Four-Resistance States in Symmetrical Multiferroic Tunnel Junctions

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Motivation

Multiferroic tunnel junctions consisting of ferromagnetic metallic electrodes and ferroelectric barrier, in which both tunneling magnetoresistance (TMR) effect and tunneling electroresistance (TER) effect can be observed, are one of the candidates for commercial multi-state storage devices. Although there have been numerous reports on the multiferroic tunnel junctions, only few attention has been attached to the multiferroic tunnel junctions with symmetrical electrodes. In general, asymmetrical electrodes is intrinsically required for achieving different barrier hights against the ferroelectric switching in ferroelectric/multiferroic tunnel junctions with single-phase ferroelectric barrier.

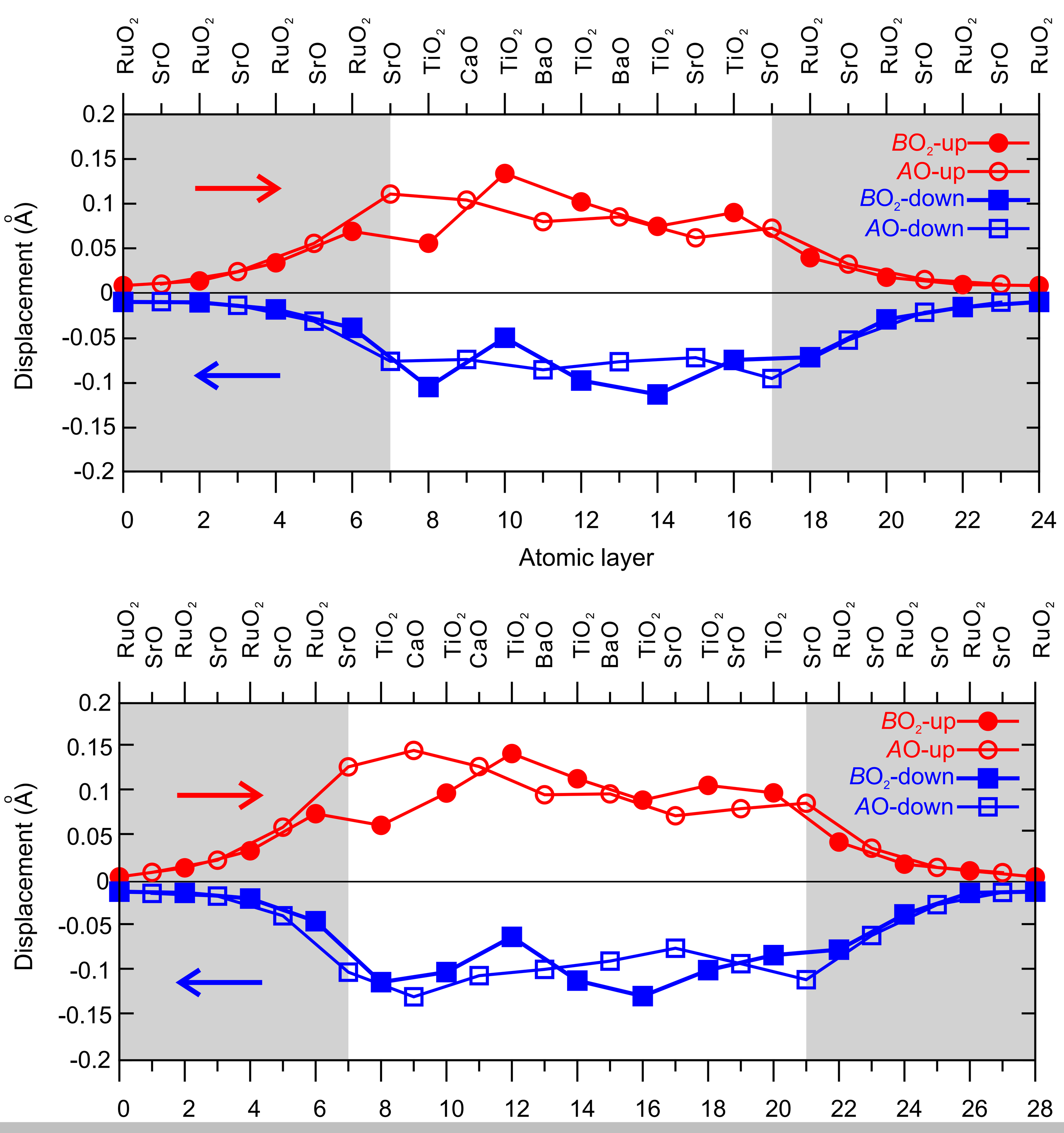
Our previous study (Gao. et al., JPCM 2013) has demonstrated the intrinsic asymmetric ferroelectricity in tricolor superlattice composed of $CaTiO_3$, $BaTiO_3$, and $SrTiO_3$. This tricolor superlattice provides a possibility to achieve multiferroic tunnel junctions with symmetrical electrodes.

In this Poster, we perform an comparative study on the TMR and TER effects in the multiferroic junctions with symmetrical and asymmetrical electrodes, and predict robust foure-resistance states in symmetrical multiferroic tunnel junctions.

Models

In Gao. et al.'s study, (CTO)-$(BTO)_2$-(STO) (CBBS) and $(CTO)_2$-$(BTO)_2$-$(STO)_2$ (CCBBS) show strong electric polarization. Hence, only these two ferroelectric compounds are considered in current study. In order to examine the existence of ferroelectricity at tricolor/electrode interfaces, we introduce seven layers of $SrRuO_3$ (SRO). Both symmetrical and asymmetrical interfaces are simulated in our study, they are named as $[(SRO)_4/CBBS/(SRO)_3]_{sym}$ and $[(SRO)_4/CCBBSS/(SRO)_3]_{sym}$ with symmetrical interfaces, and $[(SRO)_4/CBBS/(SRO)_3]_{asym}$ and $[(SRO)_4/CCBBSS/(SRO)_3]_{asym}$ with asymmetraical interfaces. Two of the models are shown in Fig. 1.

Figure 2



The survived ferroelectricity at nanoscale

Figure 2 shows the atomic displacements in the layers of *AO* and BO_2. In each hetrostructure, bistable states are observed, and there are significant changes in quantity and sign (+ or -) of the atomic displaces, which indicates the ferroelectricity at nanoscale is well preserved. The atomic displaces show asymmetrical feature under ferroelectric switching, which reveals the intrinsic asymmetric ferroelectricity. This is further confirmed by Fig. 3 that is a double-well potential profile as a function of normalized soft mode. 1.0 and -1.0 represent "up" and "down" polarization states, respectively. Compared to a symmetrical double well of single-phase ferroelectric (e.g. bulk $BaTiO_3$), the double well of $[SRO/CBBS/SRO]_{sym}$ shows asymmetrical properties, and the normalized displacement corresponding to paraelectric state deviates from zero. These features prove the asymmetrical ferroelectricity. Furthermore, the asymmetry of double well is enhanced if asymmetrical interfaces are applied (see the double well of $[SRO/CBBS/SRO]_{asym}$).

Figure 3

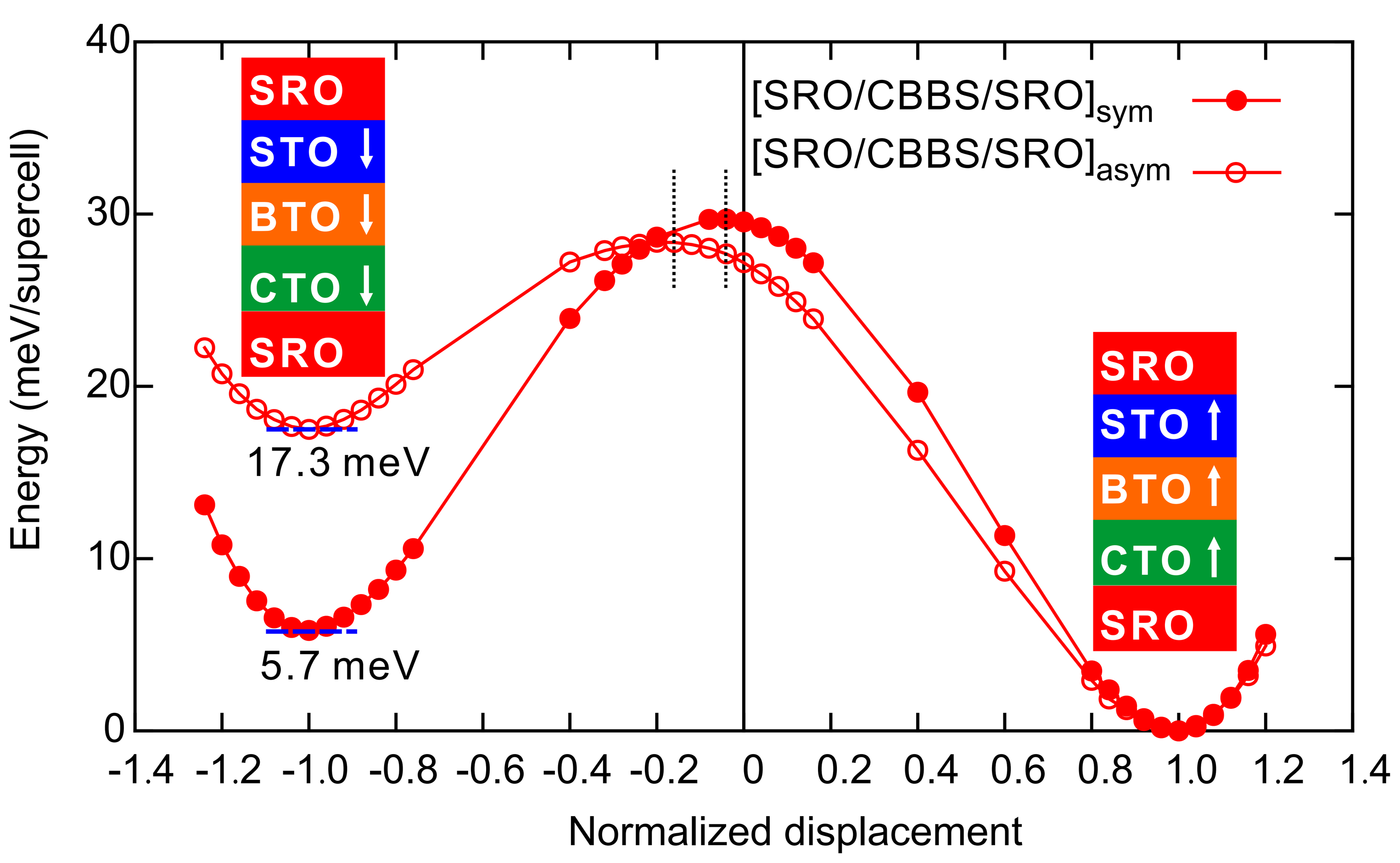
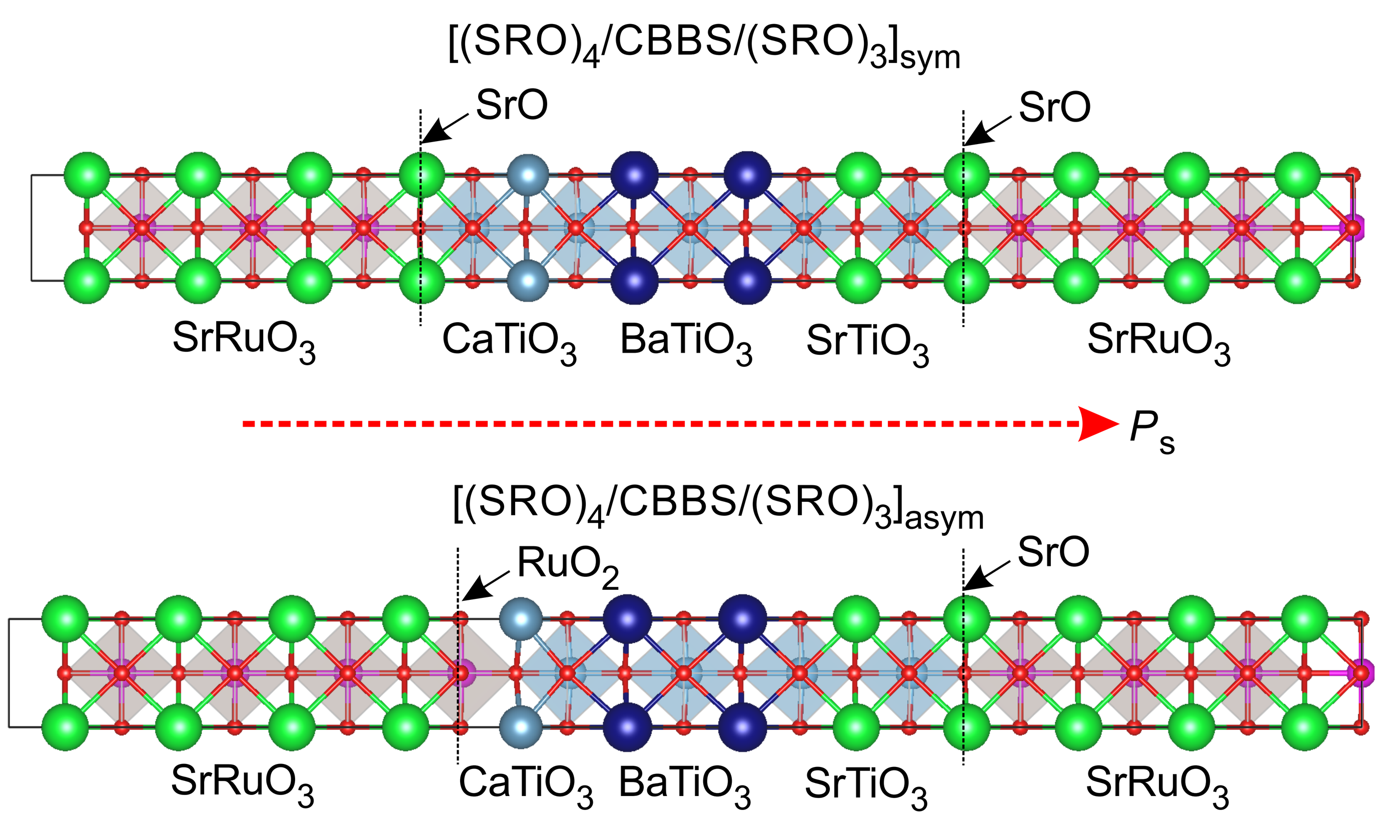


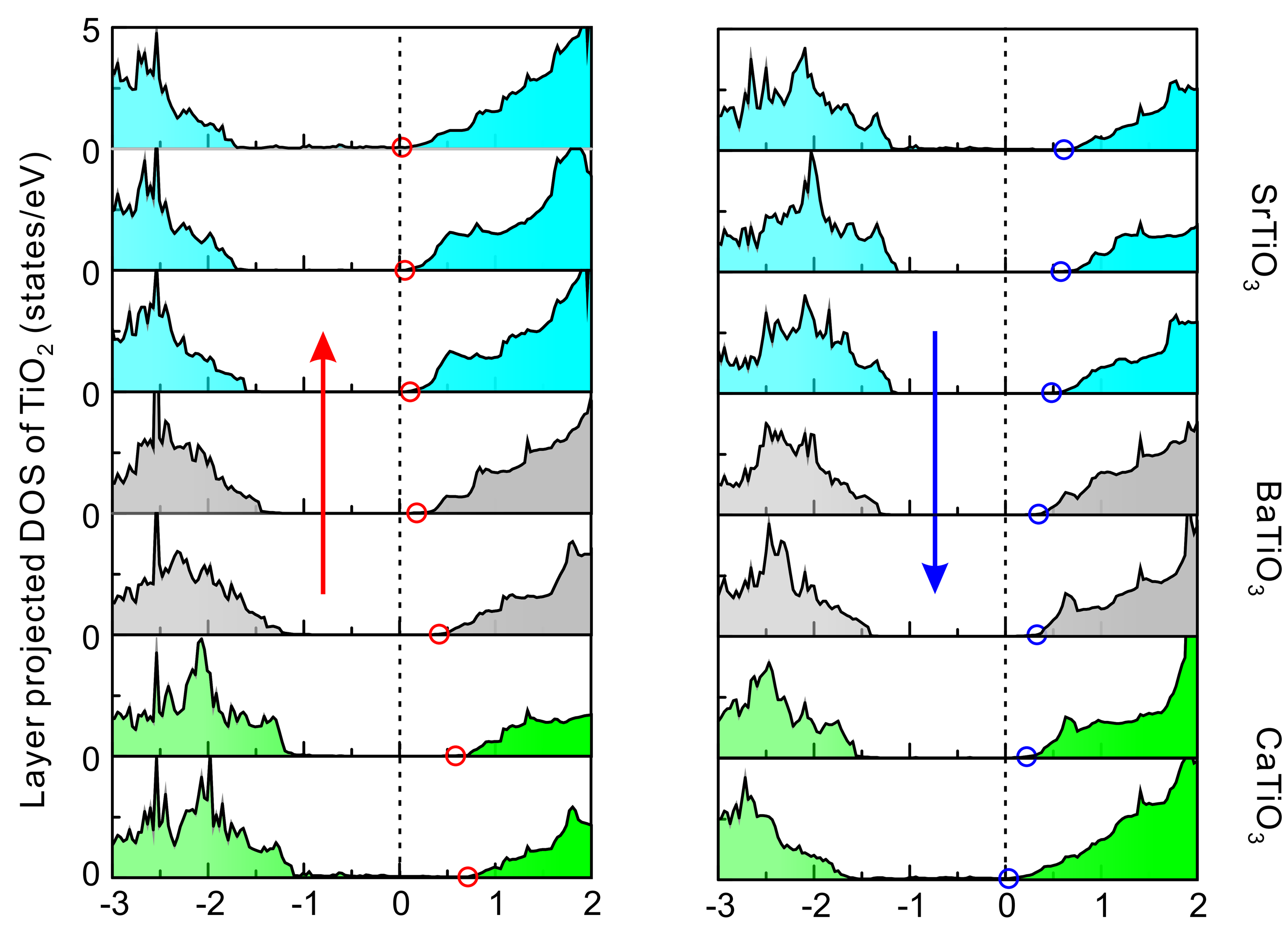
Figure 1



The effect of ferroelectric switching on electronic structure

Figure 4 shows the projected densiteis of states of TiO_2 layers in $[(SRO)_4/CCBBSS/(SRO)_3]_{sym}$.

Figure 4



The four-resistance states

Figure 5 shows TER and TER ratios in each multiferroic tunnel junction.

Figure 5

MFTJ-$[CBBS]_{sym}$

G (Siemens)	⇉	⇄	⇉:⇄ 100%	TMR 100%
↑	1.43e-09	3.58e-10	3.99	59.82
↓	1.54e-09	3.45e-10	4.46	63.43
↑:↓	0.93	1.04		
TER 100%	3.98	1.85		

MFTJ-$[CBBS]_{asym}$

G (Siemens)	⇉	⇄	⇉:⇄ 100%	TMR 100%
↑	1.45e-08	1.97e-09	7.36	76.08
↓	1.37e-08	2.62e-09	5.23	67.89
↑:↓	1.06	1.04		
TER 100%	2.91	14.11		

MFTJ-$[CCBBSS]_{sym}$

G (Siemens)	⇉	⇄	⇉:⇄ 100%	TMR 100%
↑	2.22e-11	8.42e-12	2.64	44.96
↓	8.39e-12	1.96e-12	4.28	62.15
↑:↓	2.65	4.30		
TER 100%	45.08	62.24		

MFTJ-$[CCBBSS]_{asym}$

G (Siemens)	⇉	⇄	⇉:⇄ 100%	TMR 100%
↑	2.45e-10	5.90e-11	4.15	61.21
↓	1.15e-10	4.78e-11	2.41	41.13
↑:↓	2.13	1.23		
TER 100%	36.34	10.54		

Conclusions

I. The asymmetrical ferroelectricity at nanoscale can be preserved at tricolor/electrode interfaces. II. Density functional non-equilibrium Green's function (NEGF-DFT) study shows that four well-defined resistance states can be observed in symmetrical multiferroic tunnel junctions.

II. In symmetrical multiferroic tunnel junction with $[CCBBSS]_{sym}$ barrier, the predicted TMR and TER ratio is produced above 44.9%, the functionality of this multiferroic tunnel junction is competitive to the asymmetrical SRO/BTO/SRO multiferroic tunnel junction (TMR > 64%, TER > 35% as reported by Velve. et al., Nano Lett., 2009).

III. In multiferroic tunnel junction with $[CCBBSS]_{sym}$ barrier, NEGF-DFT study predicts the electron transport is dominated by strong barrier tunneling around Γ point in polarization "up" state, whereas in polarization "dn" state the barrier tunneling is extremely weak, and only a few resonant tunneling states are observed. This is the reason why multiferroic tunnel junction with $[CCBBSS]_{sym}$ barrier shows pretty robust performance in TER compared to other junctions in this study.

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