge transfer is slightly higher for the Fe atoms sitting above anion positions and it may be related with higher Br electronegativity.
- The charge variation in the Fe interfacial layer "oscillate" in antiphase with the charge distribution in Na(Ag)Br interfacial layers, reducing electrostatic energy interaction and thus stabilizing the Fe/Na(Ag)Br interfaces.
- Magnetic moments of interfacial Fe atoms are enhanced over the corresponding bulk value.
- The enhancement of the interfacial iron magnetic moment is higher at (IC_1) Fe/Na(Ag)Br (001) interfaces.
- A small oscillatory exchange coupling have been evidenced in the case of Fe/AgBr/Fe heterostructures, in contrast with the exponentially decaying exchange coupling specific for the systems with semiconducting (insulating) spacers.

- The main contribution to the FM conductances for Fe/NaBr/Fe (001) MTJs with (IC_1) interfaces is given by the minority spin electrons while for (IC_2) interfaces by the majority spin ones.
- The main contribution to the FM conductances for Fe/AgBr/Fe MTJs is given by the majority spin electrons, independent of Fe/AgBr (001) interface structure.
- High TMR values are predicted for all Fe/NaBr/Fe (001), Fe/AgBr/Fe (001) and Fe/(Ag-Na)Br/Fe (001) MTJs.

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