



ALMA MATER STUDIORUM
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MODENA E REGGIO EMILIA

Modeling the Electric Switching of Chalcogenide Materials Below the Nanoscale Limit

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Chalcogenides

Chemical compounds consisting of at least one chalcogen ion (S, Se, or Te), and one or more electropositive elements:

GeTe, Ge₂Sb₂Te₅, ZnTe, AgInSbTe (AIST), ...



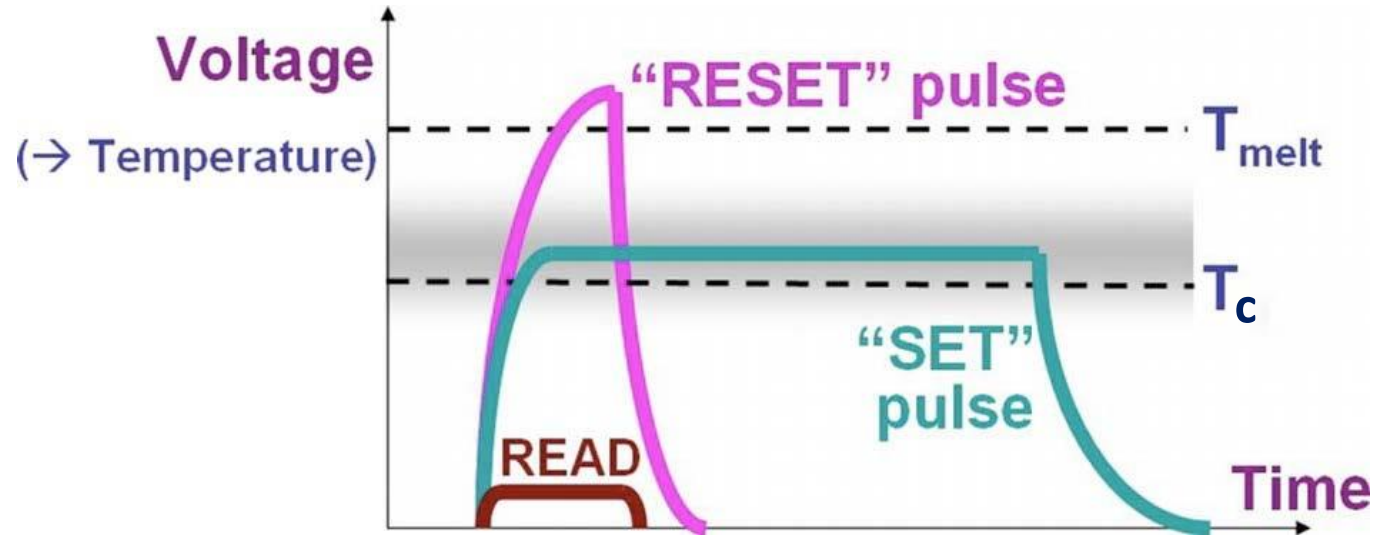
3	4	5	6	7	8	9	10
13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A		
5 B Boron 10.81	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180		
13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.948		
31 Ga Gallium 69.723	32 Ge Germanium 72.64	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.8		
49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.6	53 I Iodine 126.905	54 Xe Xenon 131.29		
81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.98	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222		
113 Uut Ununtrium 288	114 Fl Flerovium 289	115 Uup Ununpentium 288	116 Lv Livermorium 293	117 Uus Ununseptium 294	118 Uuo Ununoctium 294		

They yield (binary, ternary,...) alloys with semiconductor properties.

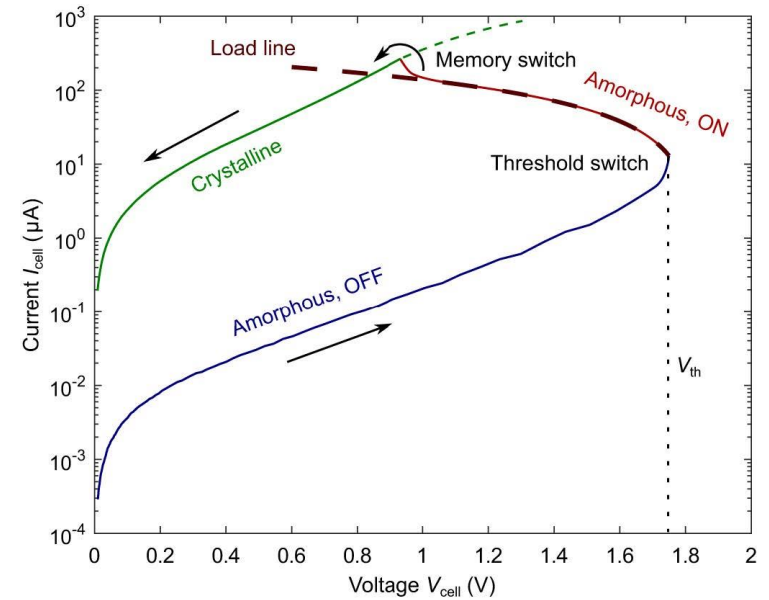
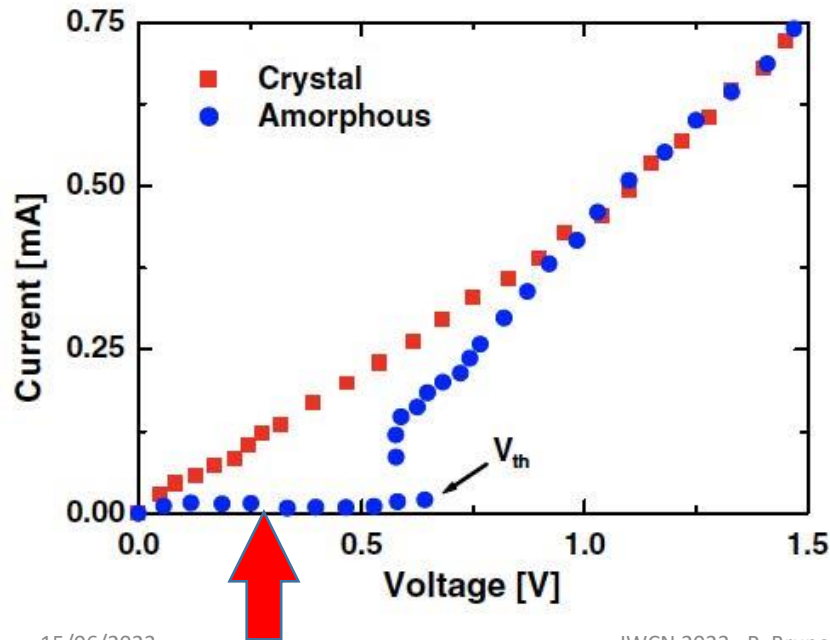
Concept first proposed by **S. Ovshinsky** (1922-2012) in 1968.

$I(V)$ characteristic: threshold-switching behavior

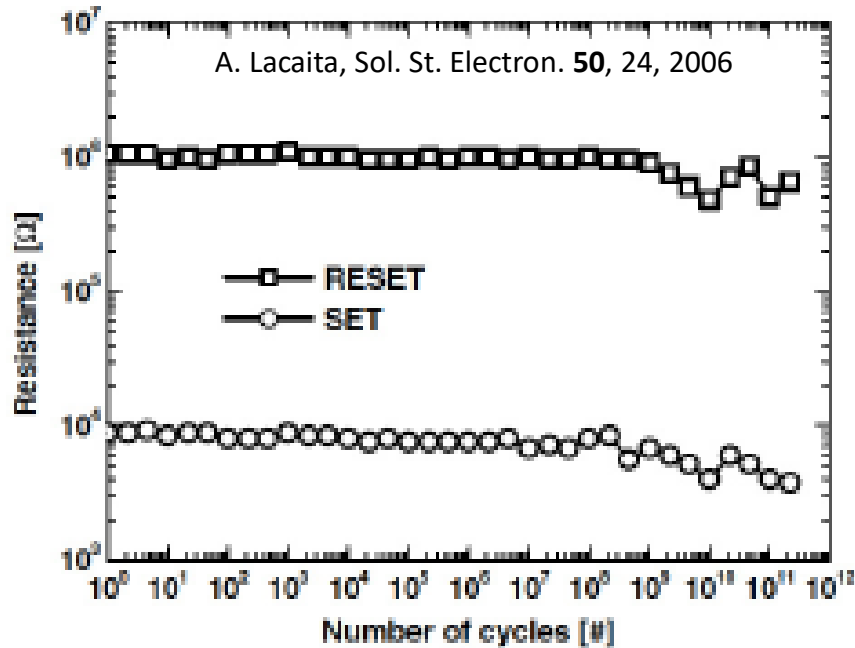
Burr et al., J Vacuum Science Technol., 2010



Le Gallo et. al., J. Phys. D (2020)



Threshold-switching: useful properties

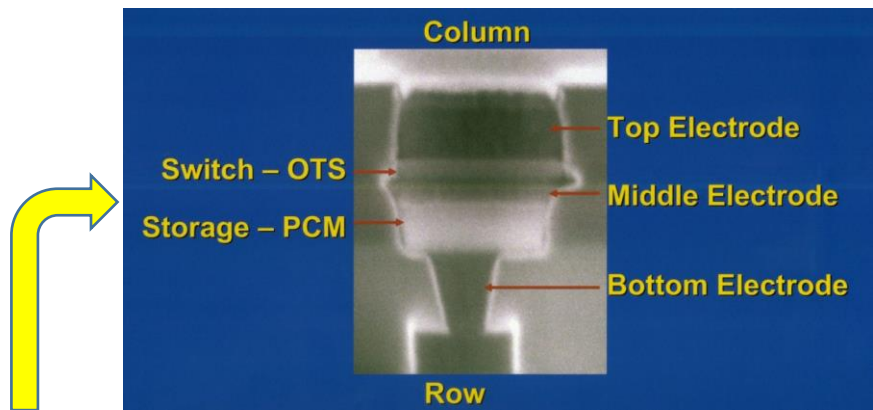


Resistivity changes by **at least 2 orders of magnitude**

Stability of the two physical states, and **large duty cycle**.

- **Large difference** in physical properties (resistivity, reflectivity) between the two (crystalline and amorphous) phases .
- **Two-state system**: possibility to store logic information («0» or «1»).
- **Fast (down to few ns) and reversible transition** between amorph. (OFF and ON) and crystalline phases induced by heating (laser irradiation or Joule effect).

Application to memories and research issues



D-C. Kau et al., 2009 IEDM Tech. Digest, 617

Optane: non-volatile memory commercialised by Micron-Intel in 2017

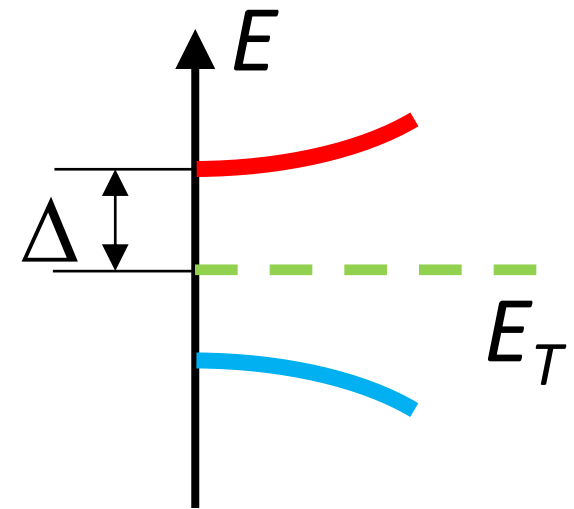
The origin (electrical, thermal or mixed electrical/thermal) of the Ovonic Switch is still a debated issue

Switching of the α -phase triggered by carrier heating

- **Localized** (trap) and **mobile** (band) states in the amorphous phase.
- Energy transfer from an external field to charge carriers.

Δ is known from optical measurements

The dispersion relation is condensed into parameter g_T / g_B



- Near threshold, **carrier heating gives rise to a positive feedback** by inducing transitions to mobile states: this determines the transition (OTS) to the low-resistivity, still-amorphous, phase.

Key features of the model – A: hydrodynamic equations

Trap-limited transport, i.e., field-assisted (Poole) transitions between localized and mobile states. The number of electrons is large enough to allow for a continuous description

$$\frac{\partial n}{\partial t} + \frac{1}{q} \frac{\partial J}{\partial z} = 0$$

Particle continuity

$$\frac{\partial n_B}{\partial t} = \frac{\partial n}{\partial t} - \frac{n_B - \tilde{n}_B}{\tau_n}$$

Local particle redistribution

$$\frac{\partial \epsilon_{\text{tot}}}{\partial t} = JF - \frac{\Delta}{q} \frac{\partial J}{\partial z} - \frac{k_B}{q} \frac{T_e - T_0}{\tau_T}$$

Energy continuity

$$\frac{\partial F}{\partial z} = -\frac{q}{\epsilon} [n - n_{\text{eq}}]$$

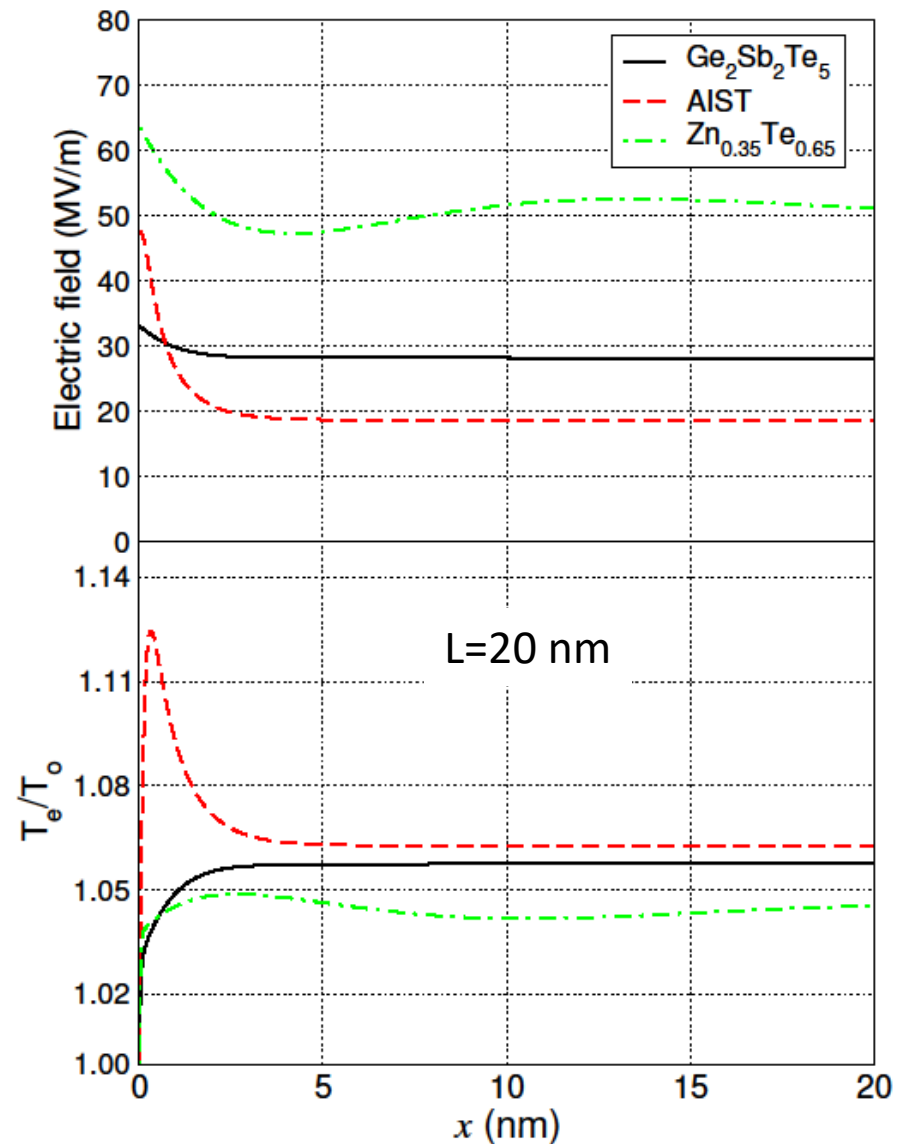
Poisson eq.

Key features of the model – B

- **Nanometric, homogeneous block of amorphous chalcogenide, with unipolar (electron) conduction.**
- Localised and mobile states; **field-assisted (Poole) transitions.**
- Electrons tend to the Fermi distribution at temperature T_e
- Equilibrium conditions at the injecting (ohmic) contact, spatial homogeneity found at the exit side (see next slide).

Spatial (in)homogeneity

In steady state, spatial inhomogeneity is found close to the injection contact.



Key features of the model – C: Numerical solution

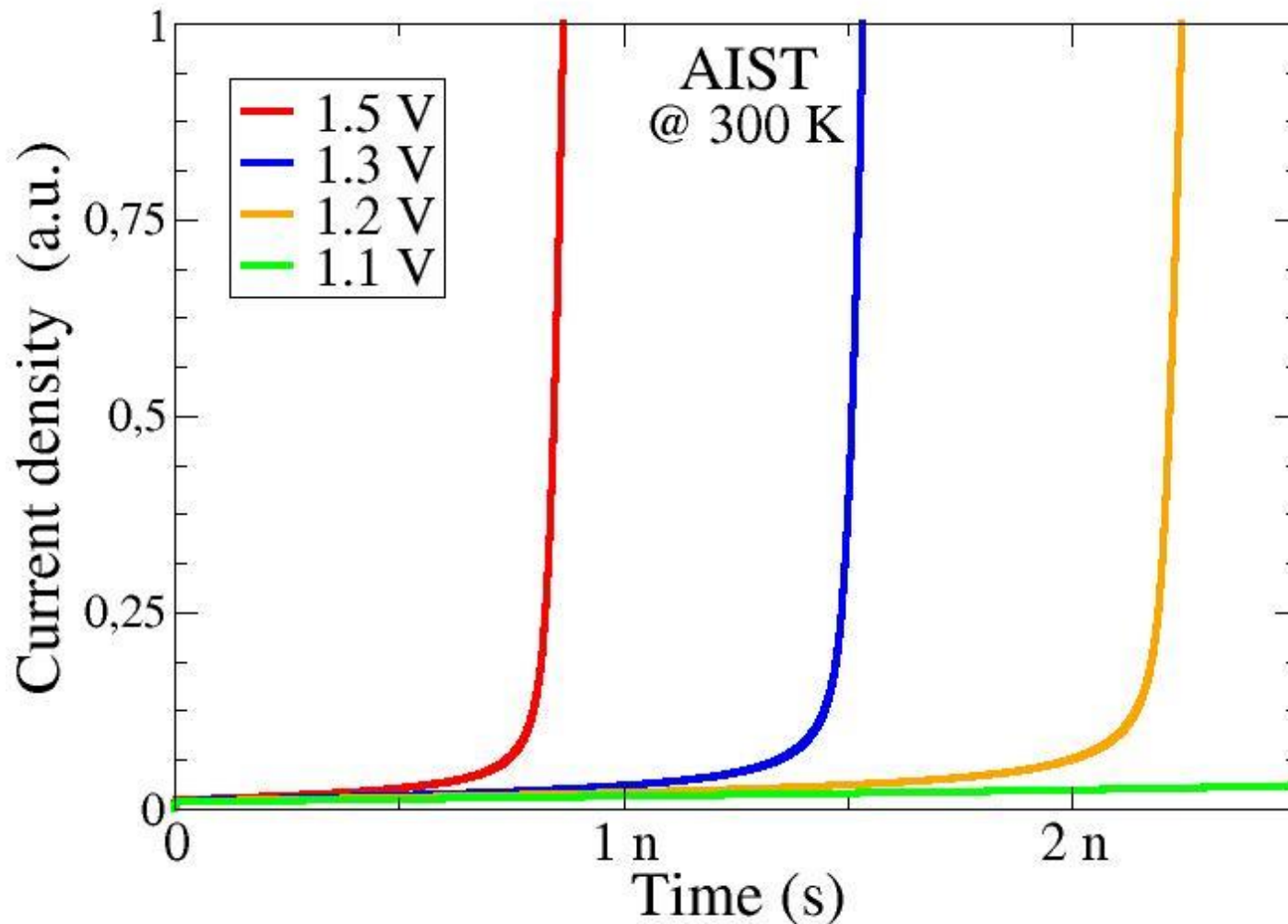
- **Forward Euler method. The complicity of the model dictates a small integration step ($\Delta t = 10^{-16}$ s).**
- No numerical instability detected during the simulations; in fact, time constants in the model have little interplay:
 - τ_T (ps) dominates up to threshold
 - τ_n (ns) controls the population relaxation
- Accuracy of about 10% is considered appropriate to compare simulation with experimental data.

Transport Aspects investigated with the model (2012-23)

- Electrical nature of OTS in chalcogenides demonstrated (Piccinini *et al.*, JAP 2012).
- Dynamics of the electron heating and the OTS onset analyzed (Cappelli *et al.*, APL 2013).
- Time-dependent operation including parasitics effect (Piccinini *et al.*, J. Phys. D, 2016).
- Role of the dispersion of the band states (Brunetti *et al.*, JCE 2020).
- Electric response in presence of a time-dependent bias (Brunetti *et al.*, Frontiers in Physics, 2022).
- **This work: comparison of transient regimes in different chalcogenides (GST-225, ZnTe, AlST) at room and high temperatures; useful for, e.g., automotive applications.**

Search for the “static” threshold voltage for OTS

Transient towards stationarity after the application of a voltage **step**. Estimated accuracy $\sim 10\%$, time span ~ 3 ns.



Experimental data about ultrafast transient regimes

- Advanced programmable setup for electrical tests (time resolution ~ 50 ps, rise/fall times of the pulse ~ 1 ns, pulse width ≤ 1.5 ns, **pulse plateau** $> V_{th}$).

Shukla *et al.*, (2017), Rev. Sci. Instrum.

- Threshold switching in the ps range demonstrated in AgInSbTe (AIST) cells and as short as 1 ns in GST 225 cells.

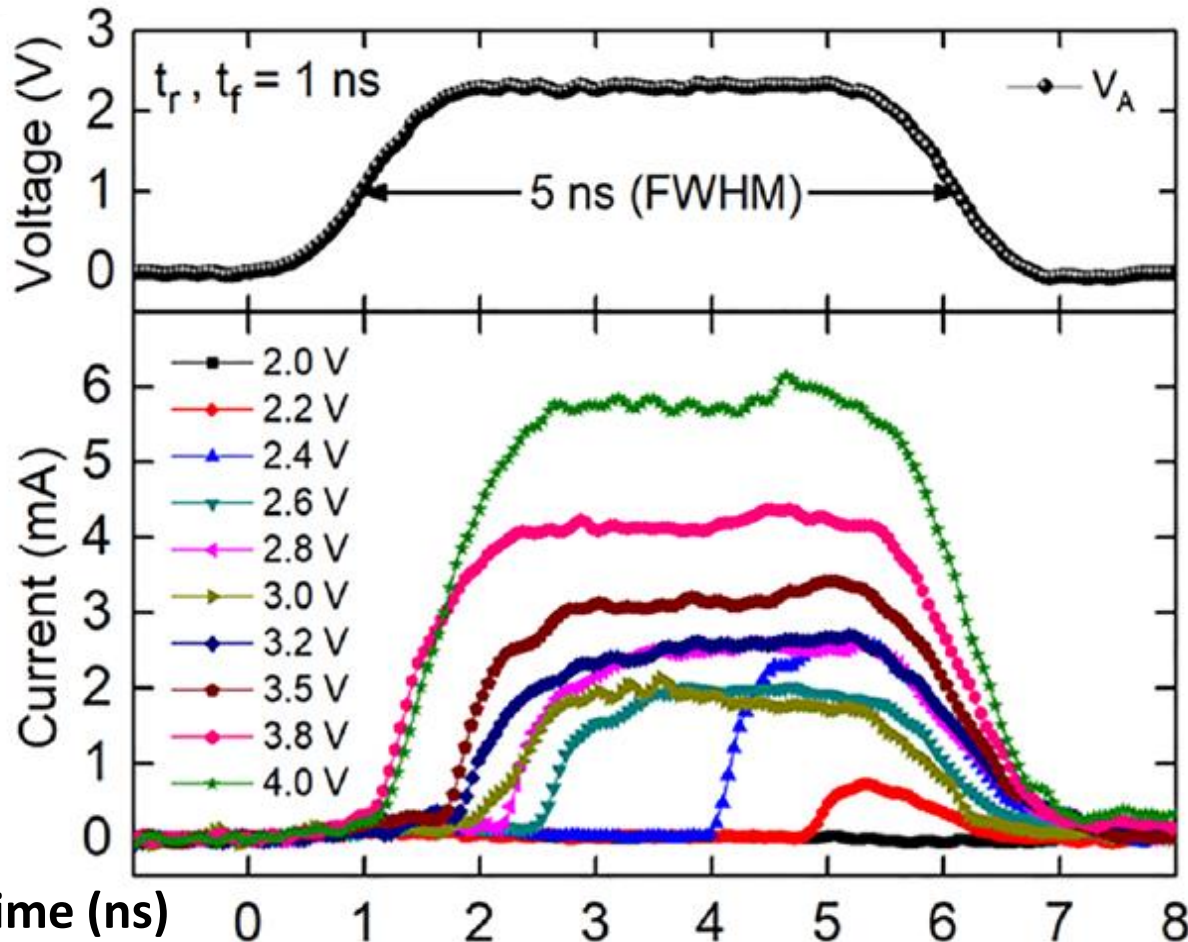
Shukla *et al.*, (2016) Sci. Rep. **6**, 37868 (AIST)

Zalden et.al., (2016) Phys. Rev. Letters (AIST)

Saxena *et al.*, (2021) Sci. Rep. **11**, 6111 (GST-225)

Experimental data about ultrafast transient regimes

Ramp voltage with finite (\sim ns) rise and fall times: threshold switching dynamics below the ns scale found in GST-225.



GST 225

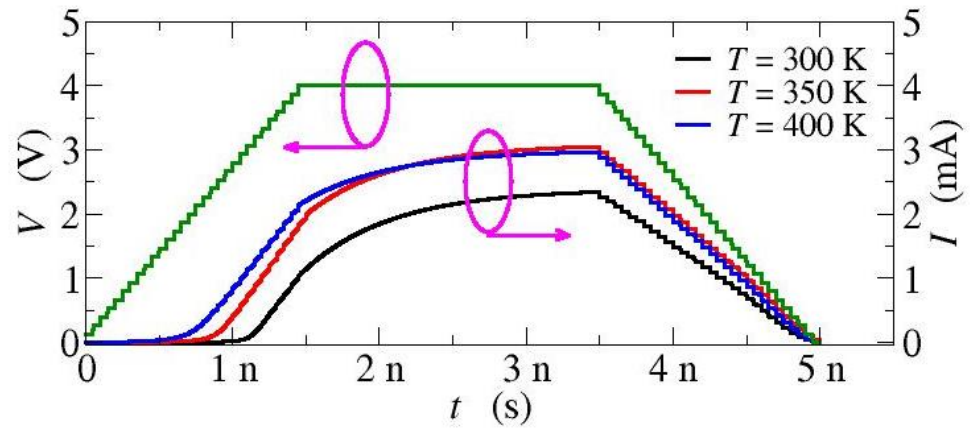
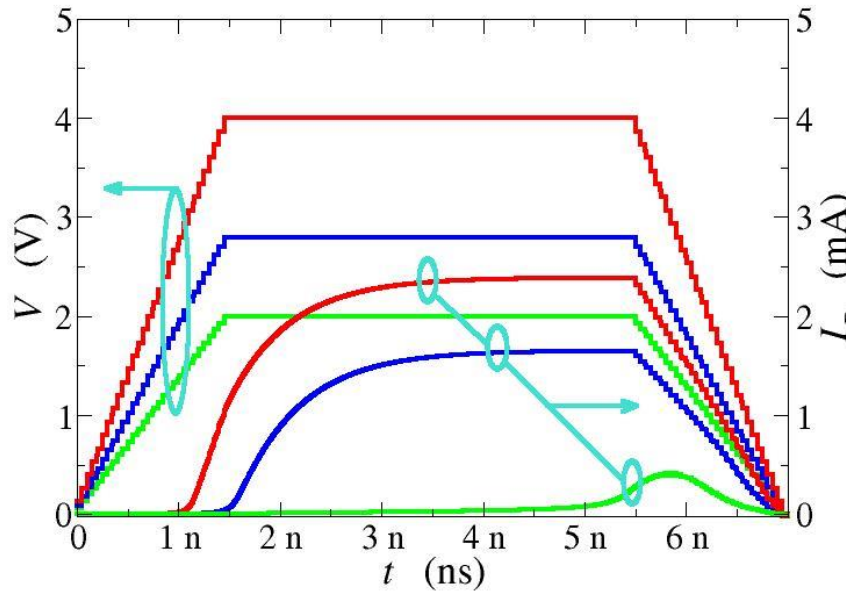
$V_{th} = 2 \pm 0.1$ V

$L = 53$ nm

$T = 300$ K

Saxena *et al.*,
(2021) *Sci. Rep.*
11, 6111.

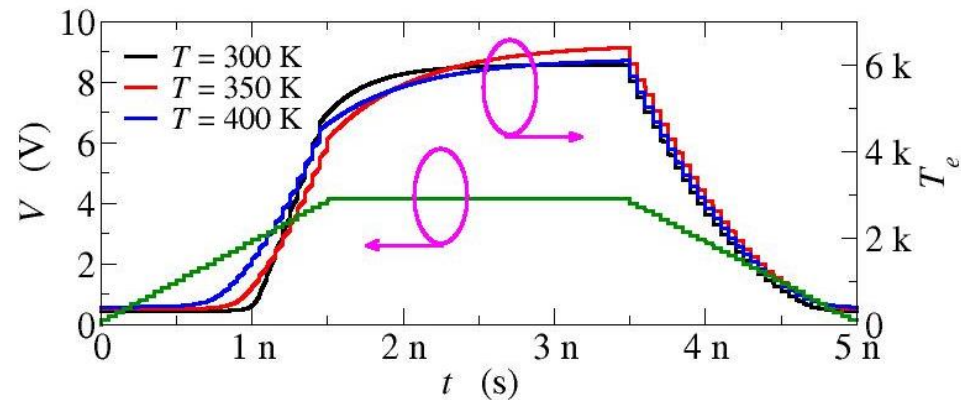
Transport dynamics: GST 225 ($T_c \cong 420$ K)



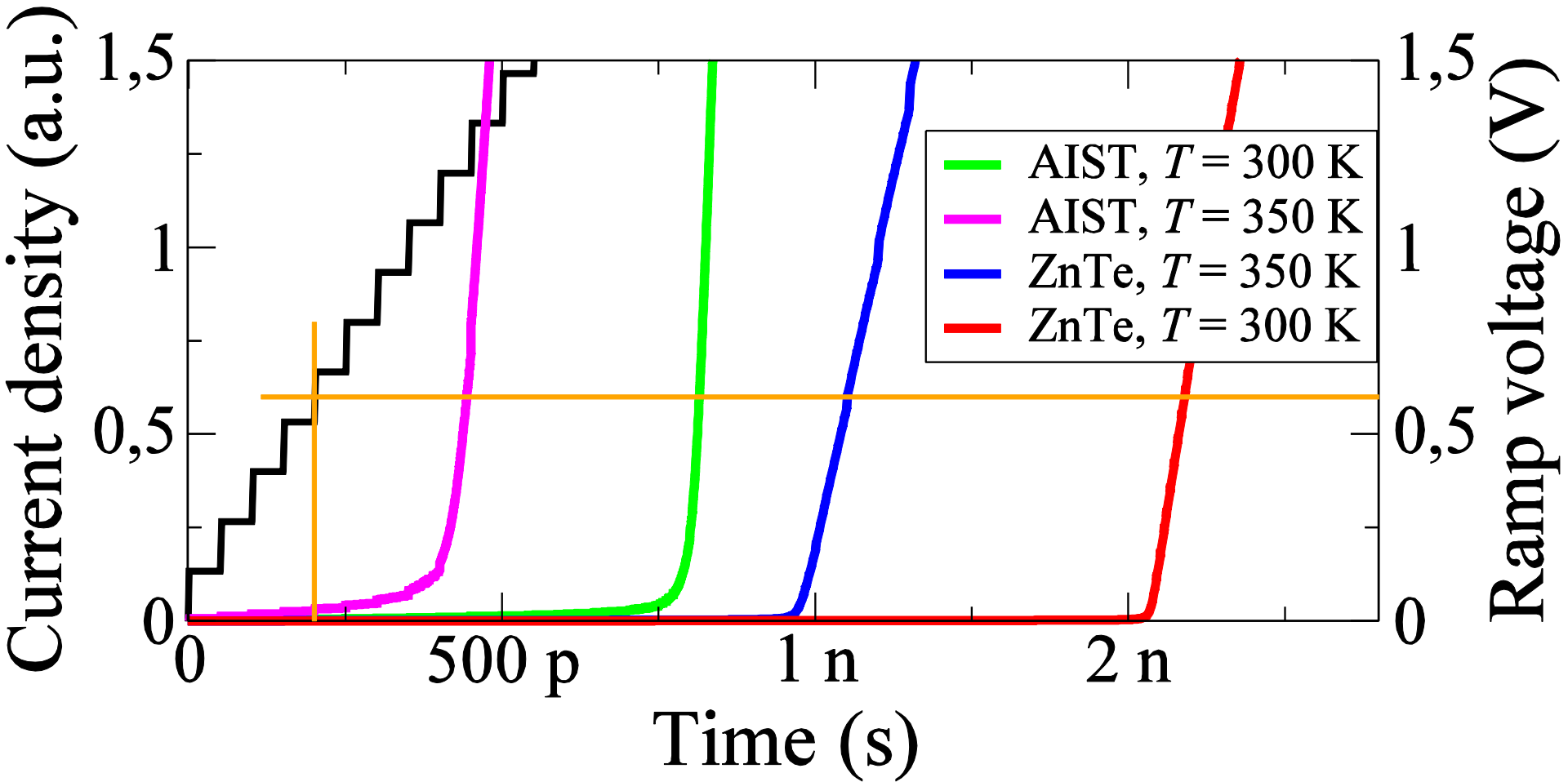
This work



R. Brunetti *et al.*, *Frontiers Phys.*,
10, 2022.

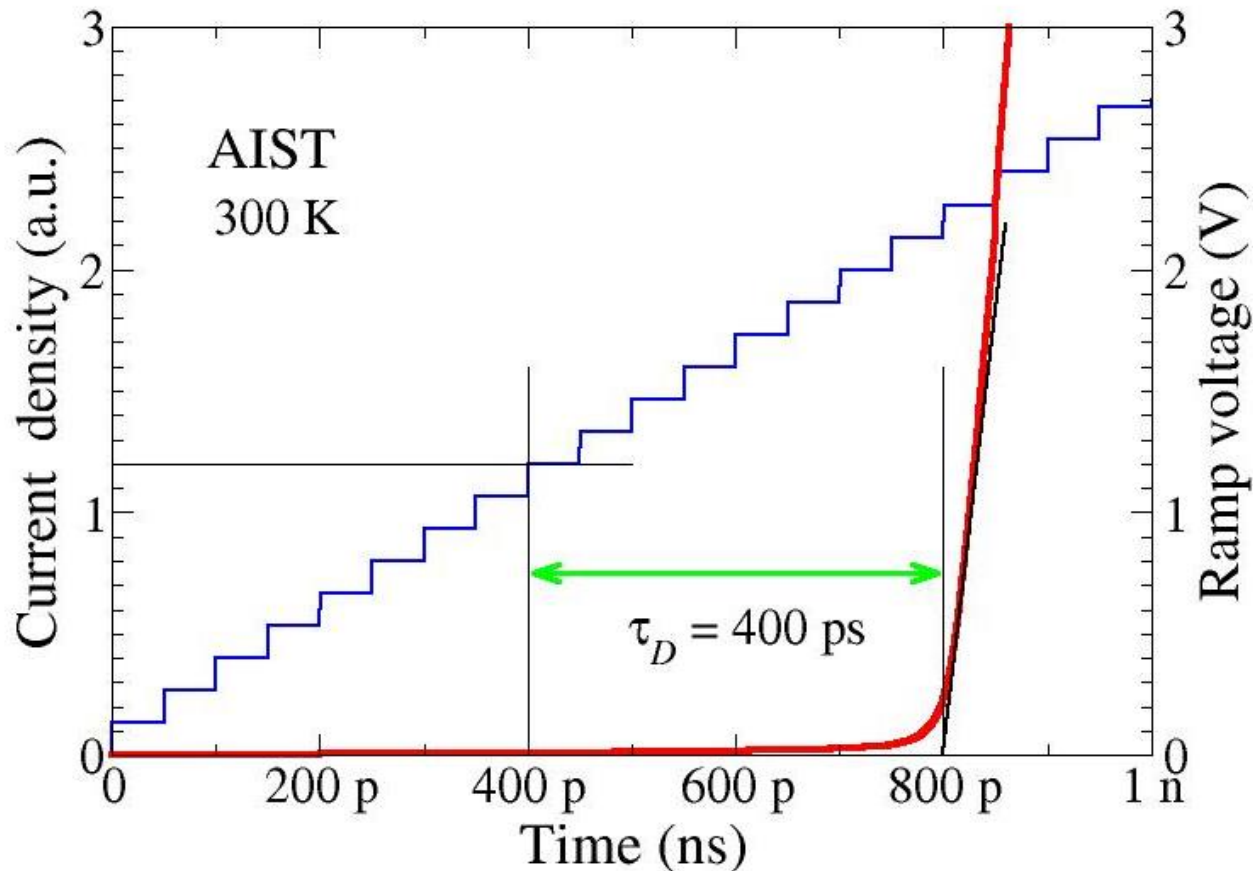


Transport dynamics: ZnTe ($T_c \cong 380$ K), AIST ($T_c \cong 450$ K)

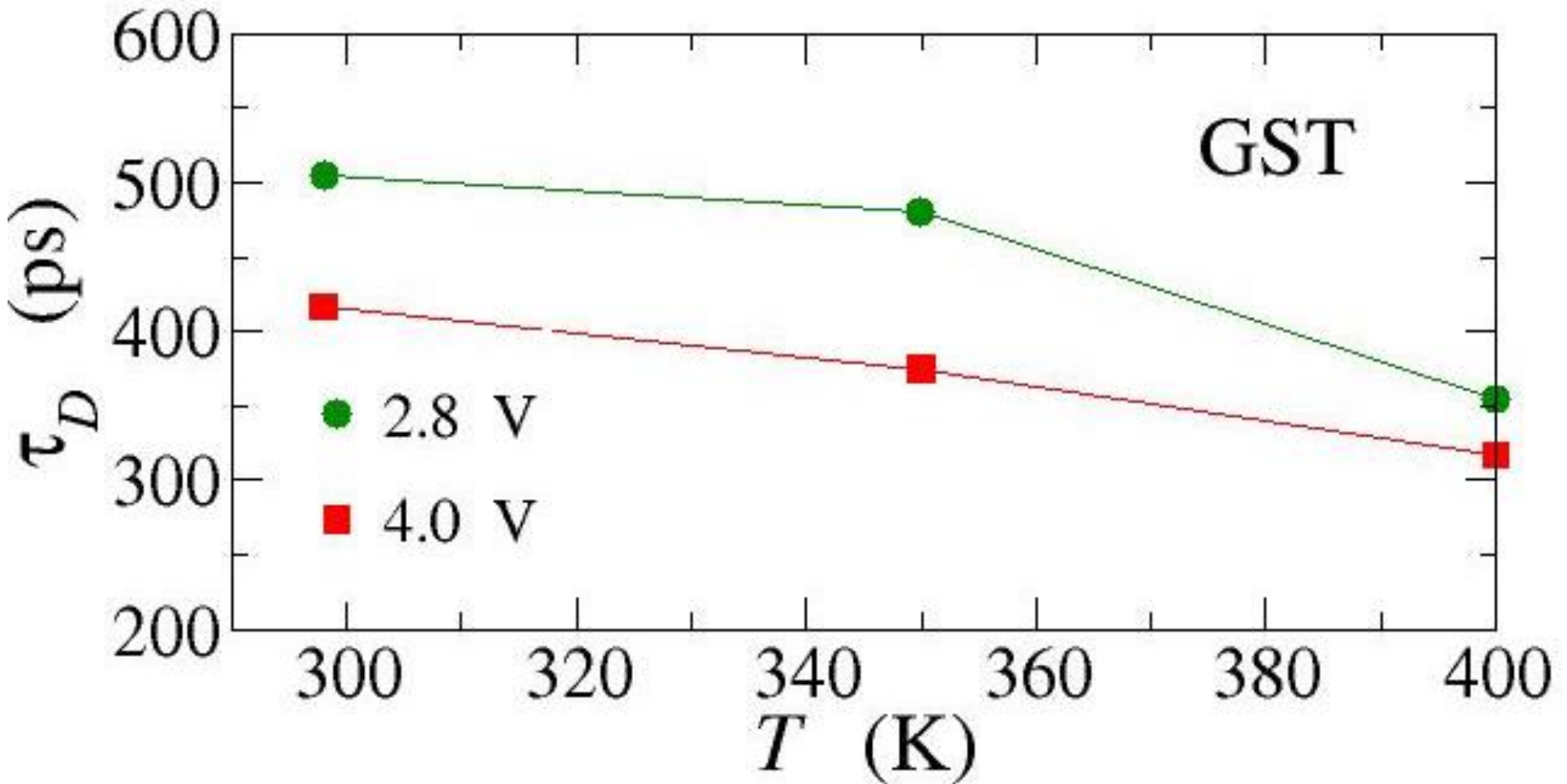


Estimate of the delay time

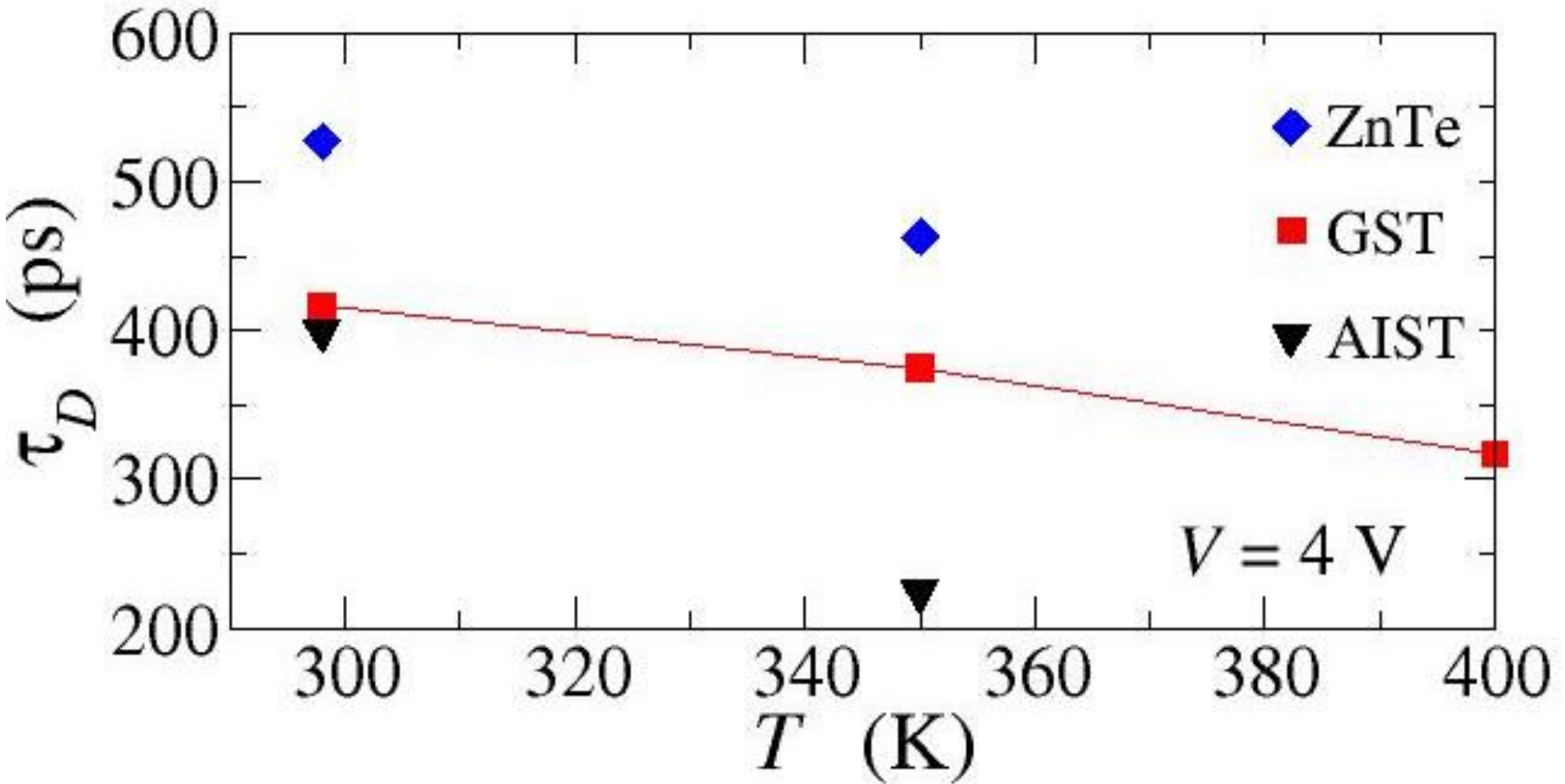
τ_D = interval between the instant when the applied voltage exceeds V_{th} and the instant when the device current rises steeply.



Delay-time – GST 225 at different plateaux



Delay-time – ZnTe, GST 225, AIST



Conclusions

- Hydrodynamic-like transport model for amorphous chalcogenides tested against experiments with voltages varying in the ns scale.
- Increase in lattice temperature reduces V_{th} and τ_D .
- **ZnTe has the longest τ_D .**
- **GST confirmed as best performing at high temperatures. Moderate change of V_{th} and τ_D .**
- **AlST shows a strong decrease of τ_D at higher T , together with the maximum V_{th} decrease.**