UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

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A first-principles study of the switching mechanism in GeTe-InSbTe phase-change superlattices

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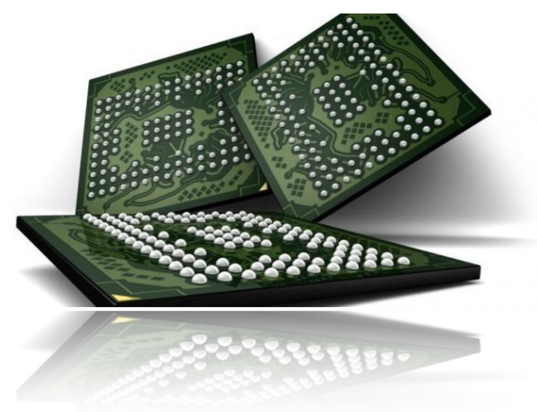

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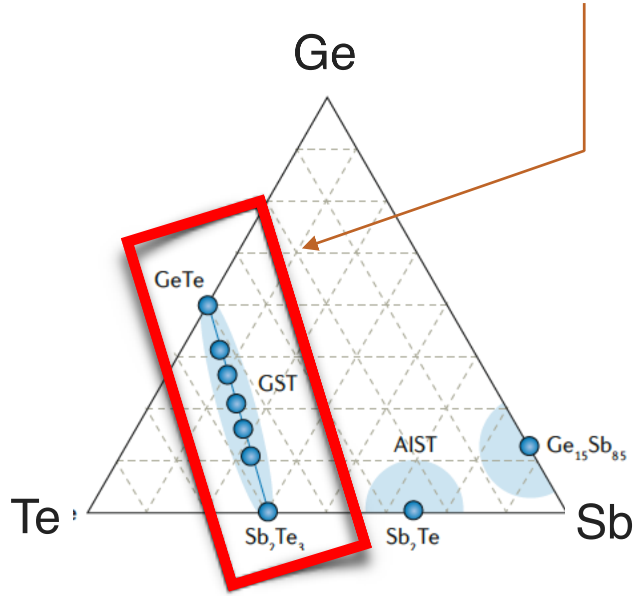
Phase change memories (PCM)

- Non-volatile memories for electronic devices
- Access time (~10-100 ns) comparable to highly fast volatile RAM
- Memory bit: nanometric region of chalcogenide materials
- Ge-Sb-Te alloys on pseudobinary GeTe-Sb_2Te_3 tie line

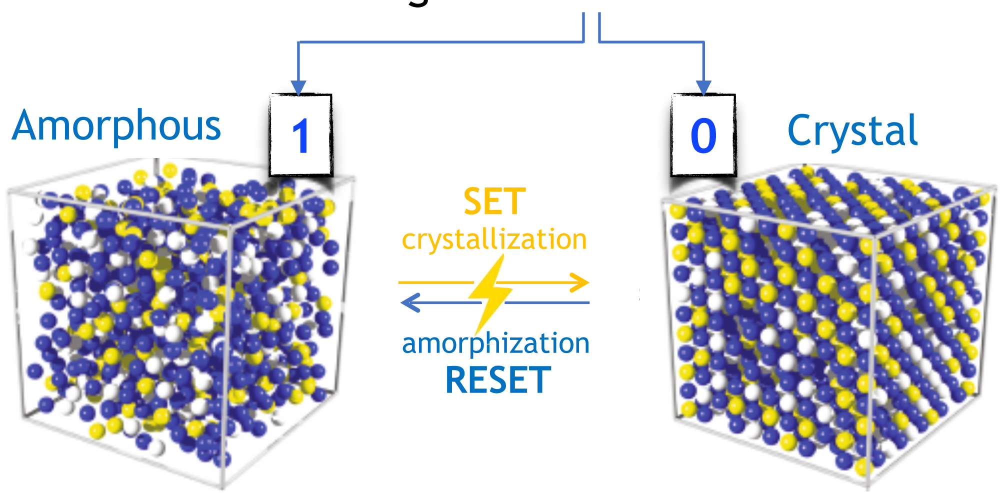


Ge–Sb–Te (GST)
Ternary diagram

Zhang, Nat. Rev. Mater. 4, 150 (2019)

Phase change memories (PCM)

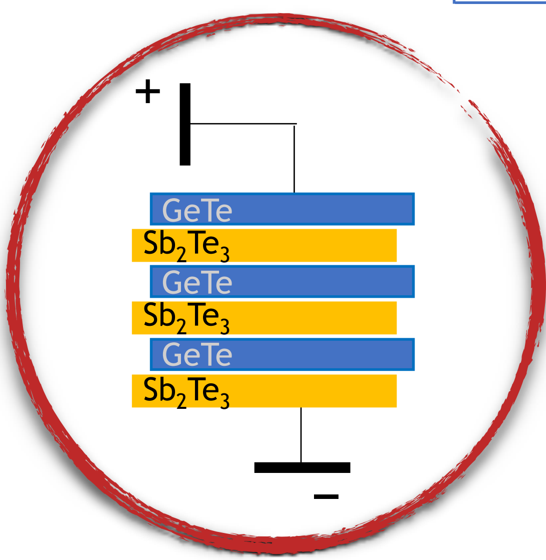
- *Rapid* & *reversible* crystal-amorphous GST switching upon Joule heating – SET/RESET programming current pulses
- Metallic *Crystal* vs. Semiconducting *Amorphous*
- High electrical contrast enables logical states discrimination in read-out

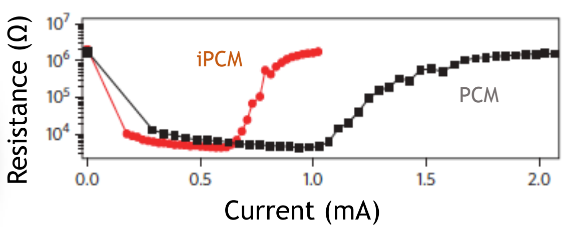


Zhang, Nat. Rev. Mater. 4, 150 (2019)

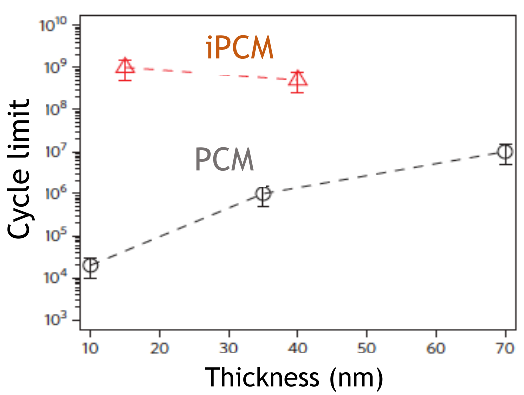
Interfacial phase change memories (iPCM)

- Based on ordered stacking of GeTe-Sb_2Te_3 layers
- Superior switching performance over conventional GST-based PCM
- Lower power consumption, improved cyclability, …





Simpson, Nat. Nanotechnol. 6, 501 (2011)



Which mechanism for iPCM switching ?

Switching mechanism & structure of logical memory states are still debated

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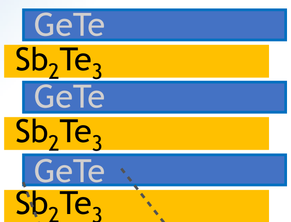
SCENARIO #1:



Structure $\longrightarrow$ SuperLattice (SL) – alternation of $(GeTe)_2$ and Sb_2Te_3 blocks

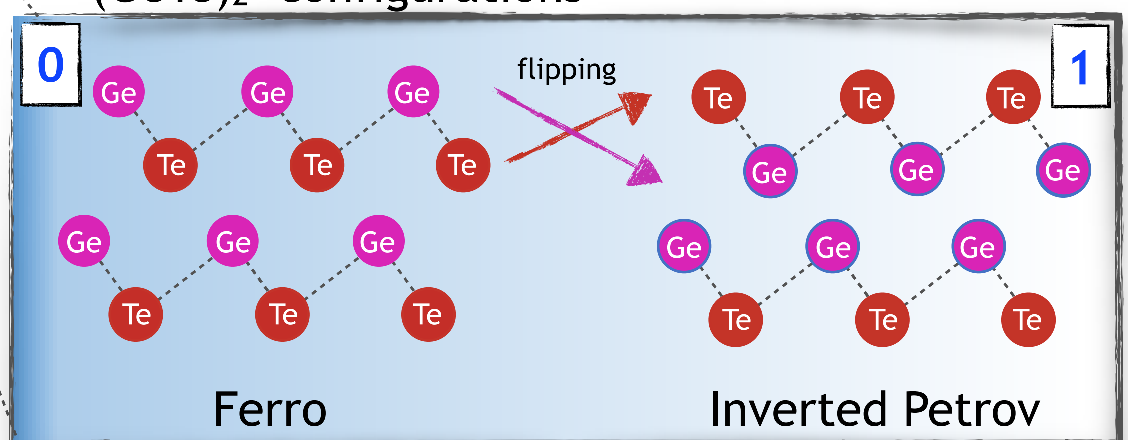
Simpson, Nat. Nanotechnol. 6, 501 (2011)

Switching $\longrightarrow$ *crystal-crystal* transformation with GeTe rearrangement in SL.

Low-(*Ferro*) vs high-resistance (*Inverted Petrov*) states via two-steps flipping process (*vertical + lateral*)

Kolobov, ACS Omega 2, 6223 (2017)
Yu, Sci. Rep. 5, 12612 (2015)

$(GeTe)_2$ configurations



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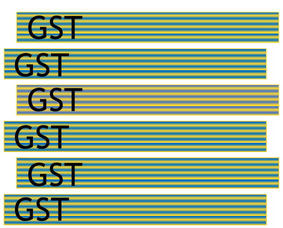
SCENARIO #2:



Structure $\longrightarrow$ tendency of Sb_2Te_3 in SL grown by MBE to incorporate GeTe bilayers to form GST-block

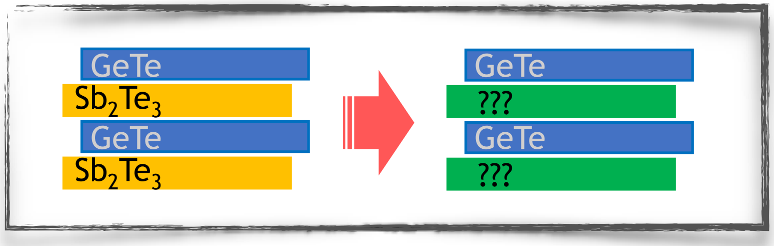
Momand, Nanoscale 7, 19136 (2015)
Wang, Cryst. Growth Des. 16, 3596 (2016)

Switching $\longrightarrow$ either thermally driven with amorphization within GST blocks or driven by reconfiguration of bilayer defects (Sb-rich/Te) at GST vdW gap

Boniardi, Phys. Status Solidi RRL 13, 1800634 (2019)
Kolobov, ACS Omega 2, 6223 (2017)
Saito, Appl. Phys. Lett. 114, 132102 (2019)

GeTe-In_3SbTe_2 superlattices

- Conceive alternative SL structure preventing GeTe-Sb_2Te_3 mixing into GST



- Retain SCENARIO #1 crystal-crystal switching mechanism

Yu, Sci. Rep. 5, 12612 (2015)

- Sb_2Te_3 replacement – Study geometry, electronic structure and switching mechanism of $(GeTe)_3$-In_3SbTe_2 SL

- In_3SbTe_2 (IST) is known phase change material with rocksalt crystalline phase and high crystallization temperature

- Use first-principles DFT methods

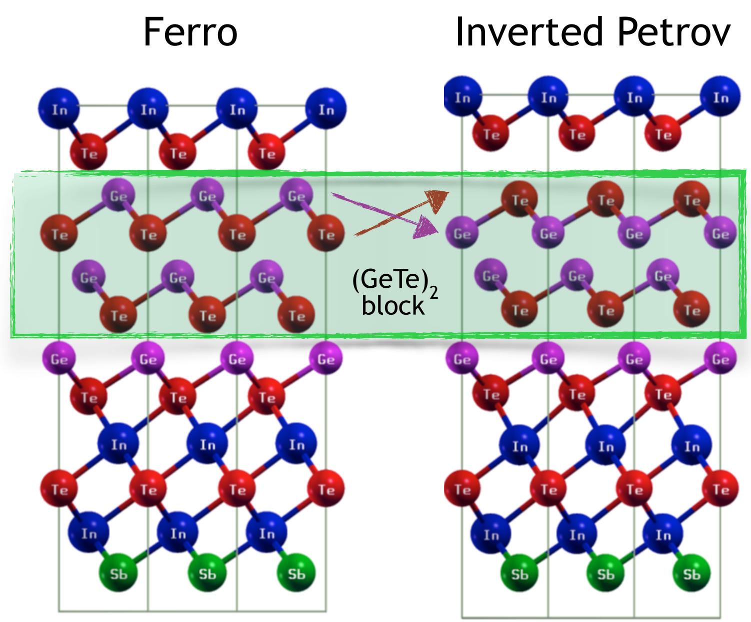
$(GeTe)_3$-In_3SbTe_2 structure

$(GeTe)_3$-In_3SbTe_2 best candidate structure:

1. $GeIn_3SbTe_3$ and $(GeTe)_2$ block Alternation
   — Low/high-resistance (Ferro/Inverted Petrov) configurations as in $(GeTe)_2$-Sb_2Te_3

2. Large 2% biaxial tensile strain of GeTe bilayers, Strain route to reduce Activation energy[1]
   — only 0.7%[2] in $(GeTe)_2$-Sb_2Te_3

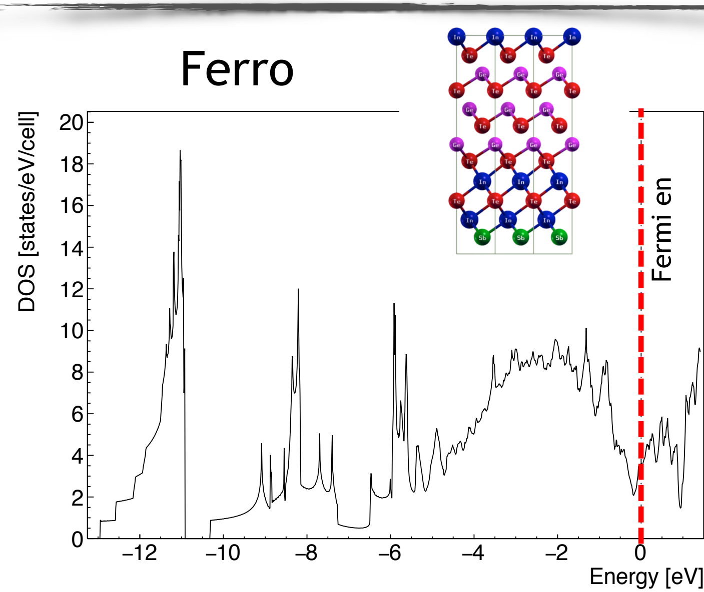
3. Low formation energy for the Ferro ground-state phase wrt parent compounds — 20 meV/at



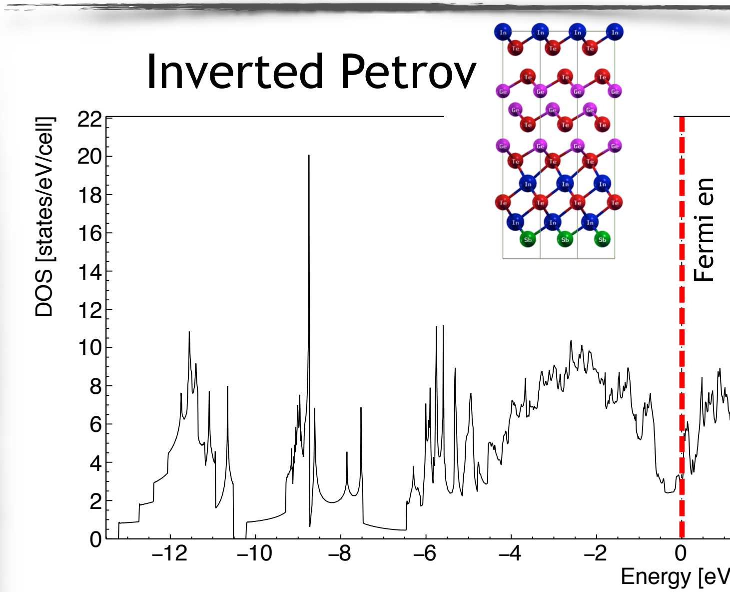
[1] Kalikka, Nat. Commun. 7 11983 (2016)
[2] Yu, Sci. Rep. 5, 12612 (2015)

$(GeTe)_3$-In_3SbTe_2 electronic properties

- Both Ferro and Inverted Petrov appear metallic from SO-corrected DOS
- Most of metallicity due to in-plane contributions ascribed to In_3SbTe_2
- Out-of-plane conductivity matters for iPCM



DOS(E_F)= 3.62 states/eV/cell



DOS(E_F)= 2.98 states/eV/cell

$(GeTe)_3$-In_3SbTe_2 conductivity

Electrical contrast in out-of-plane direction between Ferro and Inverted Petrov (IP) phases from *dc* conductivity

$$\sigma_{\mu\nu} \propto \sum_{\alpha,\mathbf{k}} \mathbf{v}_\mu(\alpha,\mathbf{k})\mathbf{v}_\nu(\alpha,\mathbf{k})\delta(\varepsilon_\mathbf{F} - \varepsilon_\alpha(\mathbf{k}))$$

$$\sigma_{zz}^{Ferro}/\sigma_{zz}^{IP} = 3.6$$

Similar value for GeTe-Sb_2Te_3 SL

Nakamura, Nanoscale 9, 9386 (2017)

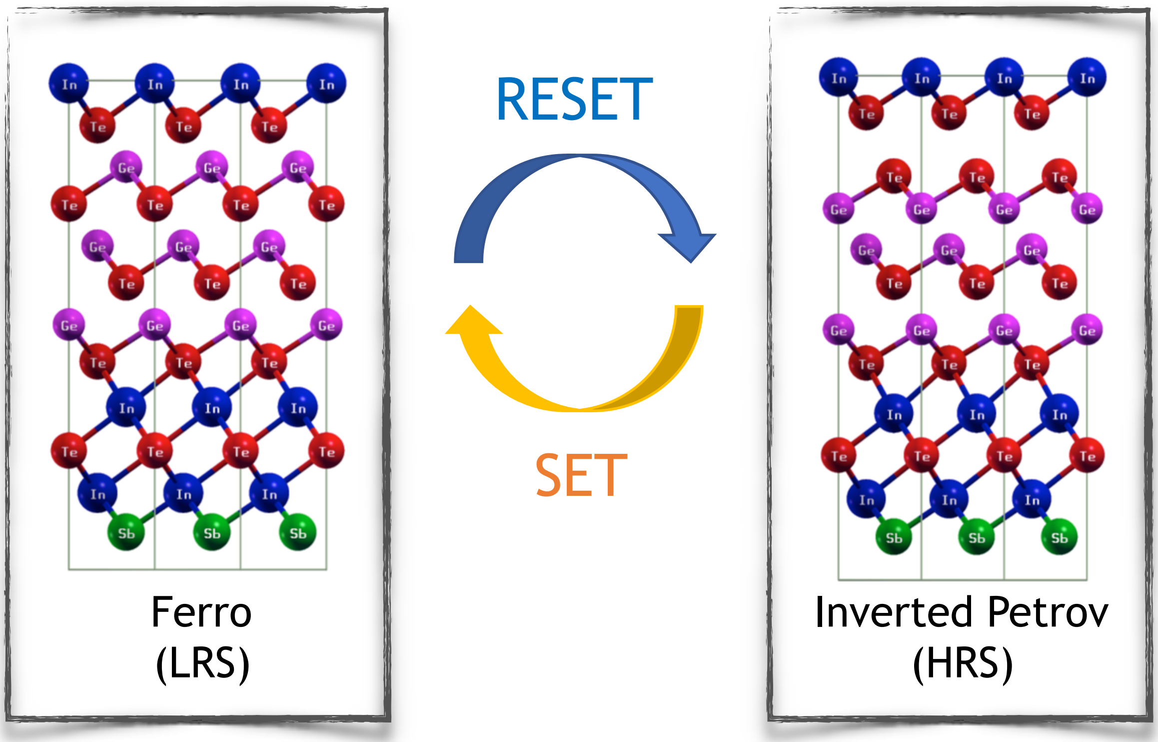
$$\sigma_{zz} \sim 10^4\, S/cm$$

- Ferro as Low-Resistive State (LRS)
- Inverted Petrov as High-Resistive State (HRS)

SET-RESET activation barriers

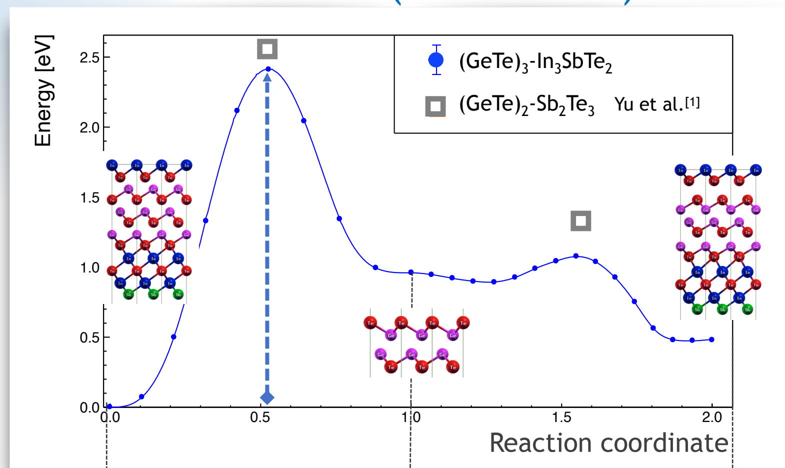
Nudged elastic band (NEB) method to compute Activation barriers between LRS and HRS states

Adopt the *vertical* + *lateral* flipping path proposed for $(GeTe)_2$-Sb_2Te_3



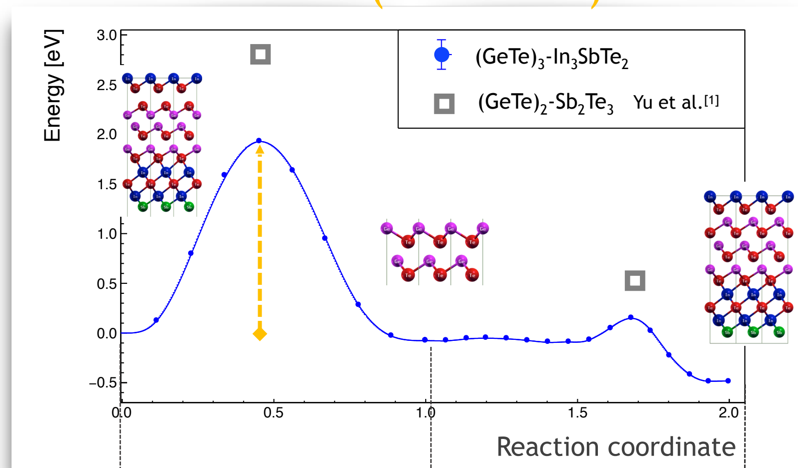
SET-RESET activation barriers

RESET (F0-IP1-IP0)



Ferro (F0) IP1 Inverted Petrov (IP0)

SET (IP0-F2-F0)



Inverted Petrov (IP0) F2 Ferro (F0)

RESET activation energy:
$(GeTe)_3$-In_3SbTe_2 = 2.41 eV
$(GeTe)_2$-Sb_2Te_3 = 2.56[1] eV

Δ = −0.15 eV

SET activation energy:
$(GeTe)_3$-In_3SbTe_2 = 1.93 eV
$(GeTe)_2$-Sb_2Te_3 = 2.84[1] eV

Δ = −0.91 eV

[1] Yu, Sci. Rep. 5, 12612 (2015)

Summary

- $(GeTe)_3$-In_3SbTe_2 as an alternative to $(GeTe)_2$-Sb_2Te_3 for iPCM realization
- In_3SbTe_2 used to possibly prevent mixing of Sb_2Te_3 and GeTe blocks
- New SL with 2% biaxially strained $(GeTe)_2$ blocks
- Ferro- and Inverted Petrov-like configurations identified as LRS/HRS
- Conductivity contrast similar to $(GeTe)_2$-Sb_2Te_3
- Reduction of activation energies for SET/RESET transformation $\longrightarrow$ Lower power consumption as compared to $(GeTe)_2$-Sb_2Te_3

Thank you