Band gap energy modelisation in Silvaco TCAD Atlas Device simulator

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Outline

- Bandgap narrowing in Silvaco
- Reverse/forward current level vs bandgap and temperature
- Simulation of radiation damage and impact of bandgap and temperature
  - Reverse bias: depletion voltage and leakage current
  - Forward bias: forward current
- Conclusions and Outlook

BANDGAP NARROWING IN SILVACO

Bandgap narrowing in Silvaco

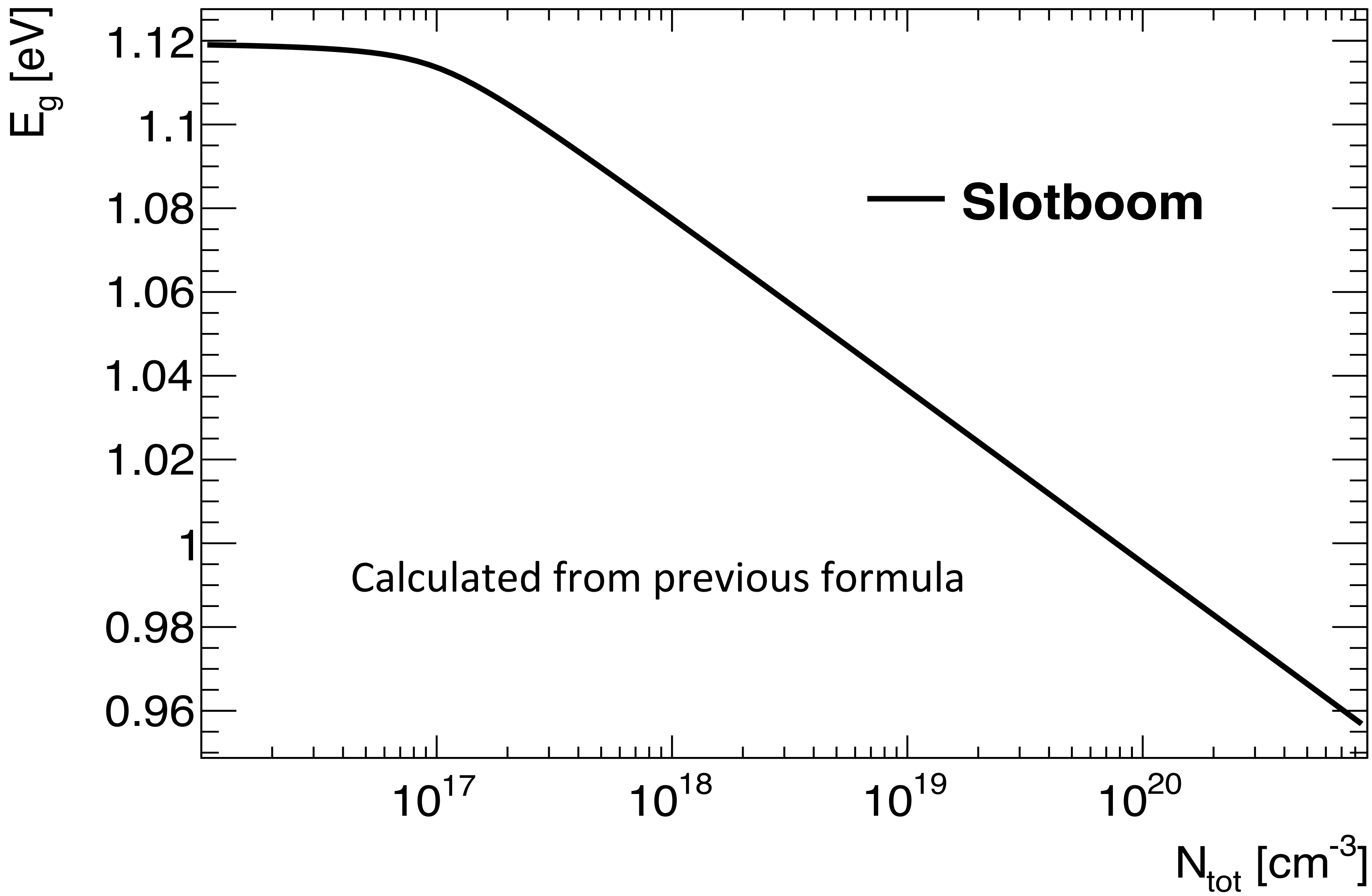
Bandgap narrowing effects in Atlas are enabled by specifying the **BGN** parameter of the **MODELS** statement. These effects may be described by an analytic expression relating the variation in bandgap, ΔE_g, to the doping concentration, N. The expression used in Atlas is from Slotboom and de Graaf [297]:

$$\Delta E_g = \mathrm{BGN.E}\left\{ ln\frac{N}{\mathrm{BGN.N}} + \left[\left(ln\frac{N}{\mathrm{BGN.N}}\right)^2 + \mathrm{BGN.C}\right]^{\frac{1}{2}}\right\} \qquad 3\text{-}46$$

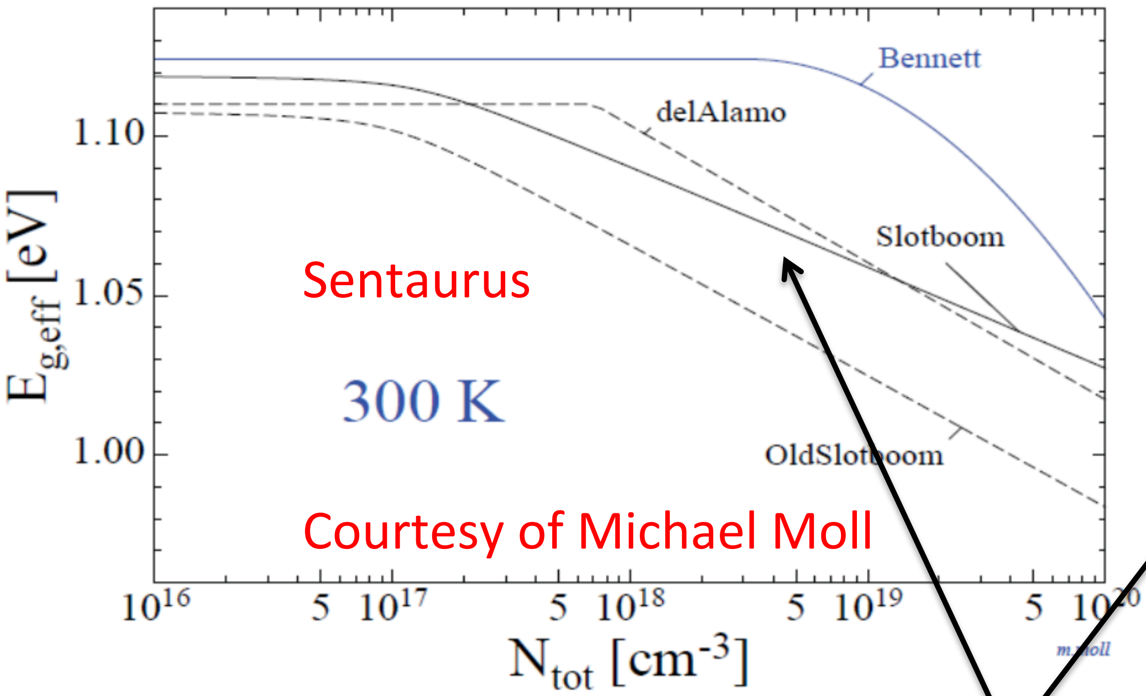
The variation in bandgap is introduced to the other physical models by subtracting the result of Equation 3-47 from the bandgap, E_g. In addition an adjustment is also made to the electric

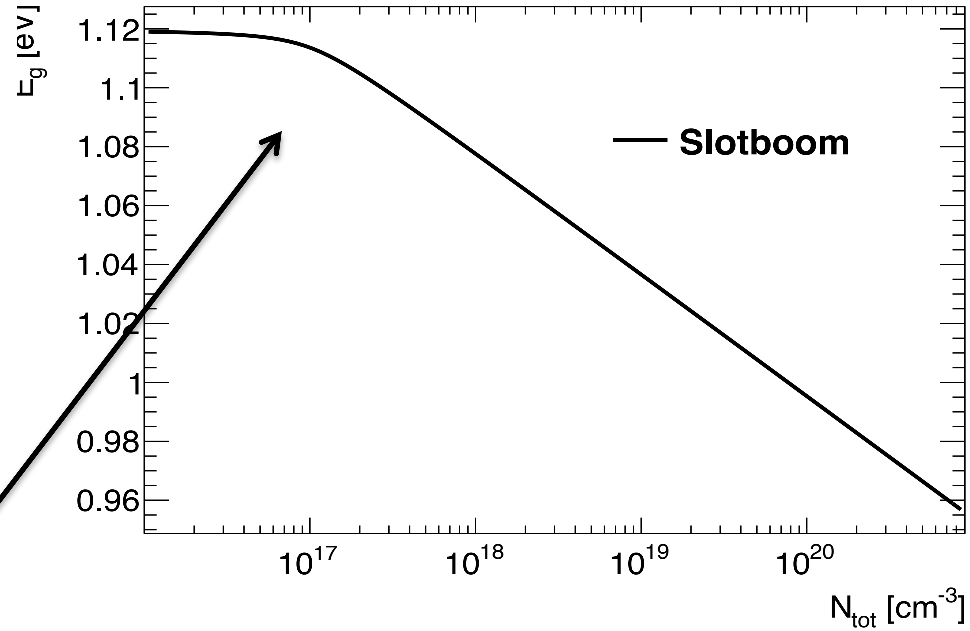
Statement	Parameter	Defaults (Slotboom)	Units
MATERIAL	BGN.E	9.0×10^{-3}	eV
MATERIAL	BGN.N	1.0×10^{17}	cm^{-3}
MATERIAL	BGN.C	0.5	

Bandgap narrowing: how it looks like



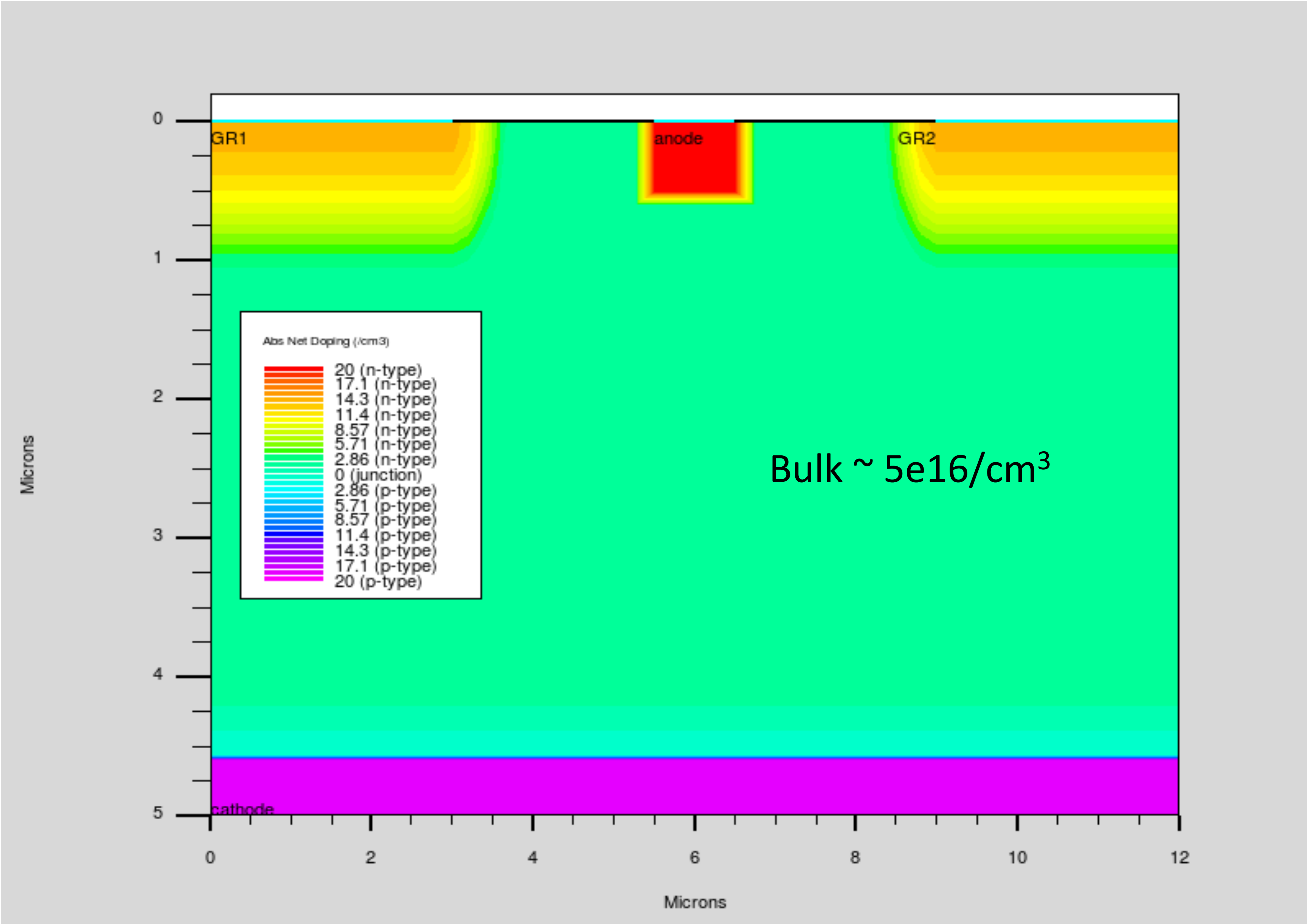
Bandgap narrowing: how it looks like



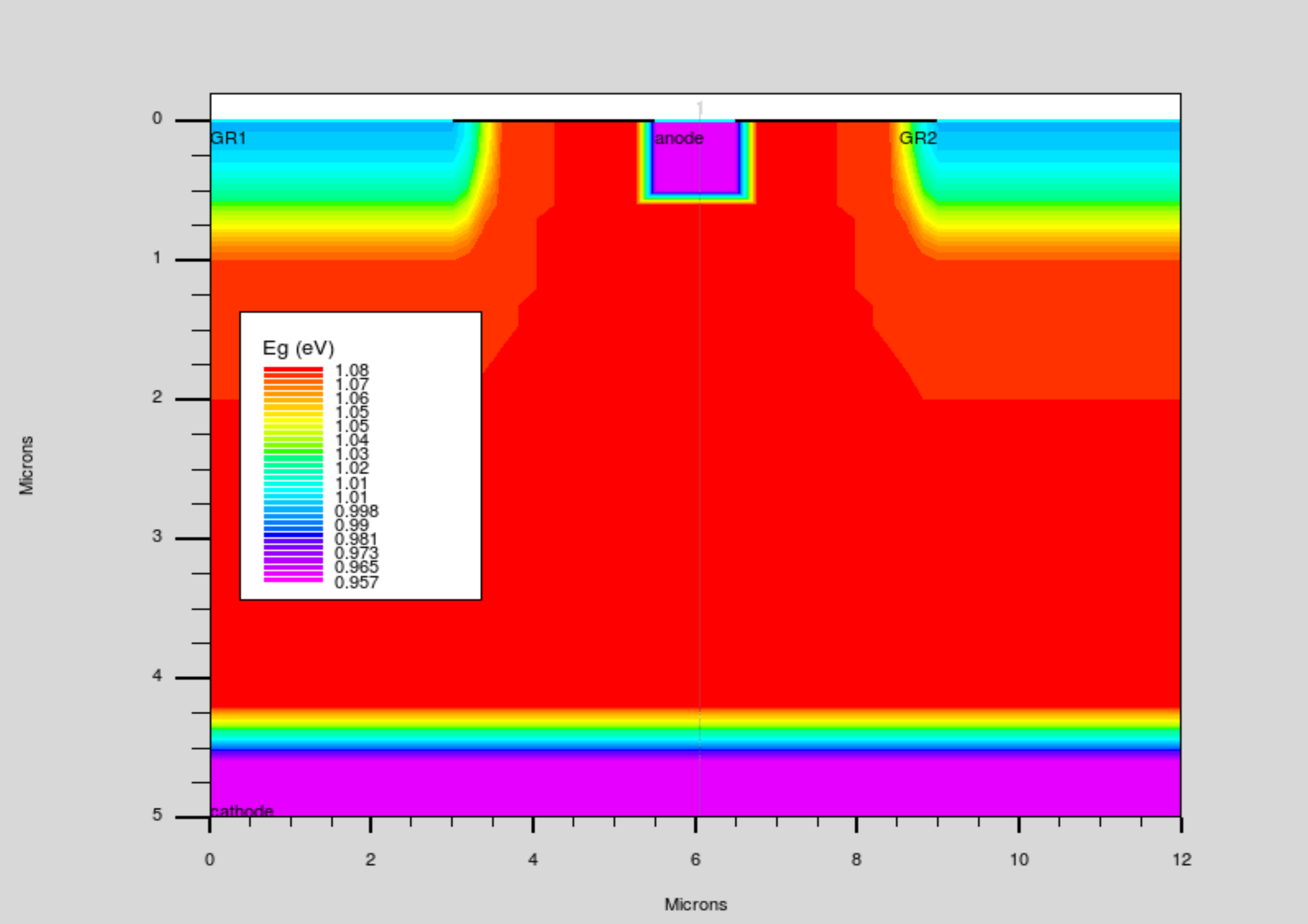


Not sizeable difference

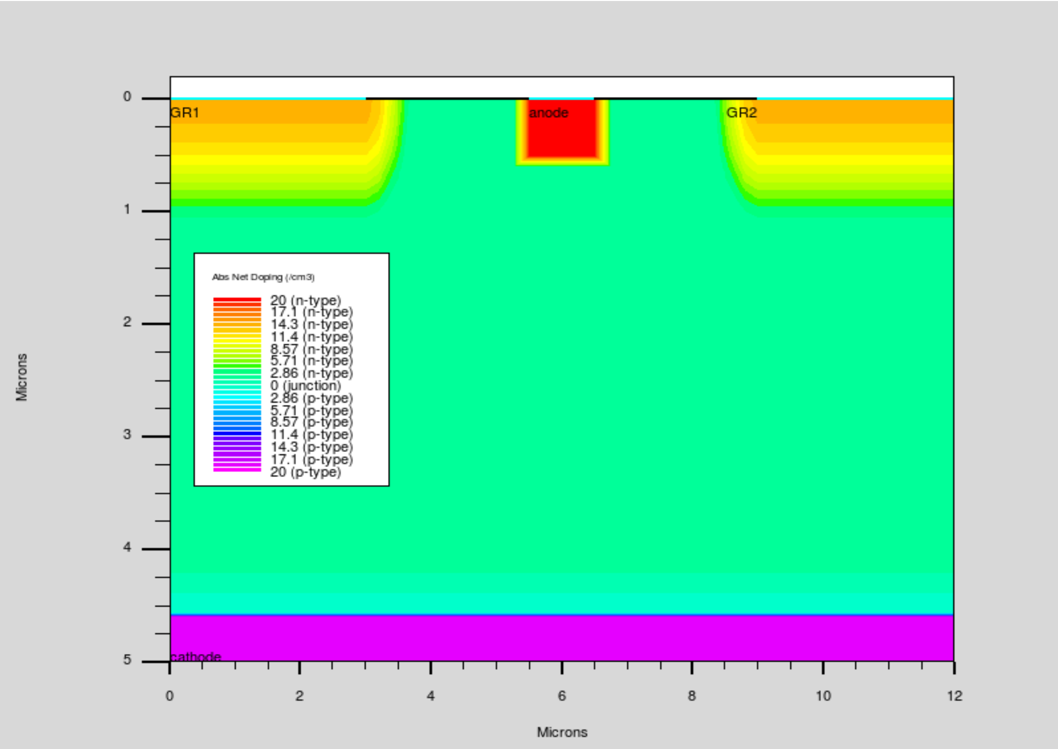
Test structure: effective doping concentration

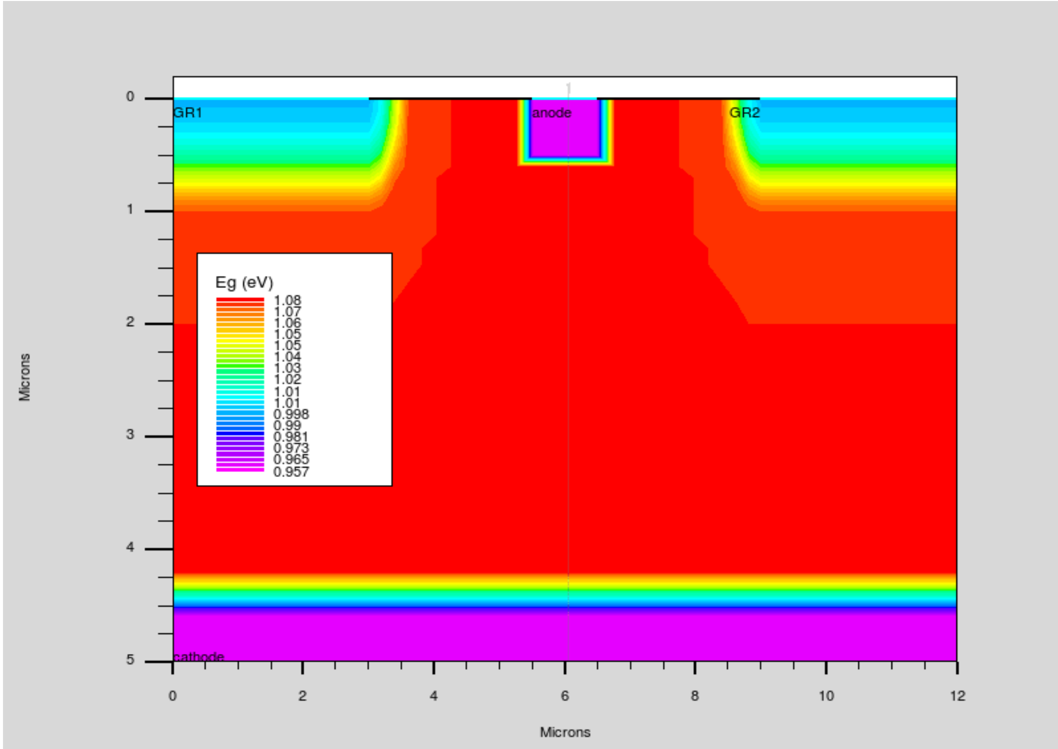


Test structure: bandgap energy in simulation



Test structure: bandgap energy in simulation





No hidden adjustments here: it is what is calculated according to the formulas

Temperature dependence of Eg

- Both Silvaco Atlas and Synopsys Sentaurus use the same parameterization for Eg(T)*:

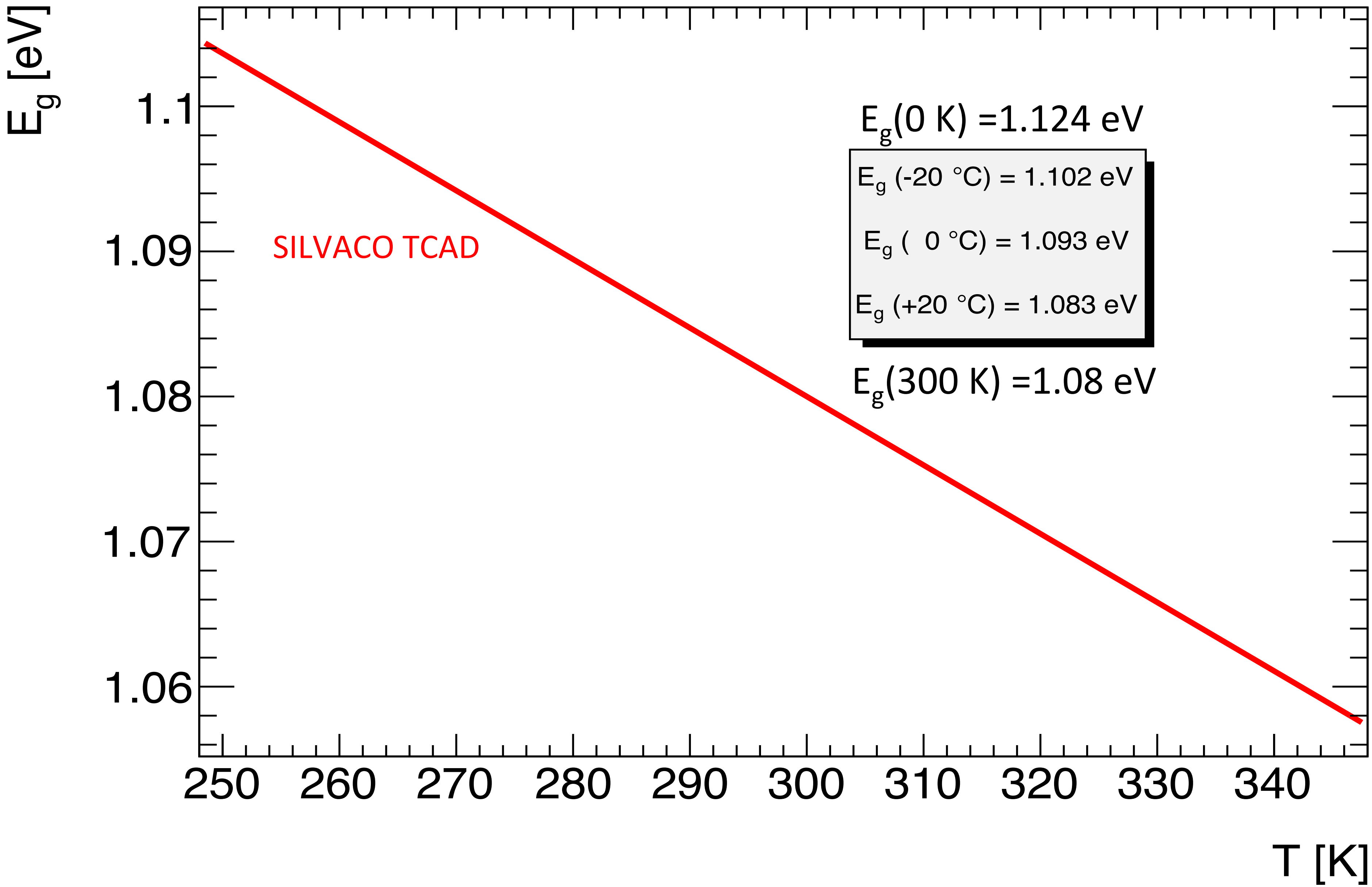
$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T+\beta} = E_g(300) + \alpha\left[\frac{(300)^2}{300+\beta} - \frac{T^2}{T+\beta}\right] \equiv E_g(T_{ref}) + \alpha\left[\frac{(T_{ref})^2}{T_{ref}+\beta} - \frac{T^2}{T+\beta}\right]^*$$

parameter	value
α	4.73×10^{-4} eV/K
β	636 K

- The very well known difference between the two is that:
  - Eg(300K) = 1.08 eV in Silvaco Atlas
  - Eg(0K) = 1.1696 eV in Synopsys Sentaurus (⇔ Eg(300K)~1.12 eV)

* S. M. Sze, Physics of semiconductor devices. John Wiley & Sons, 1981

How do Eg change with temperature?



Reminder: why 1.08 eV?

[redacted]

To: Marco Bomben Cc: [redacted]

Reply-To: [redacted]

RE: silicon bandgap energy value

Hi Marco,

I suspect this is an historical value. You do find references in the literature to the bandgap of silicon being 1.08 eV.

These references tend to be older so I would imagine that as the manufacturing of silicon wafers has improved, the bandgap has shifted slightly with 1.11 ev being settled on.

It is quite a fundamental parameter, changing the default in the software would have quite an effect on users so we probably decided to stick with the slightly lower value, as you know, the user can always set theory own value.

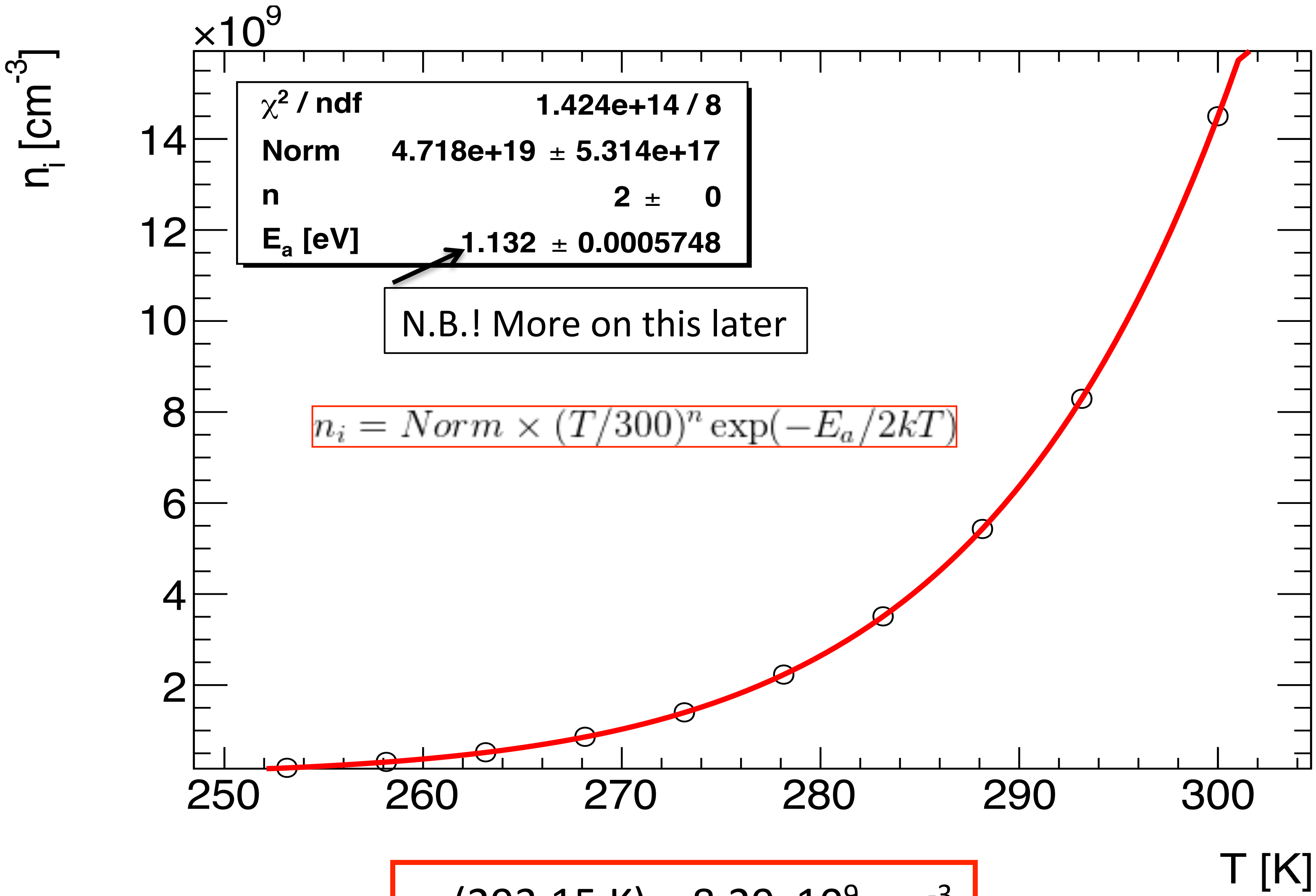
Sze lists it as 1.12 and you see references to 1.1 as well, so there is a bit of a variation out there.

Regards,

[redacted]

Silvaco Europe Ltd.

Intrinsic concentration vs temperature

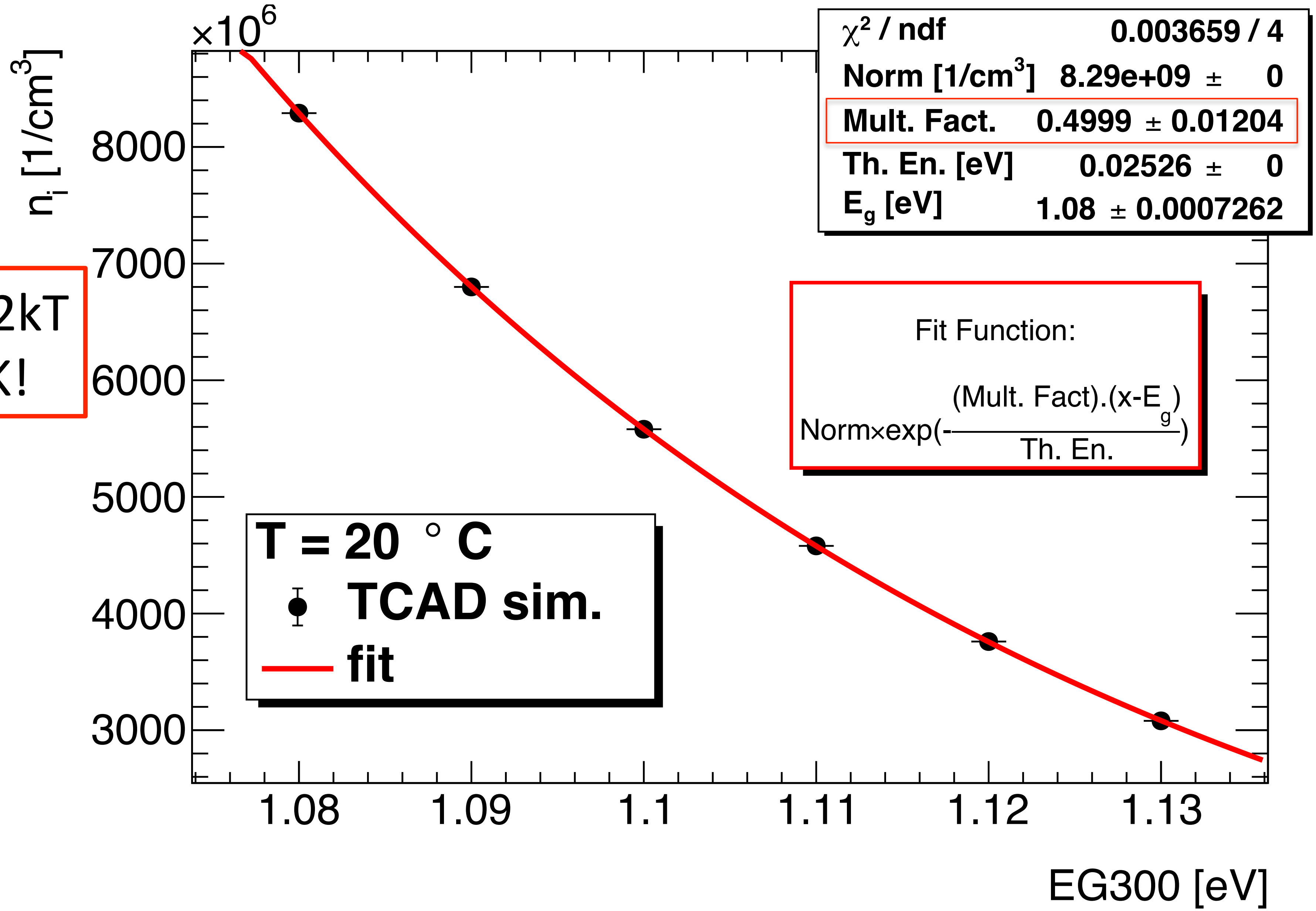


Eg fixed at 1.08 eV →

n_i (293.15 K) = 8.29x10^9 cm^{-3}
n_i (300 K) = 1.45x10^{10} cm^{-3}

Consistent with literature

Intrinsic concentration vs bandgap



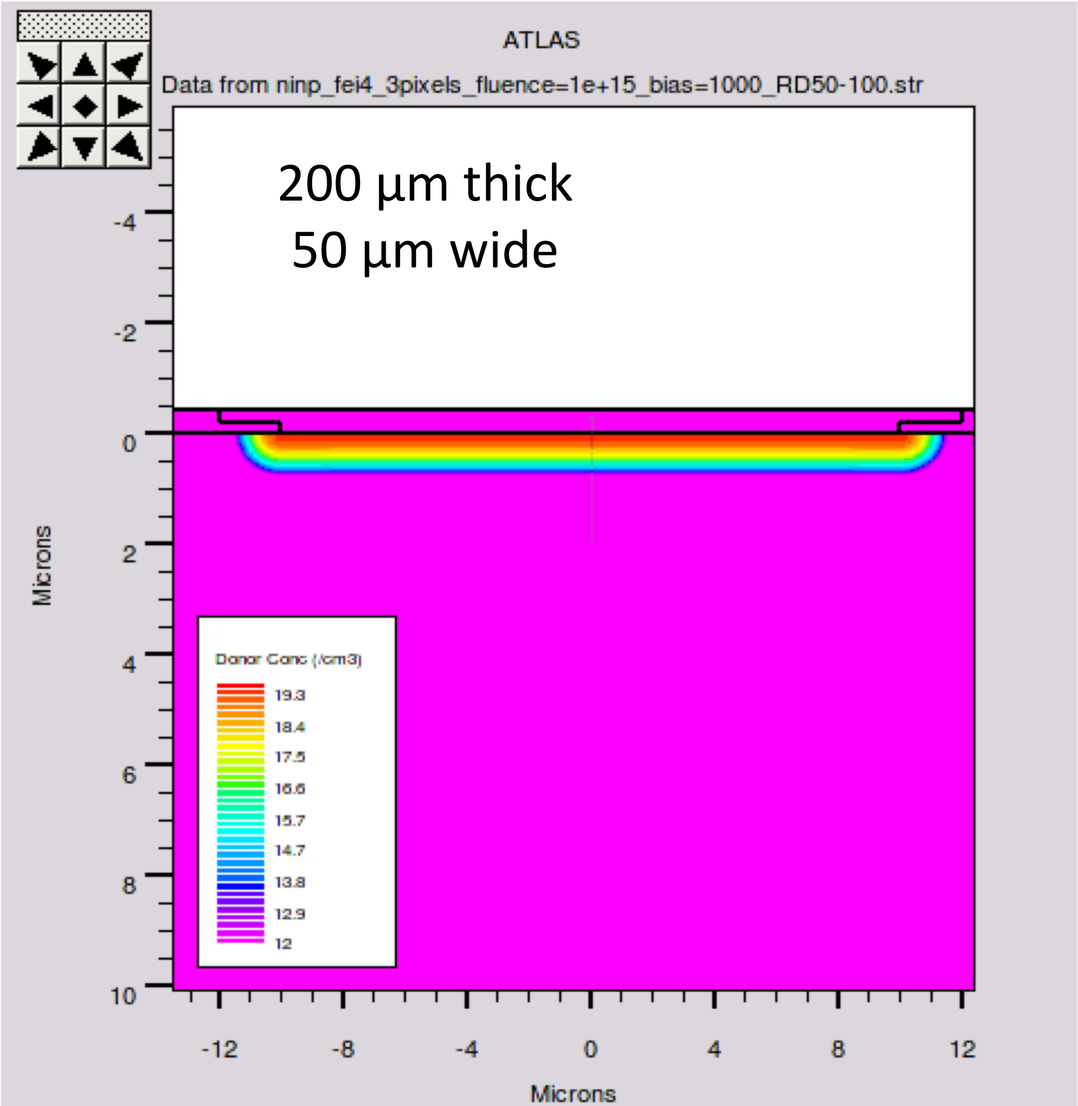
~$-E_g/2kT$
=> OK!

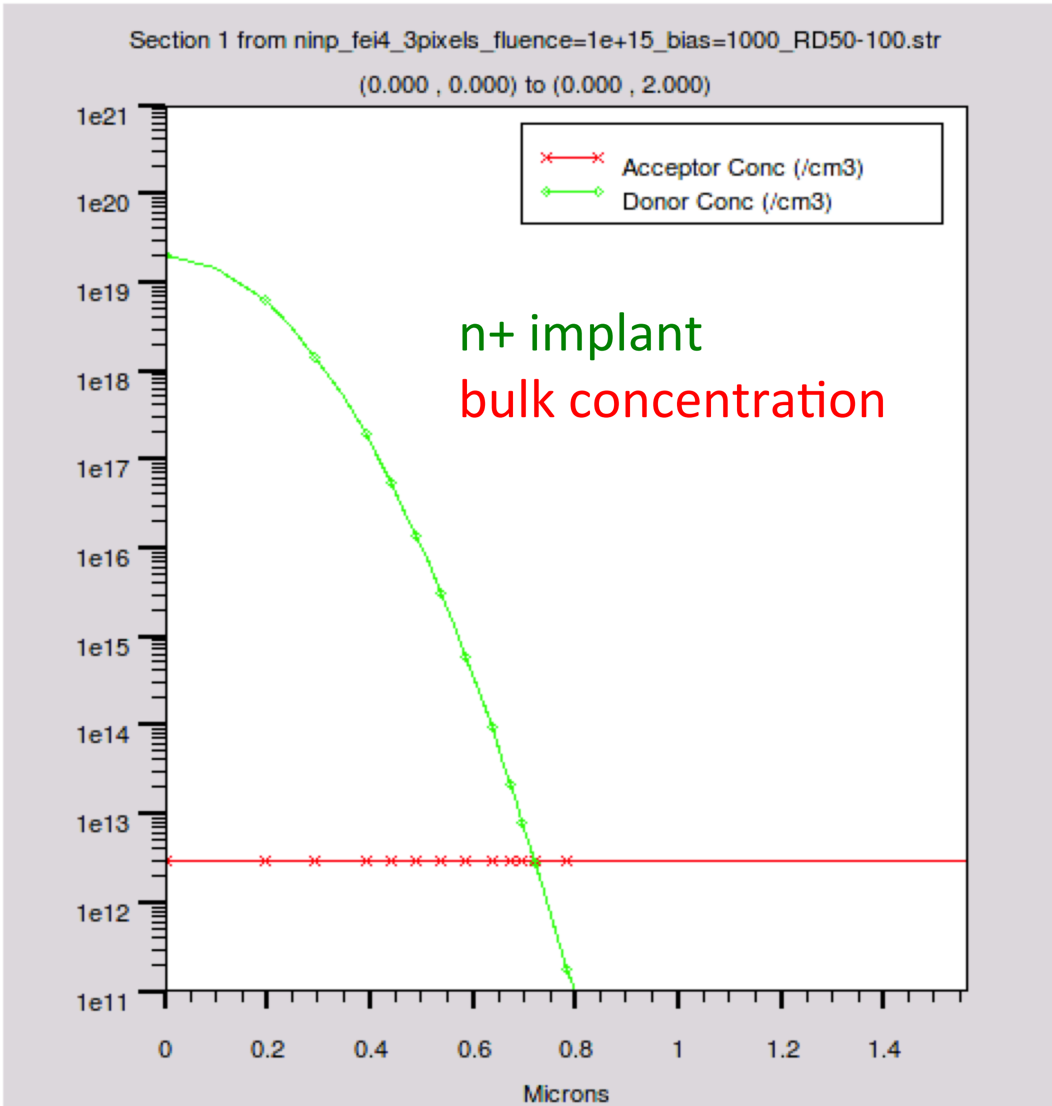
Bandgap narrowing in Silvaco: summary

- Bandgap narrowing as a function of doping works as expected
- Bandgap narrowing with temperature works as expected
- Intrinsic concentration scaling with temperature works as expected
- And value at 293.15 K is in agreement with literature when Eg(300 K) = 1.08 eV is used
- Intrinsic concentration scaling with bandgap works as expected

REVERSE CURRENT LEVEL VS BANDGAP

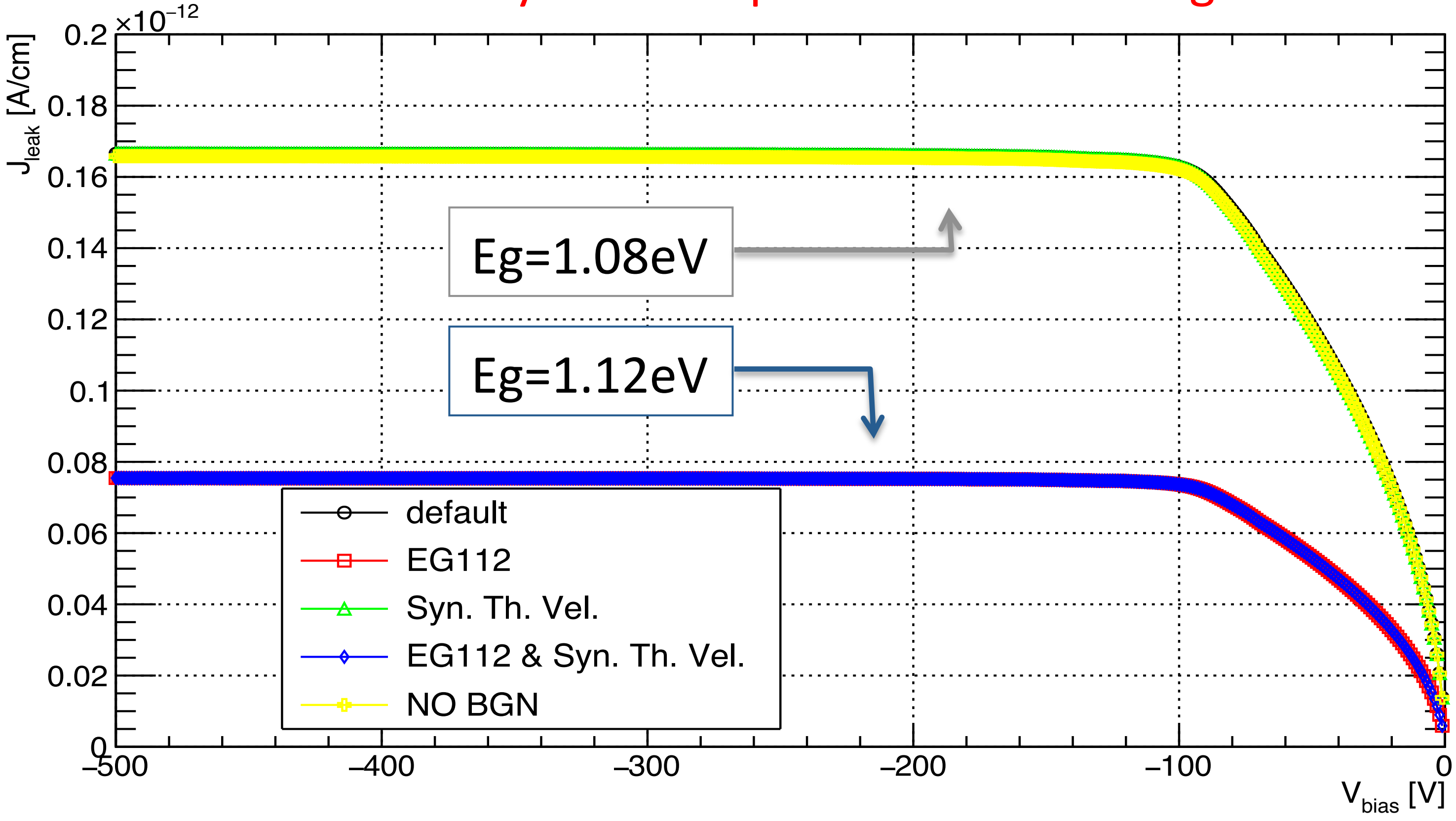
Structure


ATLAS
Data from ninp_fei4_3pixels_fluence=1e+15_bias=1000_RD50-100.str
200 µm thick
50 µm wide
Microns
Donor Conc (/cm3)
19.3
18.4
17.5
16.6
15.7
14.7
13.8
12.9
12
-4
-2
0
2
4
6
8
10
-12
-8
-4
0
4
8
12
Microns


Section 1 from ninp_fei4_3pixels_fluence=1e+15_bias=1000_RD50-100.str
(0.000 , 0.000) to (0.000 , 2.000)
Acceptor Conc (/cm3)
Donor Conc (/cm3)
n+ implant
bulk concentration
1e21
1e20
1e19
1e18
1e17
1e16
1e15
1e14
1e13
1e12
1e11
0
0.2
0.4
0.6
0.8
1
1.2
1.4
Microns

Reverse leakage current vs Eg and carr. vel.

The only relevant parameter here is Eg



default	using default Silvaco parameters values
EG112	setting $E_g^{Sil}(300) = 1.12$ eV
Syn. Th. Vel.	setting thermal velocities to the values used by Synopsys tool
EG112 & Syn. Th. Vel.	combination of the two above
NO BGN	turning off the model for bandgap narrowing based on the concentrations

Simulated leakage current vs prediction

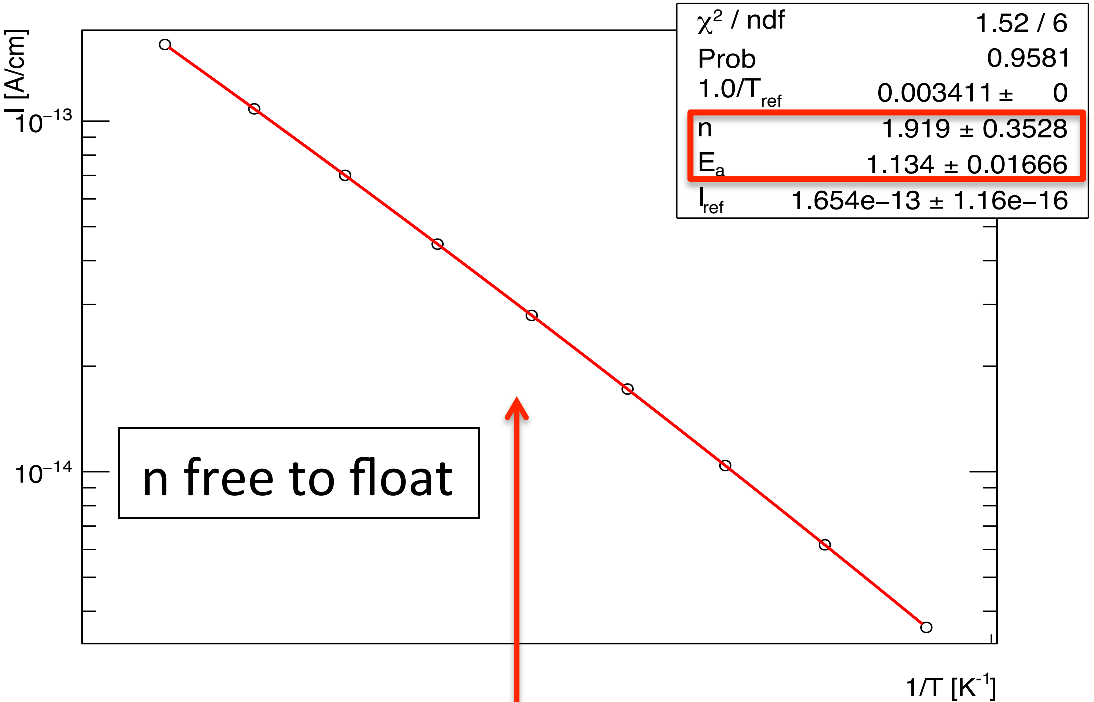
n_i (293.15 K) = 8.29×10^9 cm^{-3} Aw = 1e-8 cm^3 $\tau_g \sim 4 \times 10^{-5}$ s

Predicted $I = q n_i A w/2/\tau_g \sim 1.6 \times 10^{-13}$ A

Simulated $I \sim 1.65 \times 10^{-13}$ A

➔ Everything is consistent

Leakage current vs Temperature, Φ = 0

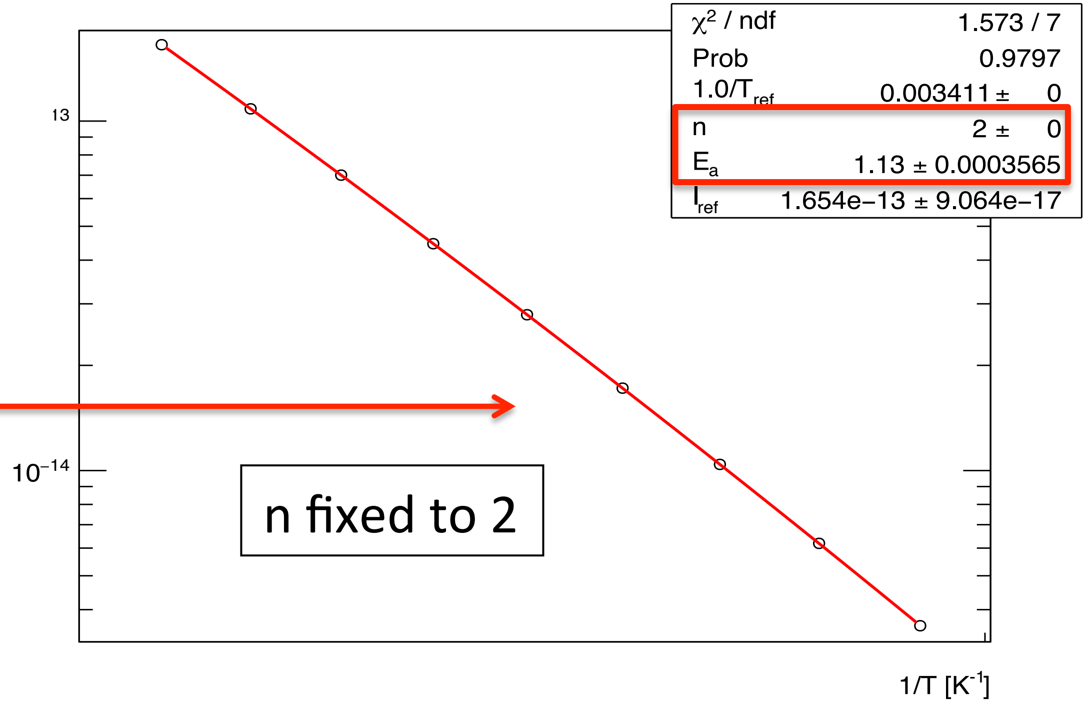


I vs 1/T

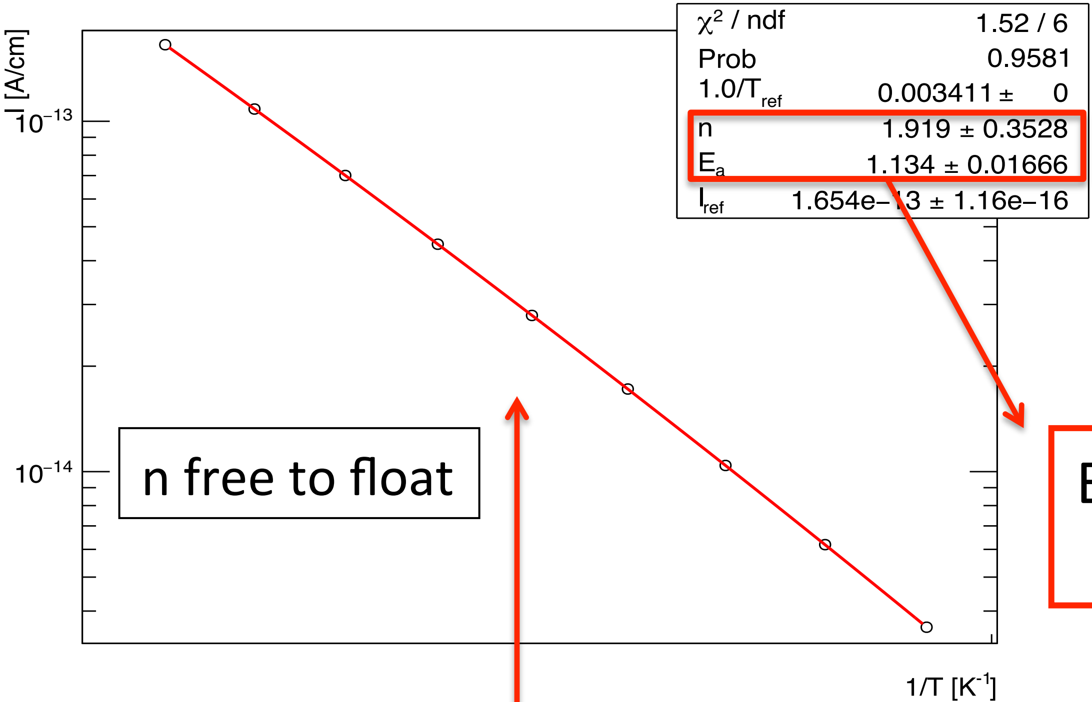
I evaluated at V_{depl} + 50 V

(V_{depl} does not depend from T)

$$I = I_{ref}\left(\frac{T}{T_{ref}}\right)^{n} exp\left[-\frac{E_a}{2k_B}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right]$$



Leakage current vs Temperature, $\Phi = 0$



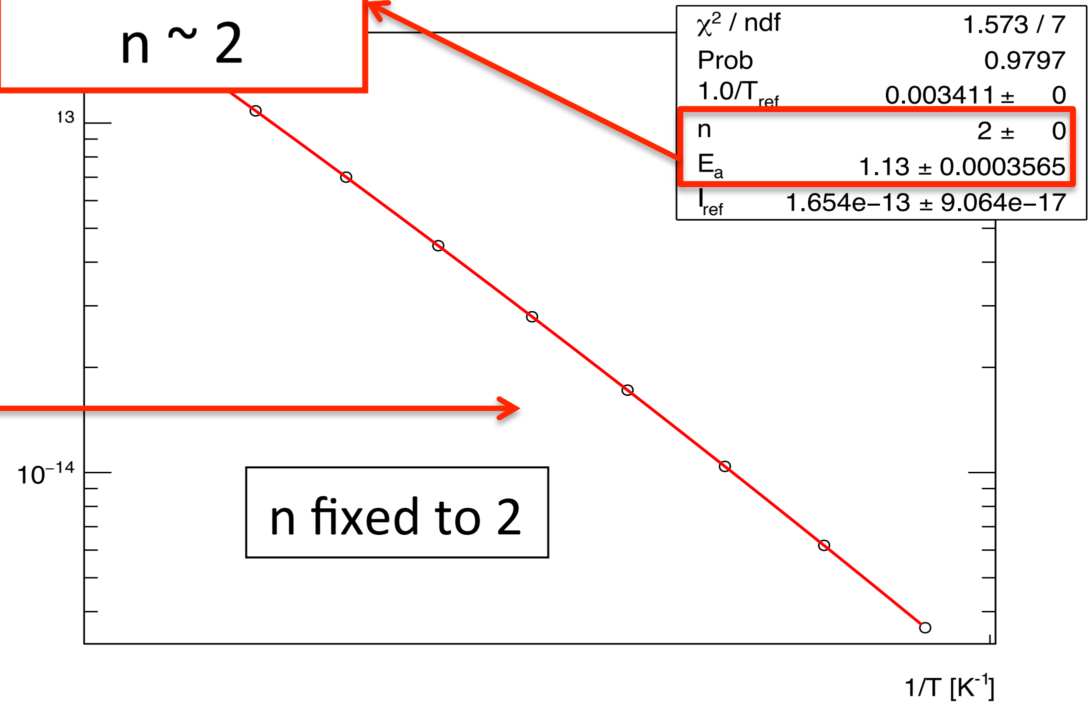
I vs 1/T

I evaluated at V_{depl} + 50 V

(V_{depl} does not depend from T)

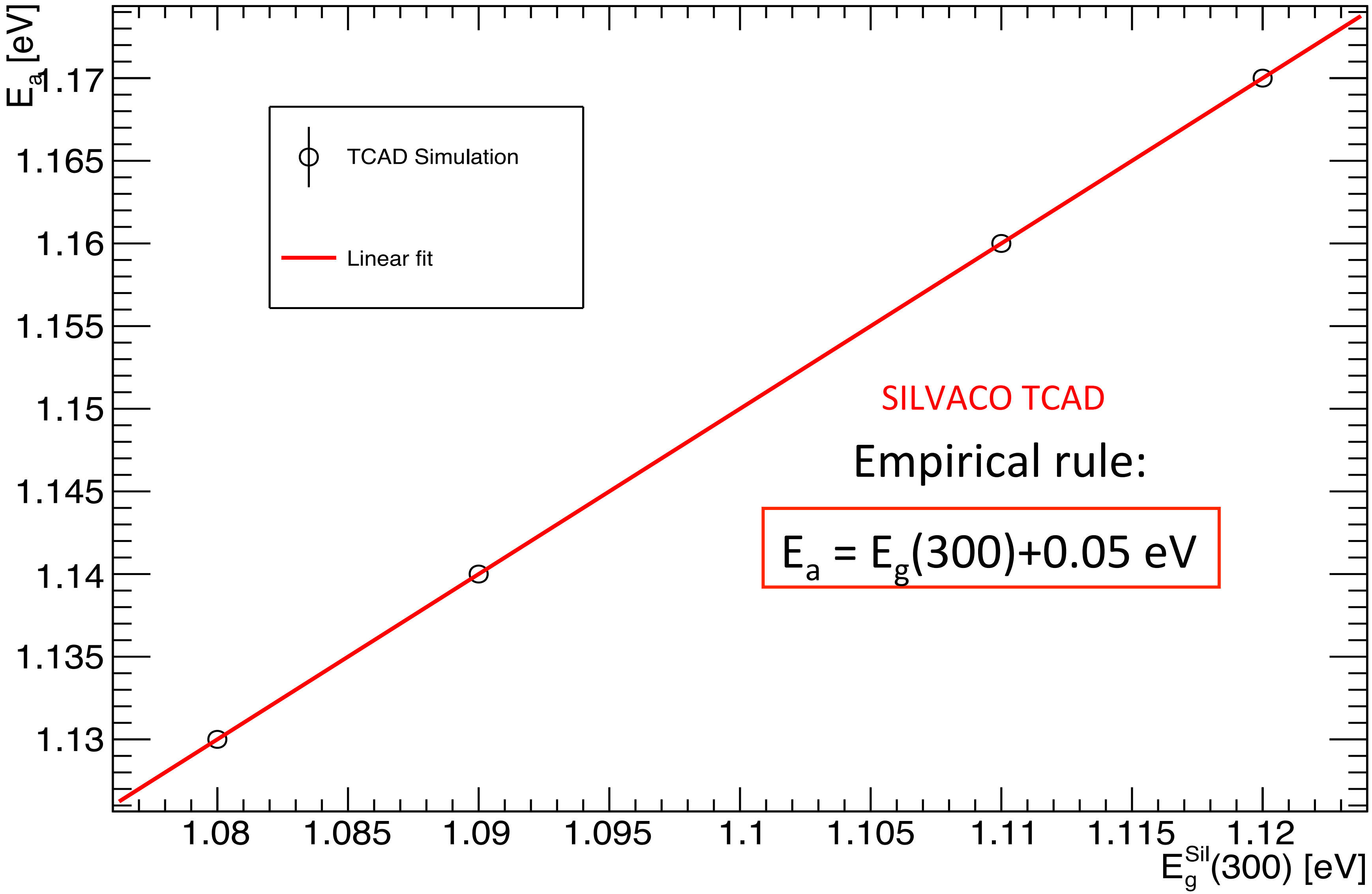
Ea ~ 1.13 eV

n ~ 2

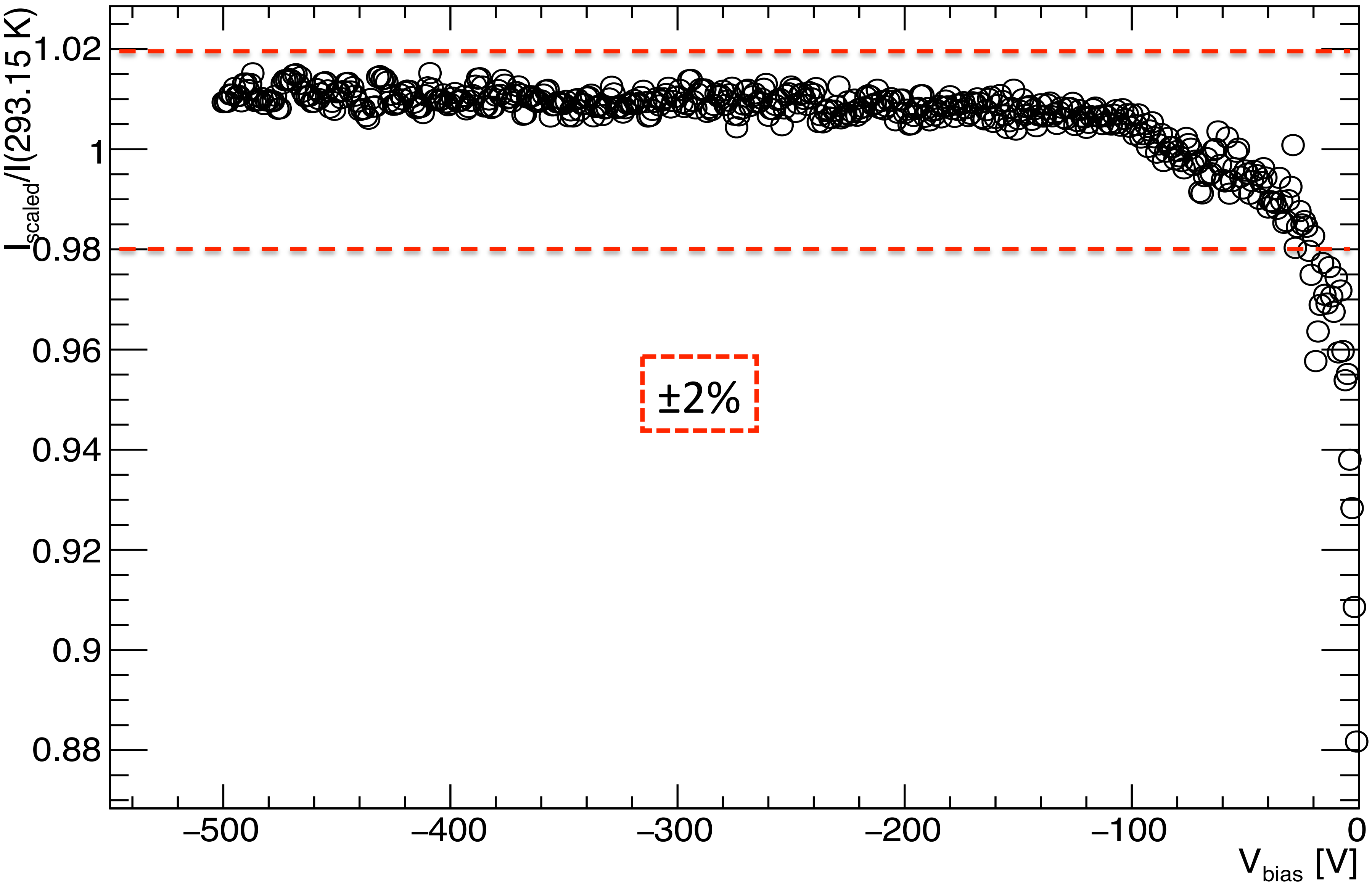


$$I = I_{ref}\left(\frac{T}{T_{ref}}\right)^{n} exp\left[-\frac{E_a}{2k_B}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right]$$

E_a vs E_g(300K) − Φ = 0

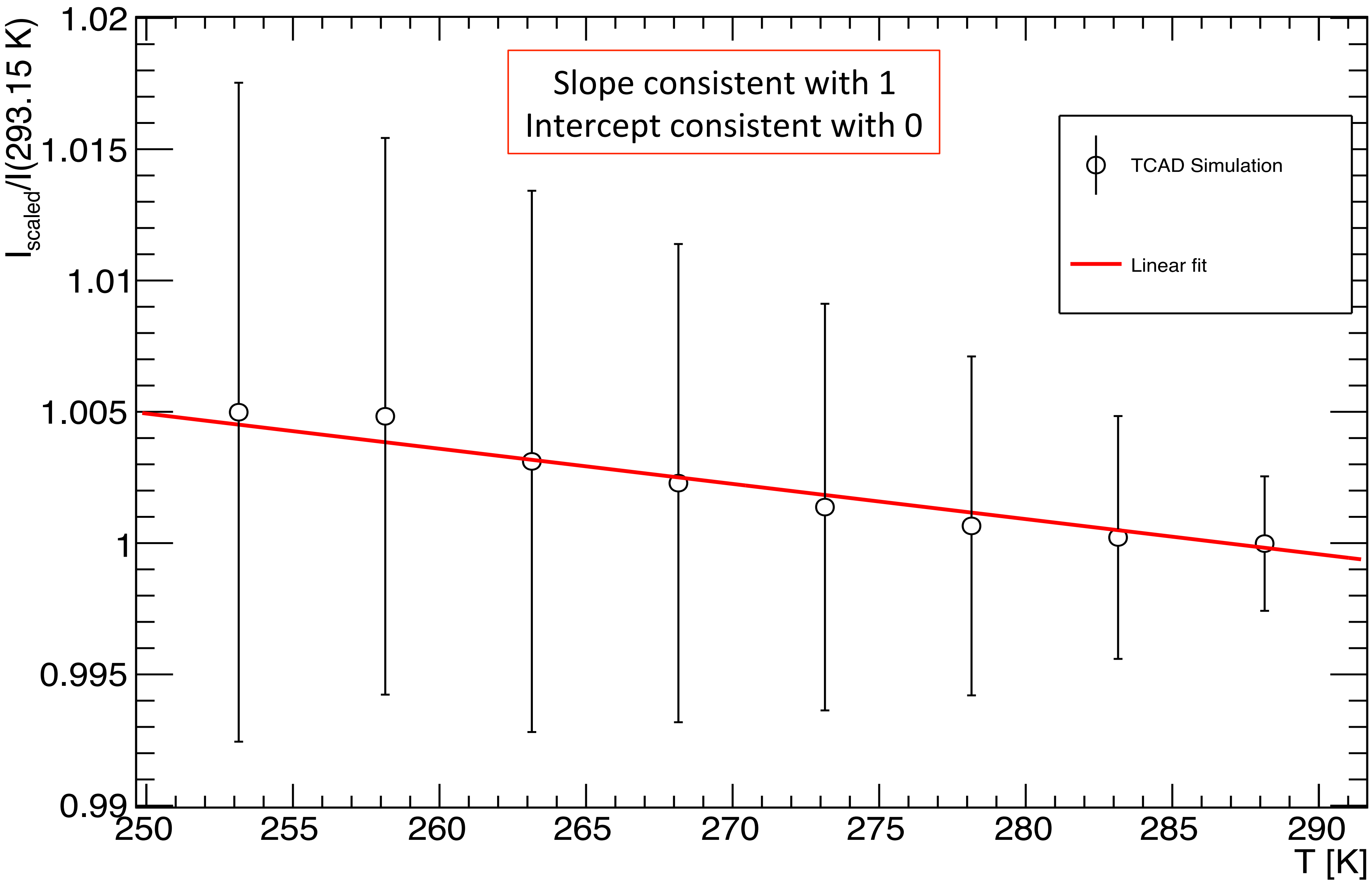


(Reverse current @ -20 C scaled to 20 C)/I(20 C)

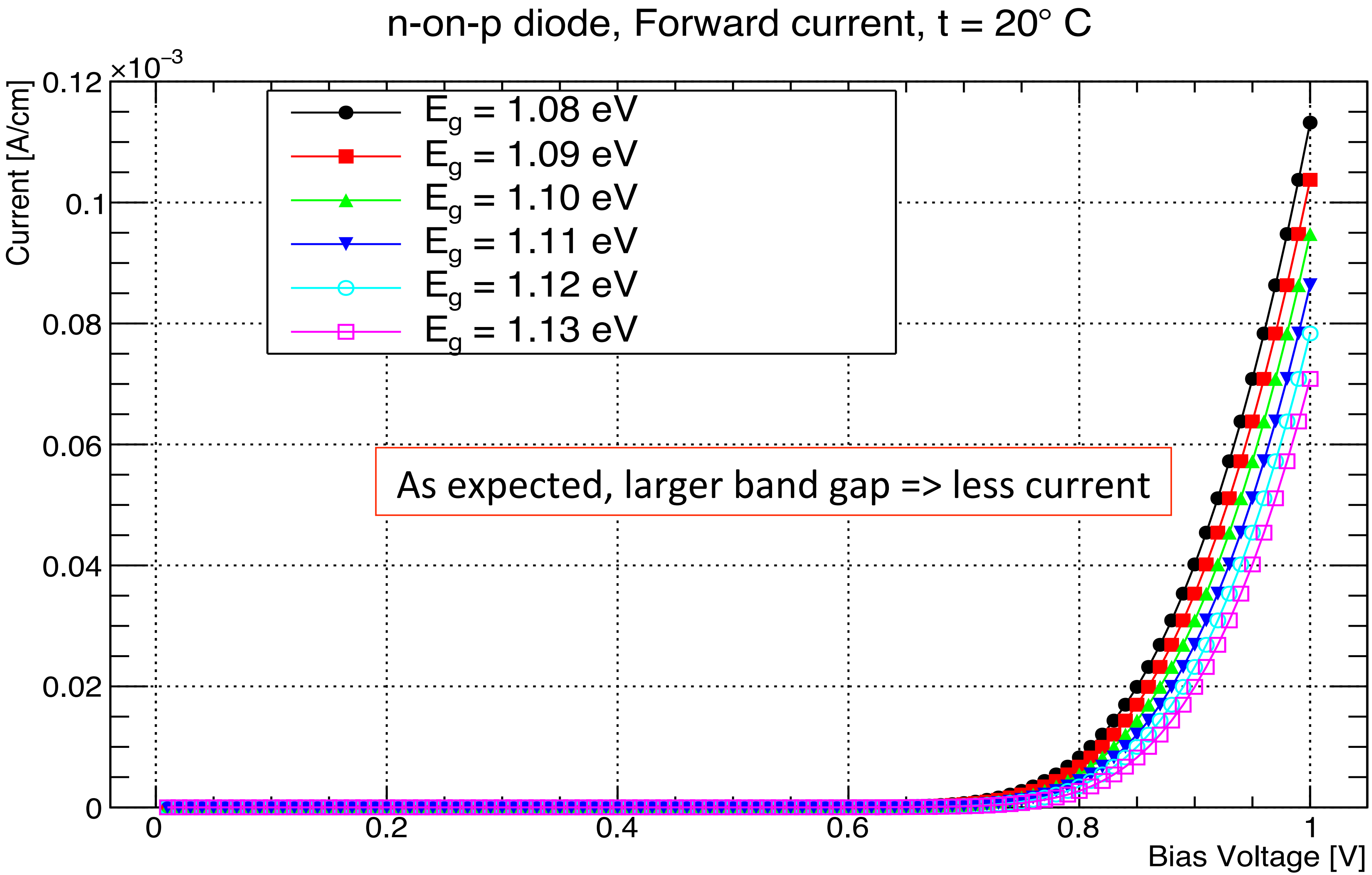


Ratio of Reverse currents scaled to 20 C

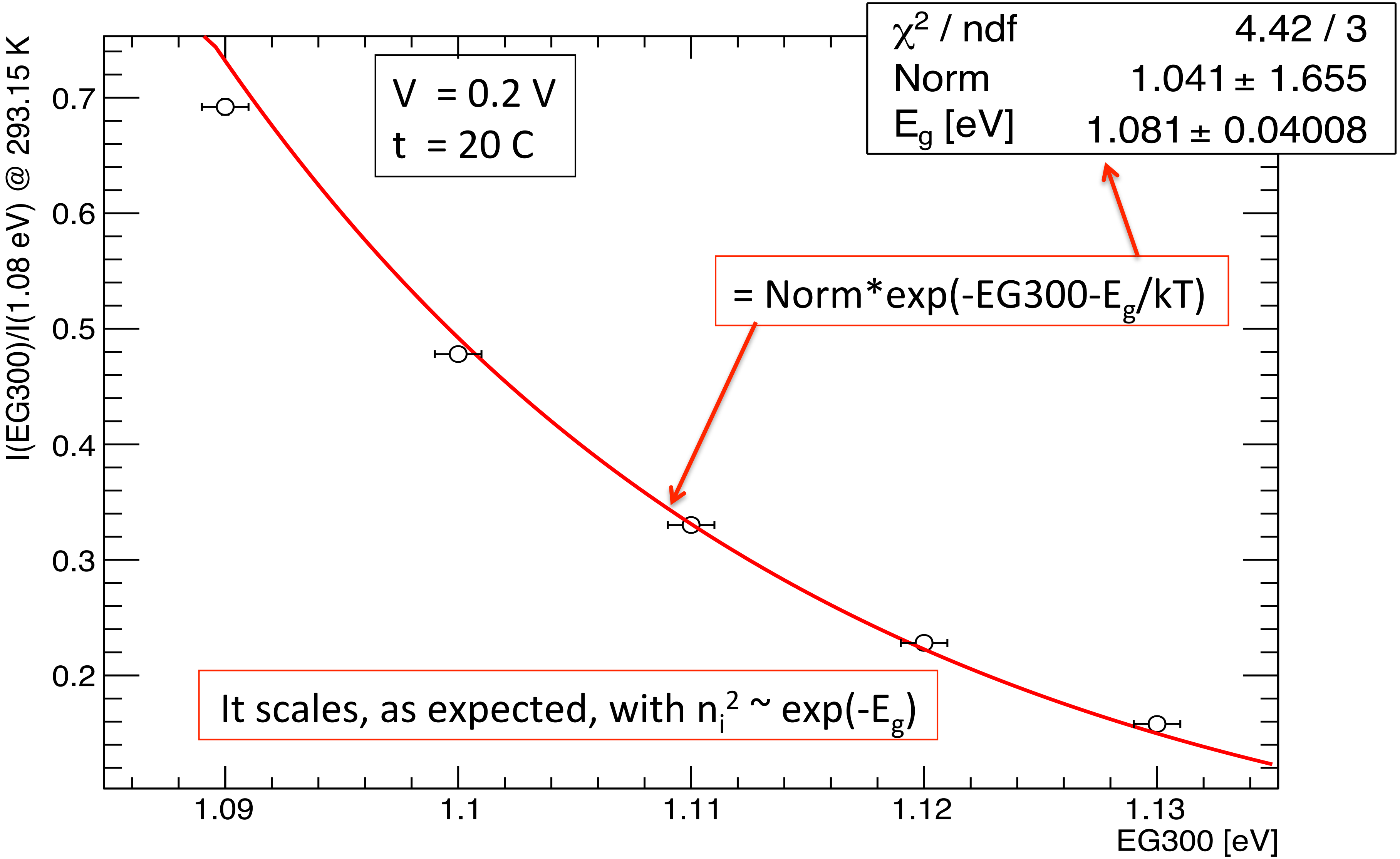
1% the accuracy on average of the rescaling



Forward current before irradiation



Forward current/I(1.08 eV) before irradiation



Reverse/forward current level vs bandgap: Summary

- Reverse current scales with the expected functional form
- The activation energy to be used is Ea = EG300+0.05 eV
- Rescaling of leakage current works at 1% level
- Forward current scales as expected with $\exp(-E_g/kT)$

SIMULATION OF RADIATION DAMAGE AND IMPACT OF BANDGAP

Radiation damage model considered

Effects of Interface Donor Trap States on Isolation Properties of Detectors Operating at High-Luminosity LHC
F. Moscatelli et al.
IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 64, NO. 8, AUGUST 2017

"Perugia 2017" in the following

TABLE II

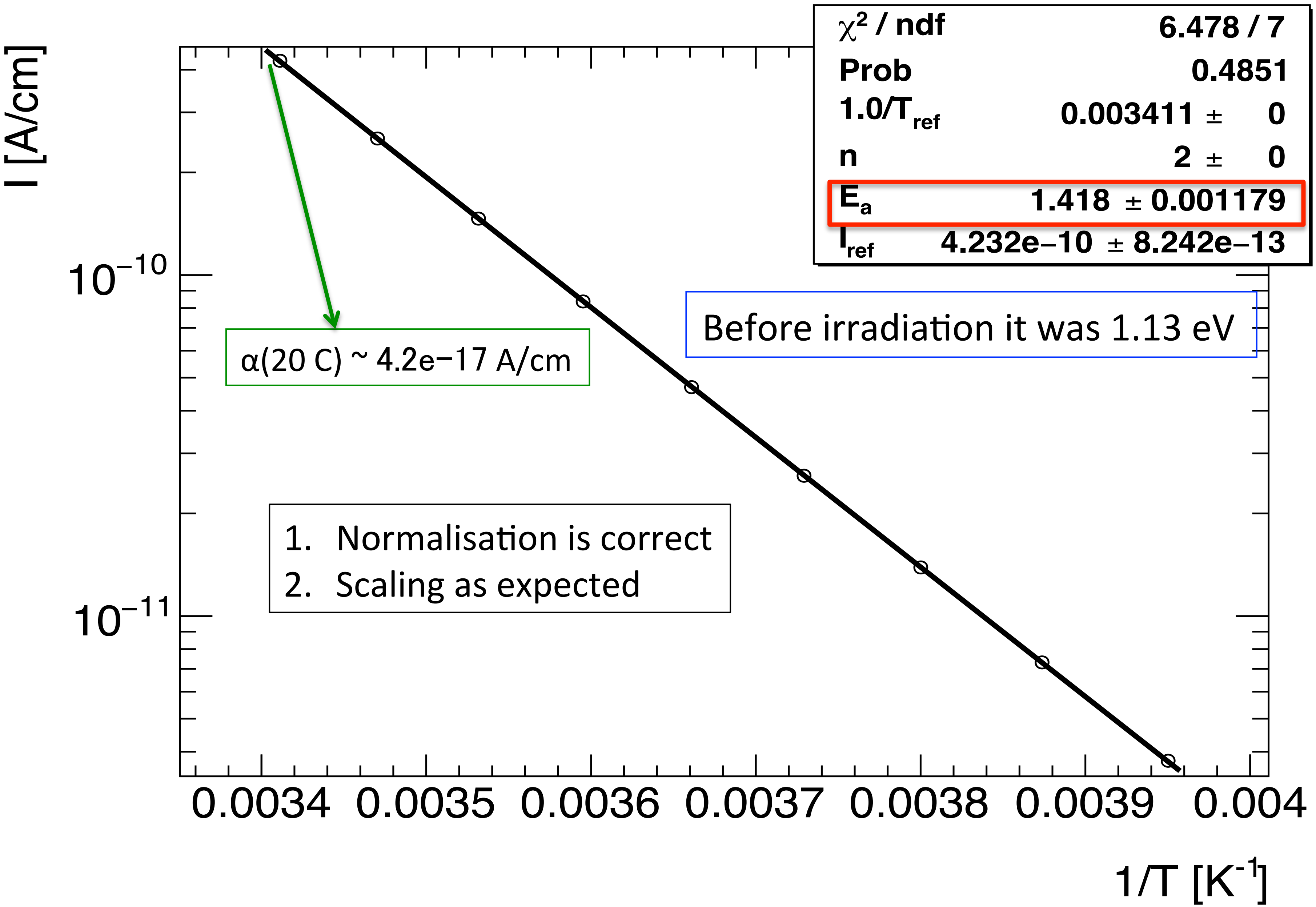
RADIATION DAMAGE MODEL FOR P-TYPE SUBSTRATES (UP TO 7×10^{15} N/CM^2)

Type	Energy (eV)	σ_e (cm^{-2})	σ_h (cm^{-2})	η (cm^{-1})
Acceptor	Ec-0.42	1×10^{-15}	1×10^{-14}	1.613
Acceptor	Ec-0.46	7×10^{-15}	7×10^{-14}	0.9
Donor	Ev+0.36	3.23×10^{-13}	3.23×10^{-14}	0.9

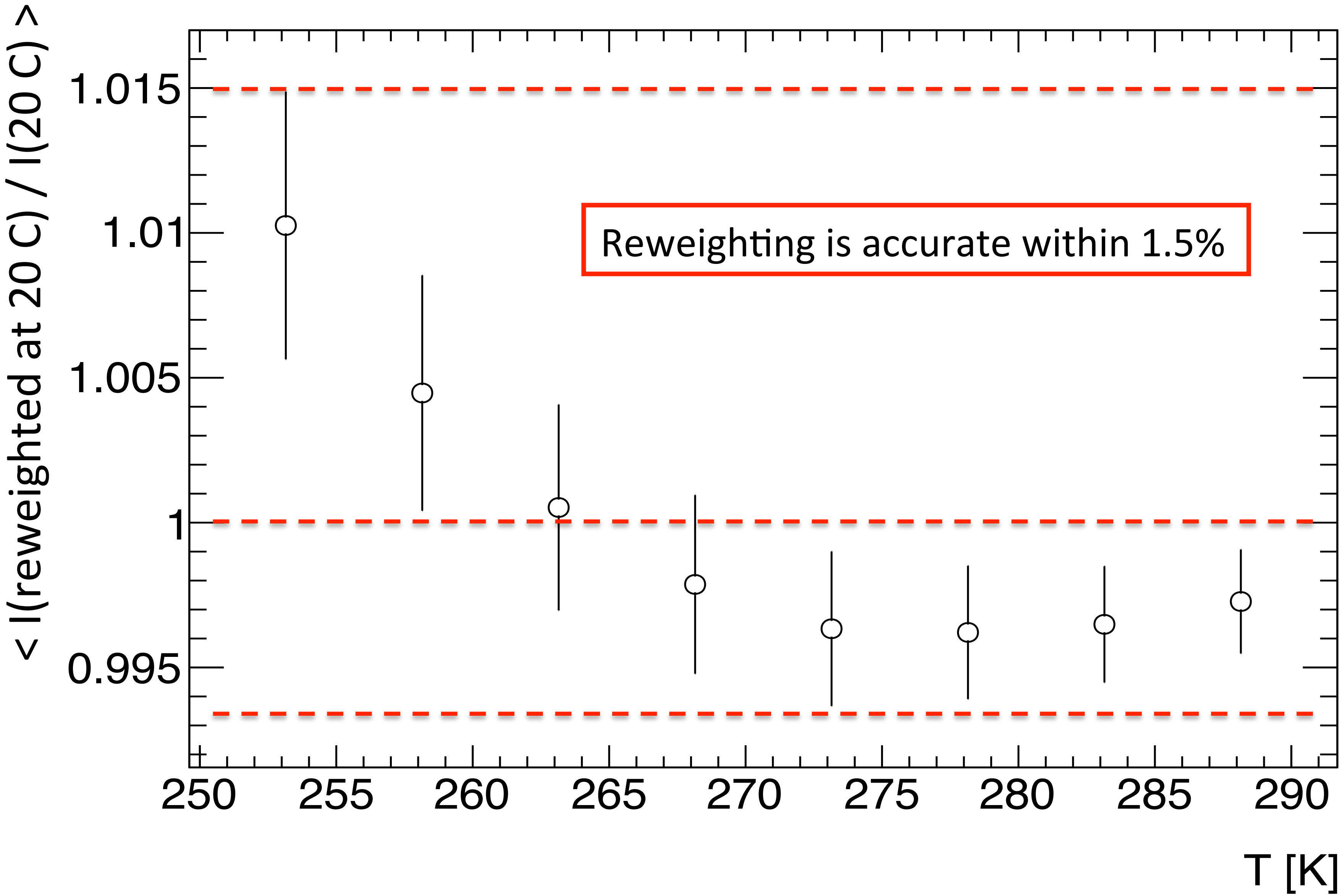
Reminder: in my presentation in Torino* I have showed that good agreement between simulators is found when EG300 = 1.08 eV is chosen and the thermal velocities are corrected à la Synopsys

* Bomben, 28th RD50 WS, Torino, June 2016

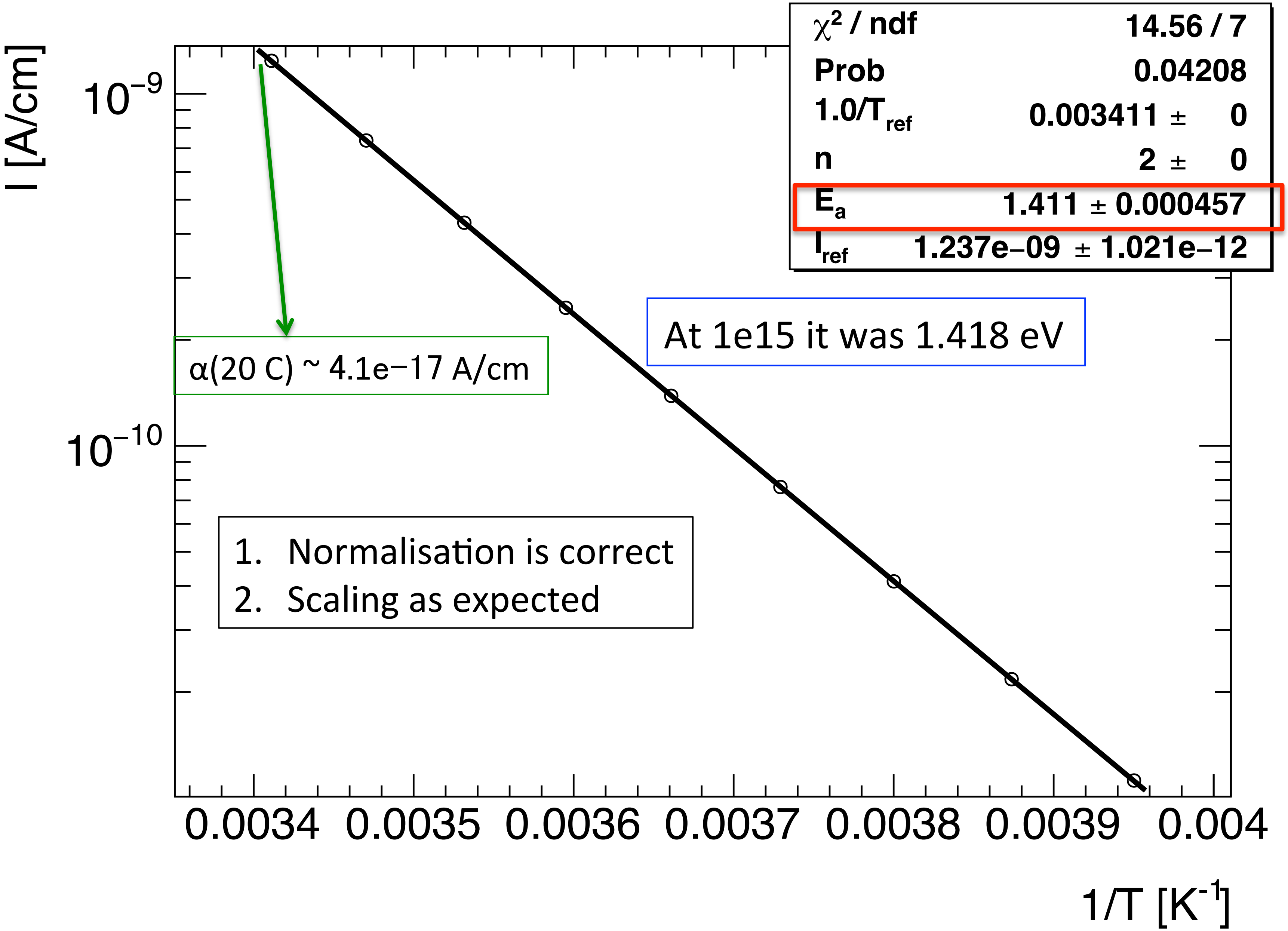
Perugia 2017, $\Phi = 1\text{x}10^{15}\ n_{eq}/cm^2$



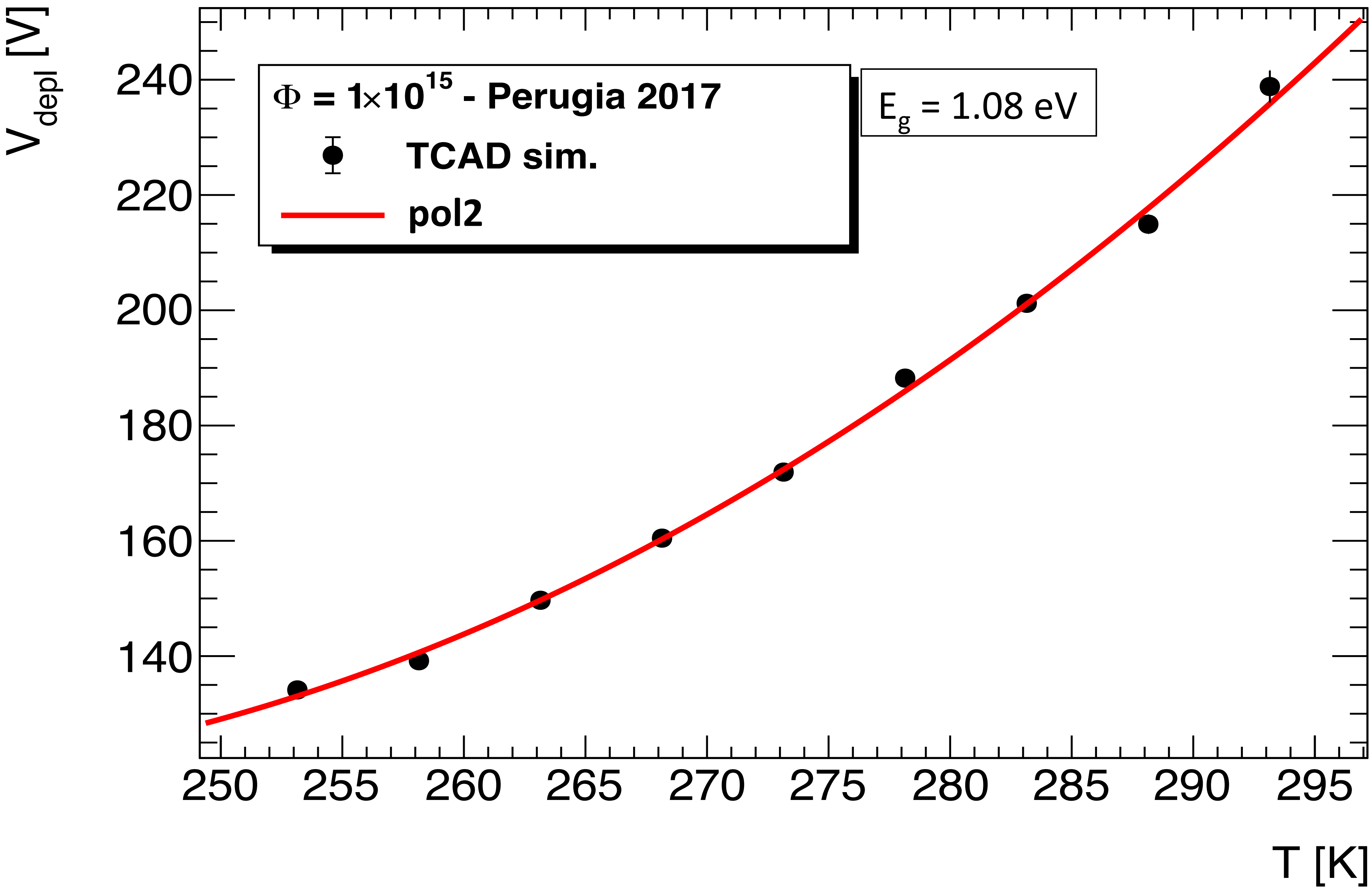
Reweighting leakage current with Ea = 1.48 eV



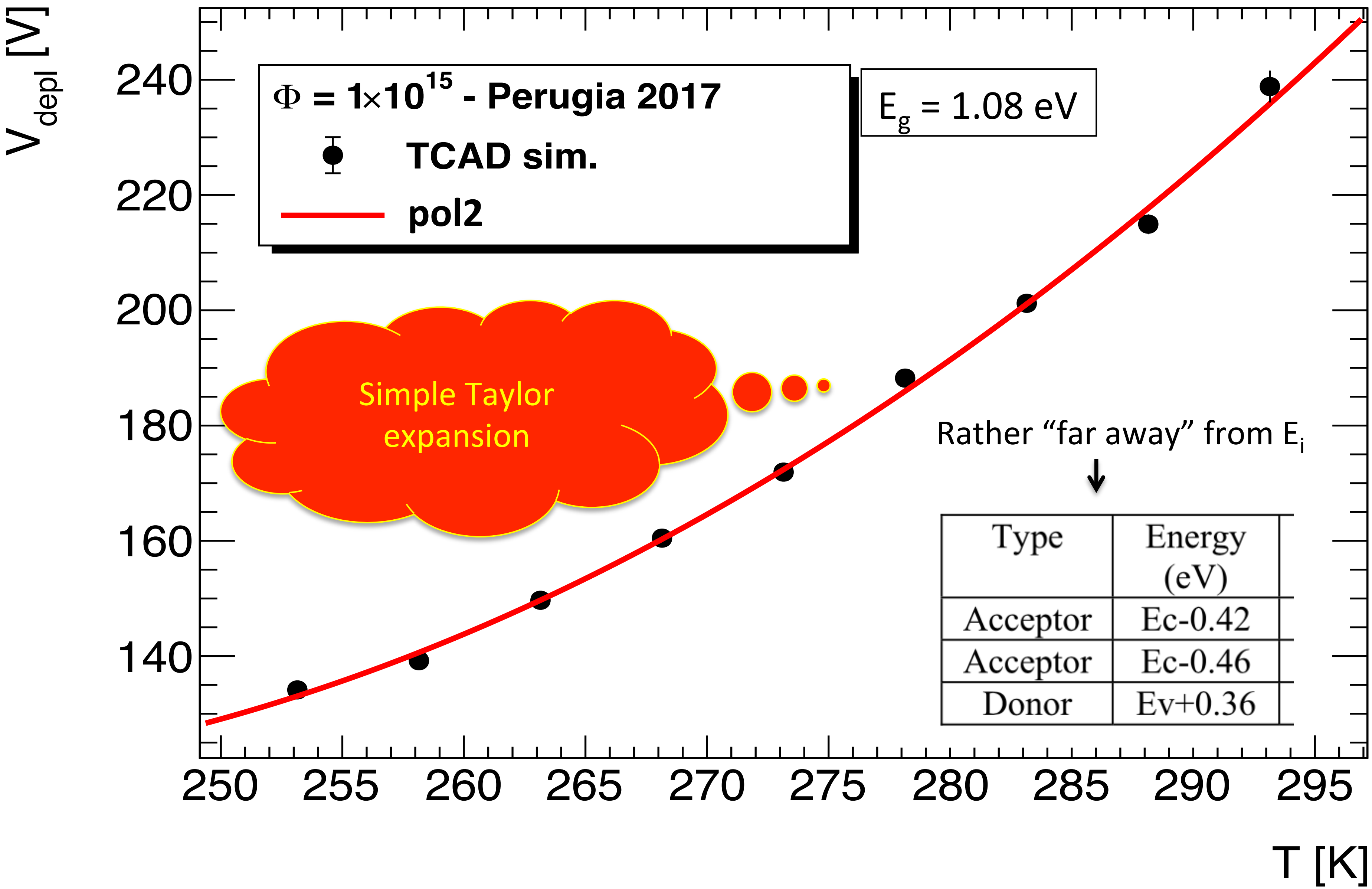
Perugia 2017, $\Phi = 3x10^{15}\ n_{eq}/cm^2$



Extra: depletion voltage vs temperature

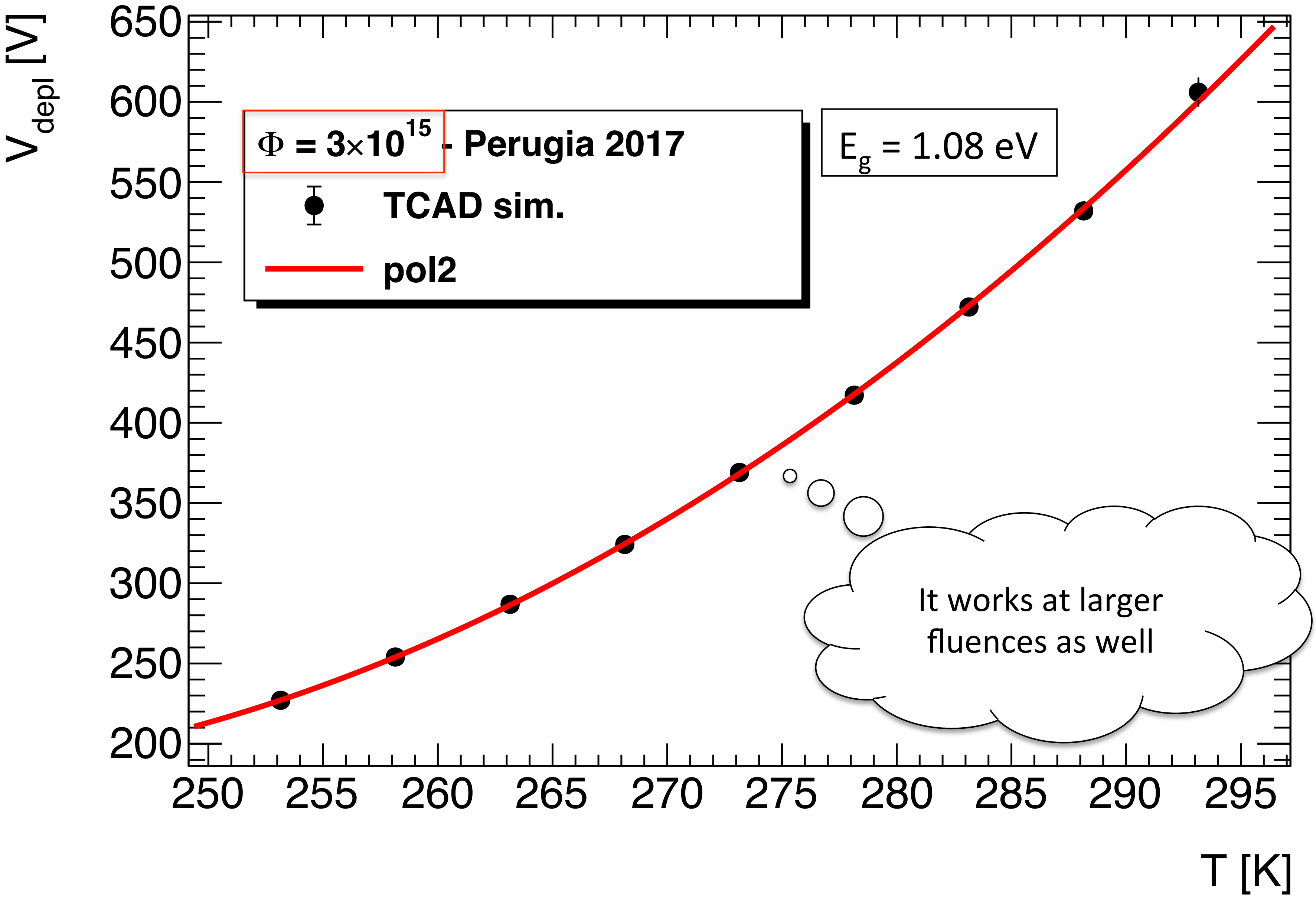


Extra: depletion voltage vs temperature

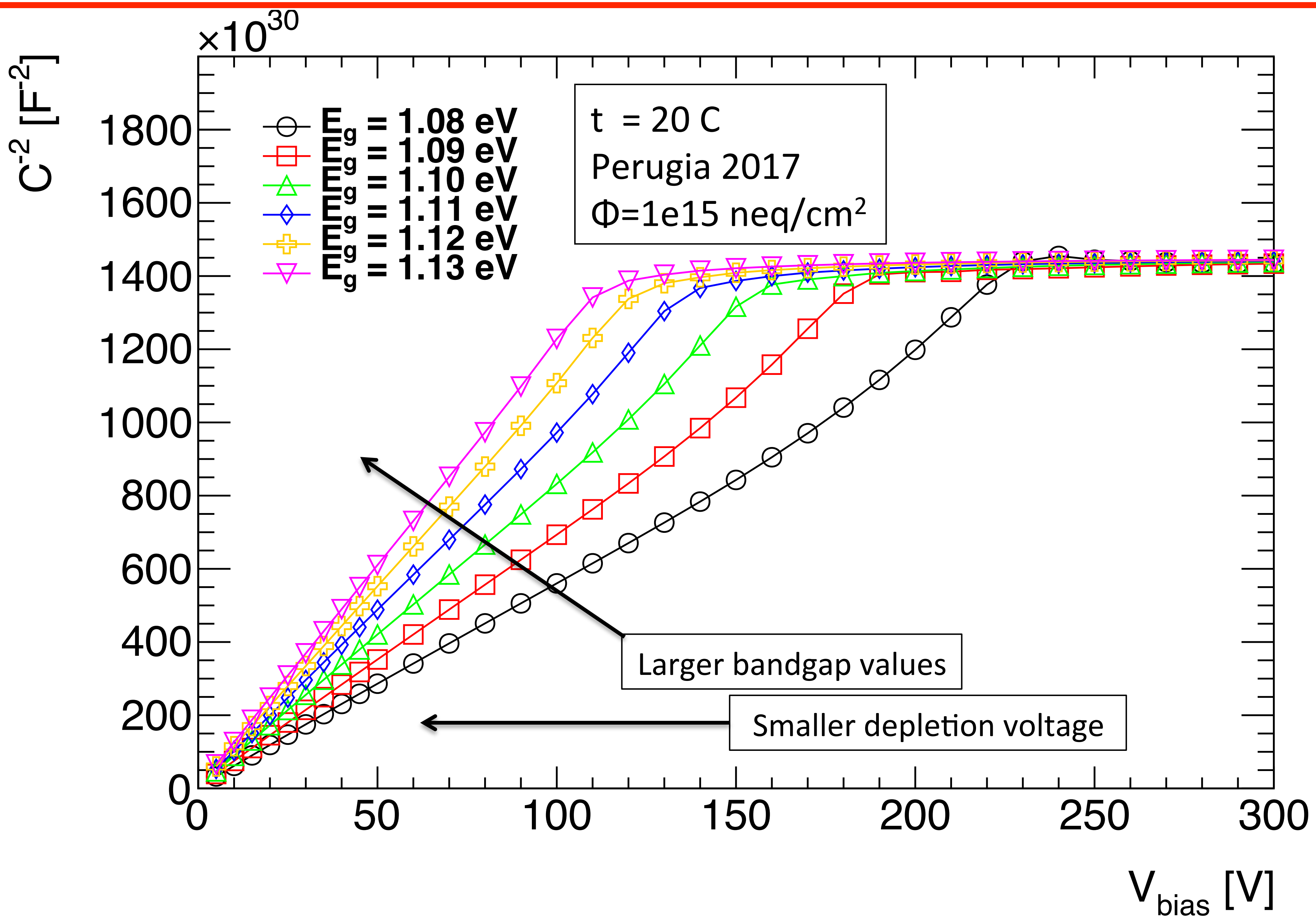


Type	Energy (eV)
Acceptor	Ec-0.42
Acceptor	Ec-0.46
Donor	Ev+0.36

Extra: depletion voltage vs temperature

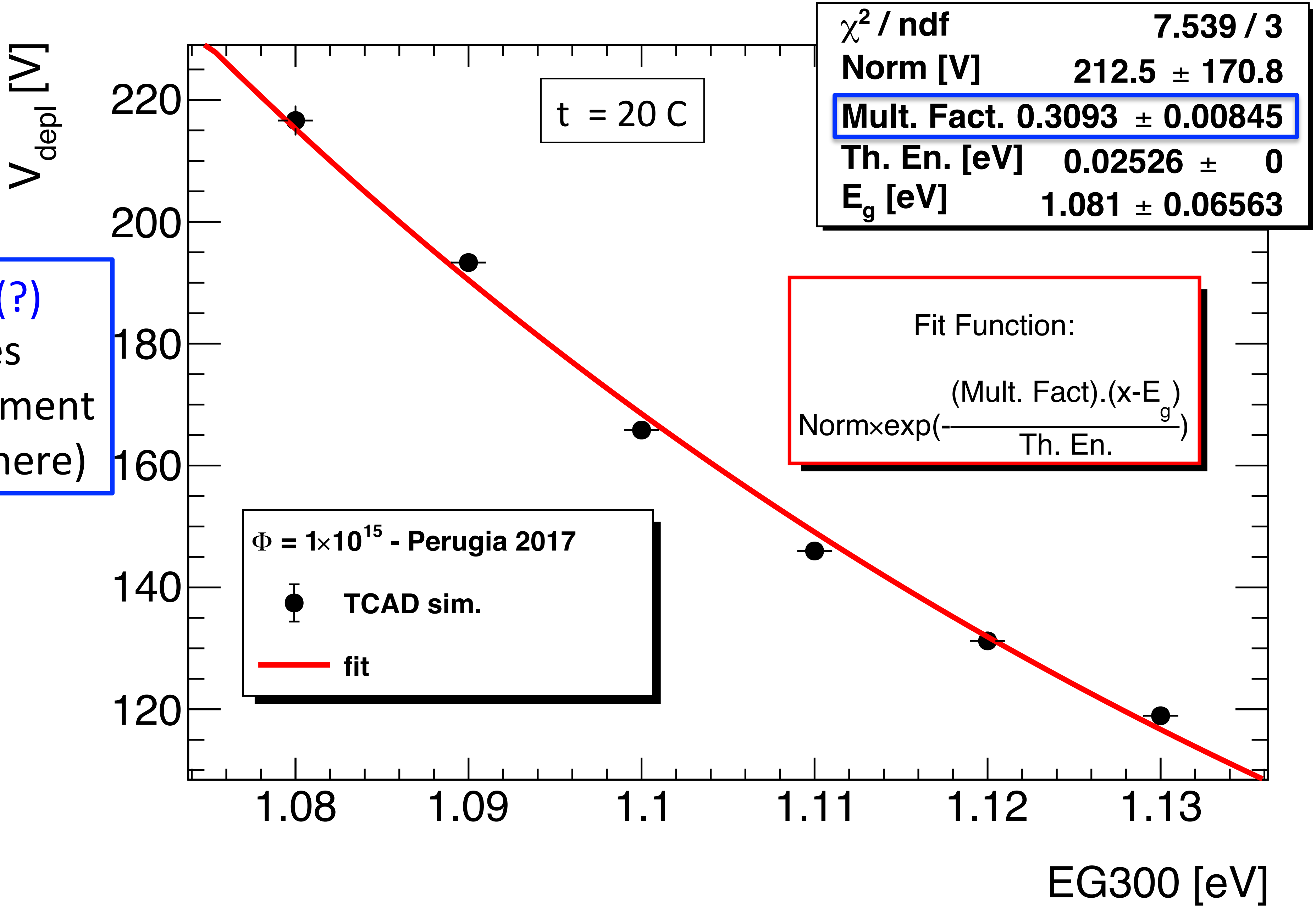


Depletion voltage vs EG300



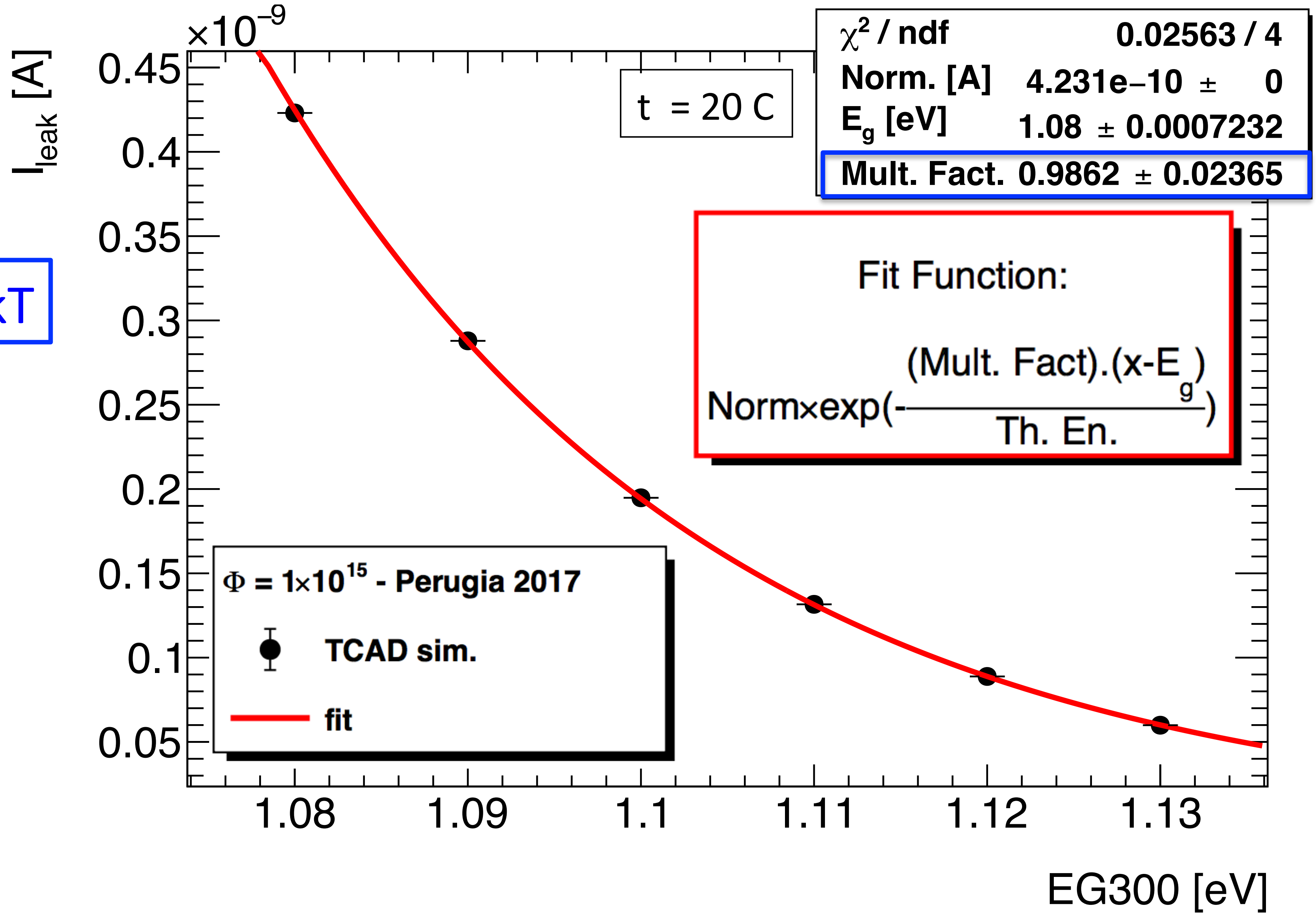
Depletion voltage vs bandgap

- ~$-E_g/3kT$(?)
- pol2 gives better agreement (not shown here)

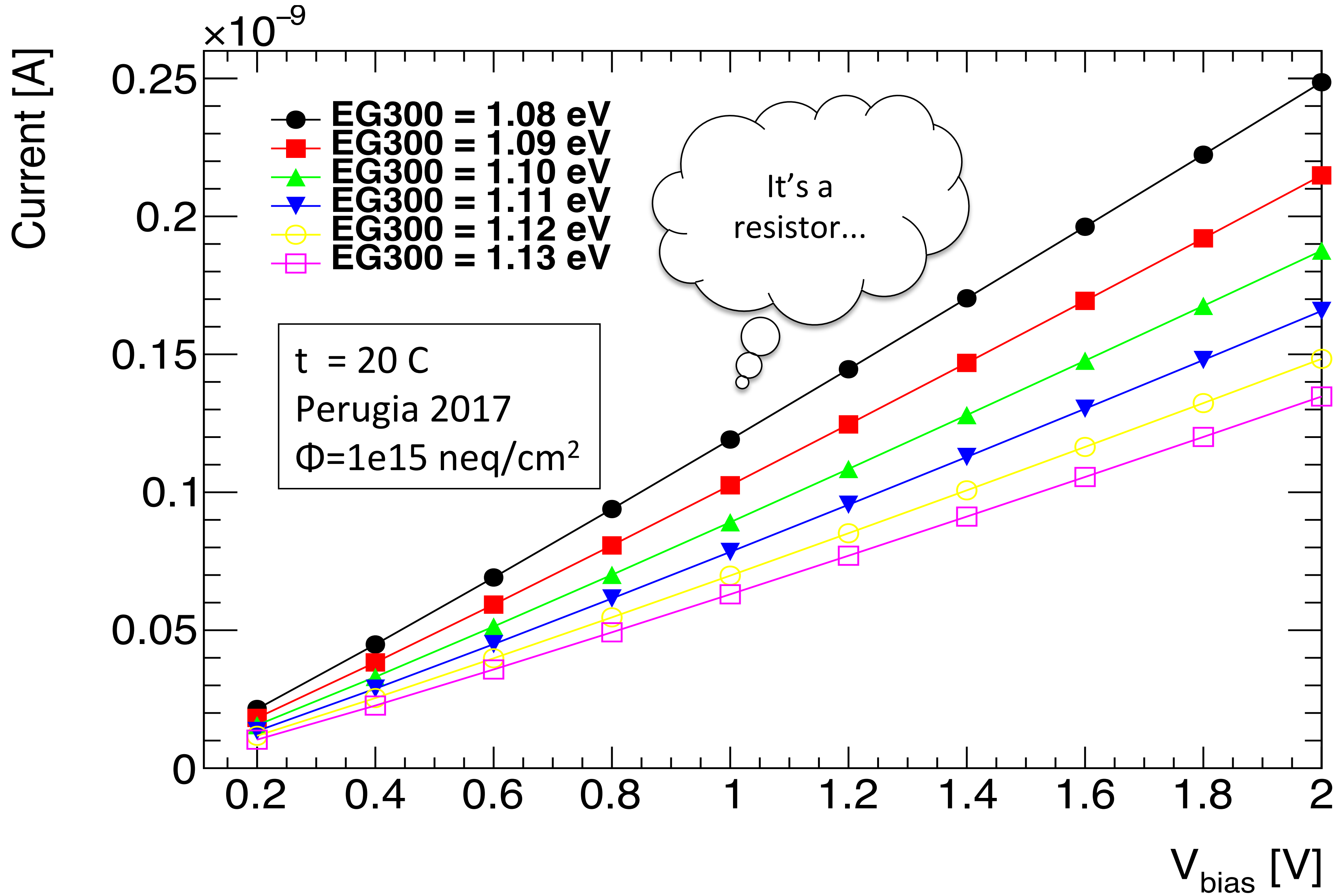


Leakage current vs bandgap

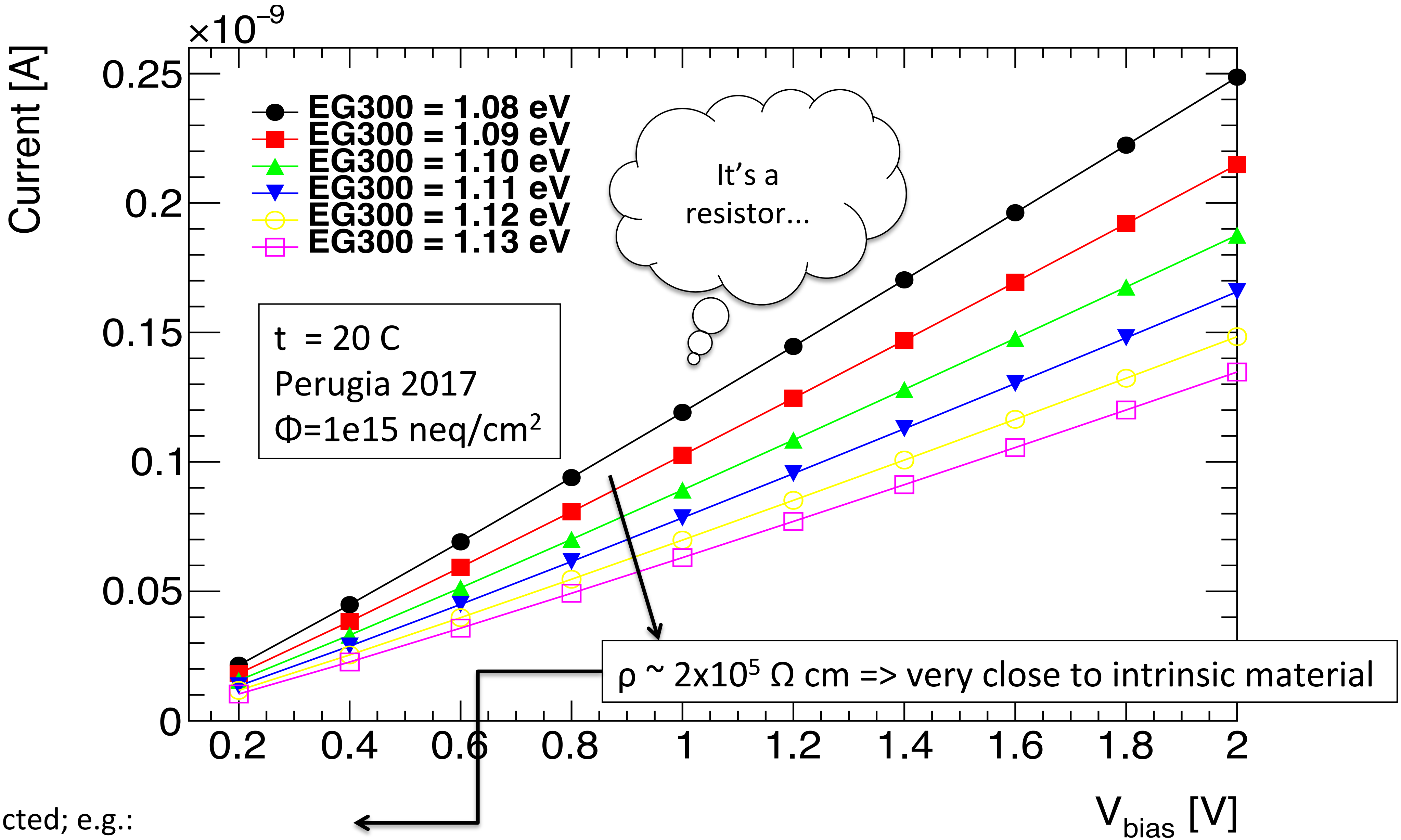
~$-E_g/kT$



Forward current after irradiation

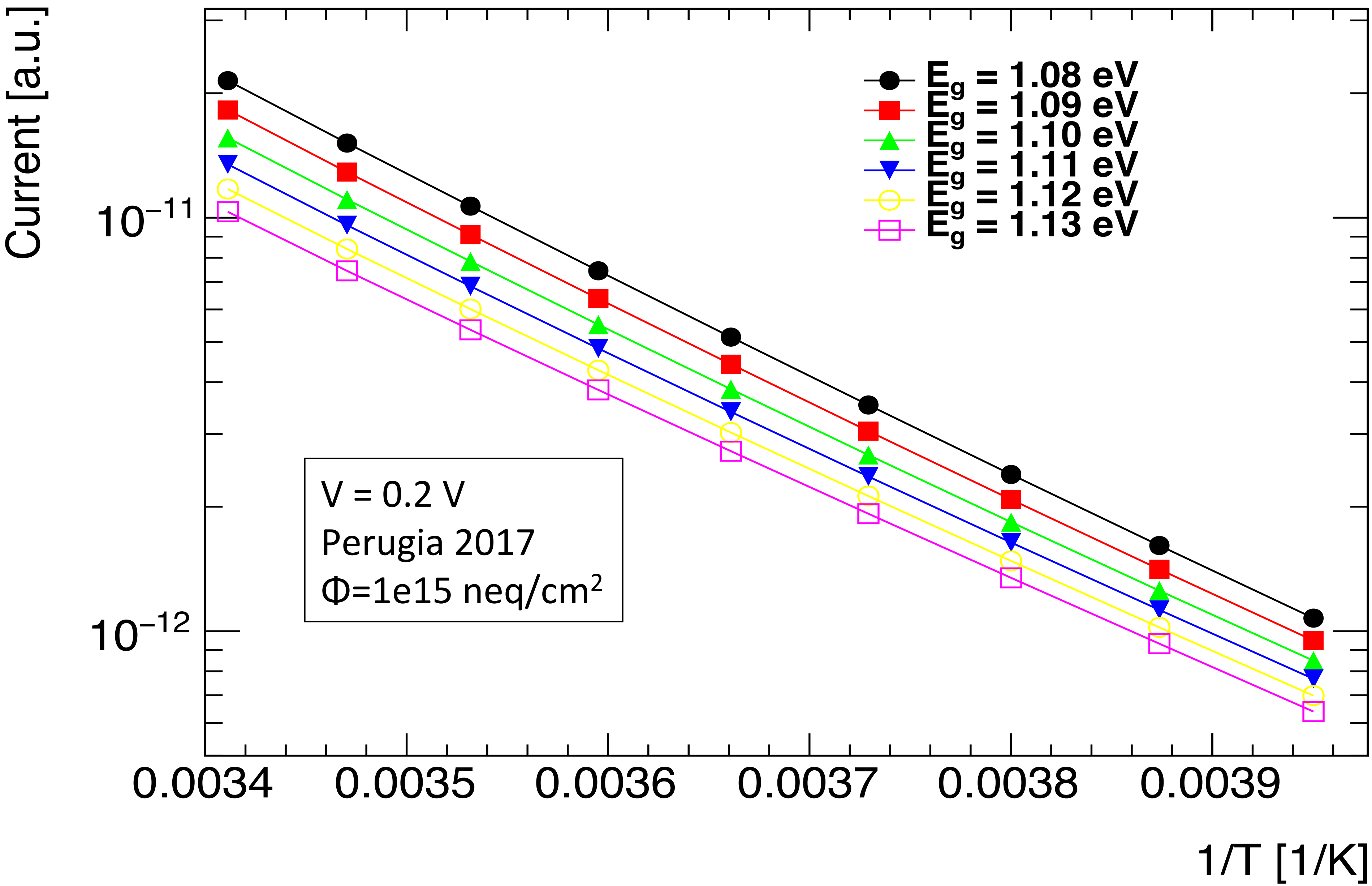


Forward current after irradiation

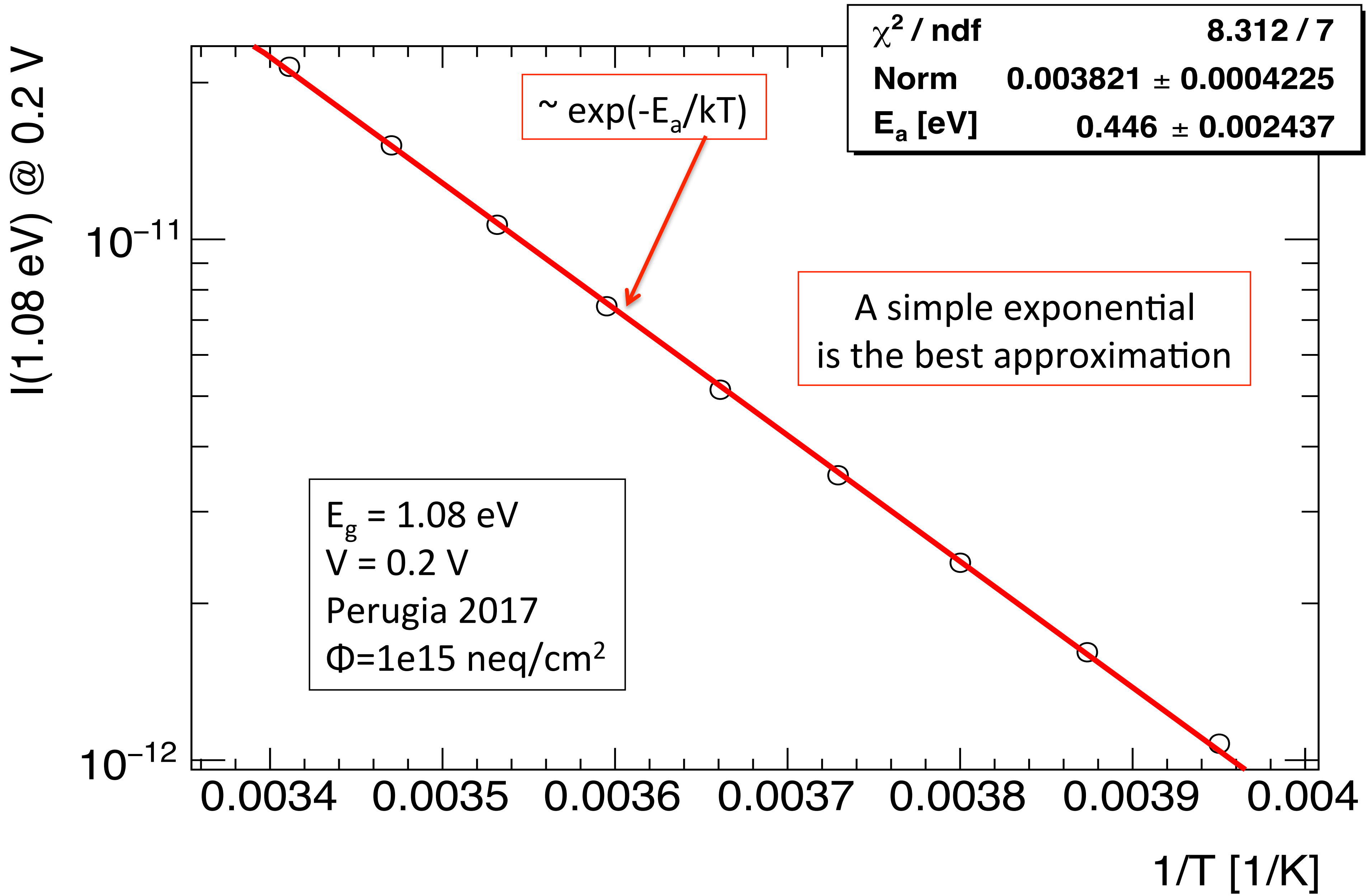


Expected; e.g.:
G. Lutz, NIM A 377 (1996) 234-243

Forward current after irradiation vs temperature



Forward current after irradiation, E_g = 1.08 EeV



Simulation of radiation damage and impact of bandgap: Summary

- Reverse current still scales with the same functional form
- Activation energy rather different (1.48 eV) => Model dependent?
  - To be checked with other models
- Depletion voltage dependence on (T,E_g) “small” on ranges tested
  - Due to position of traps wrt intrinsice energy
  - To be checked with other models
- Forward current scales as expected with bandgap and energy

CONCLUSIONS AND OUTLOOK

Conclusions and Outlook

- Despite the low default bandgap value at 300 K predictions seem to be consistent in Silvaco Atlas device simulator
- Reverse current scales as expected when the correct activation energy is used
- Forward current scales as expected
- After irradiation things gets more complicated
- Yet the current scales with temperature with the same functional form
- More fluences / models to be investigated
- Extra: predicted depletion voltage vs temperature needs more investigation (in contact with Perugia group)
- Outlook: the situation is more clear; possible to make robust predictions
- Silvaco used and to be used for ATLAS digitizer
- Collaboration with MPI too; see next talk

Acknowledgements

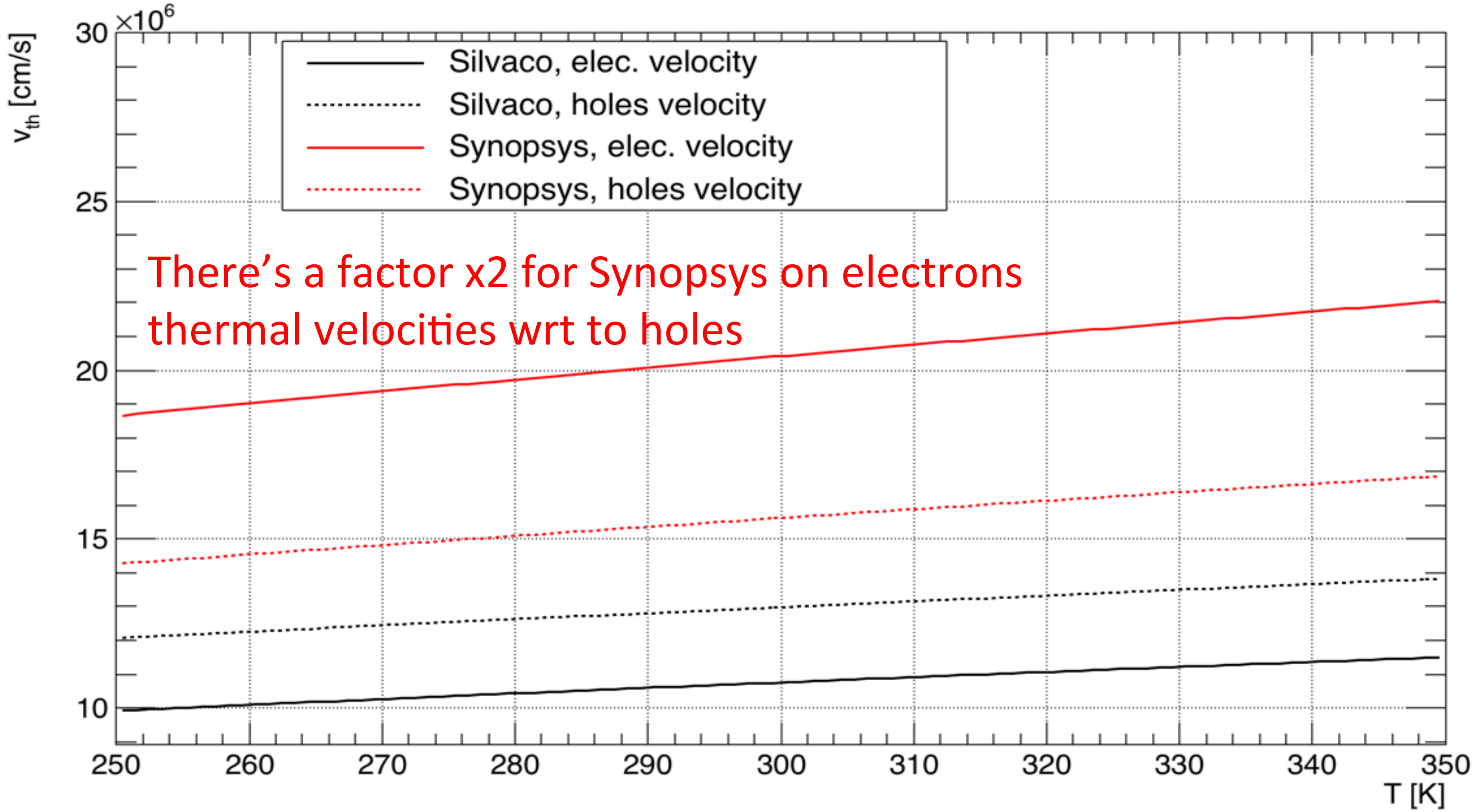
- Michael for suggesting studies to further understand “what’s going on”
- Rogelio, Perugia and MPI group for giving Silvaco a chance
- Luciano Bosisio (Uni. of Trieste) for great discussions
- LPNHE group for supporting me
- My girlfriend (a biologist) for listening to me while getting mad at EG300 default value
- and...

THANK YOU FOR YOUR ATTENTION

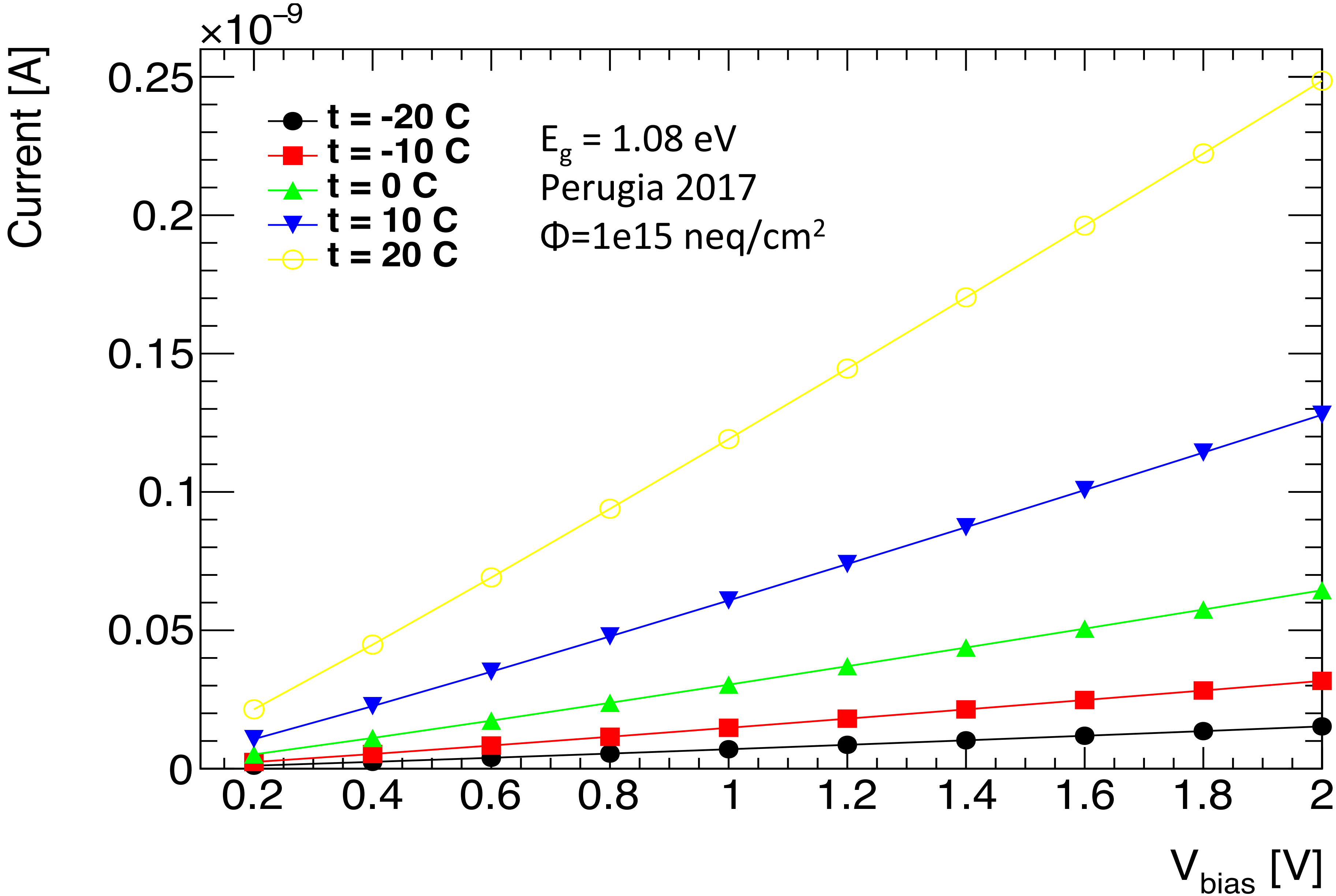
Backup

Reminder

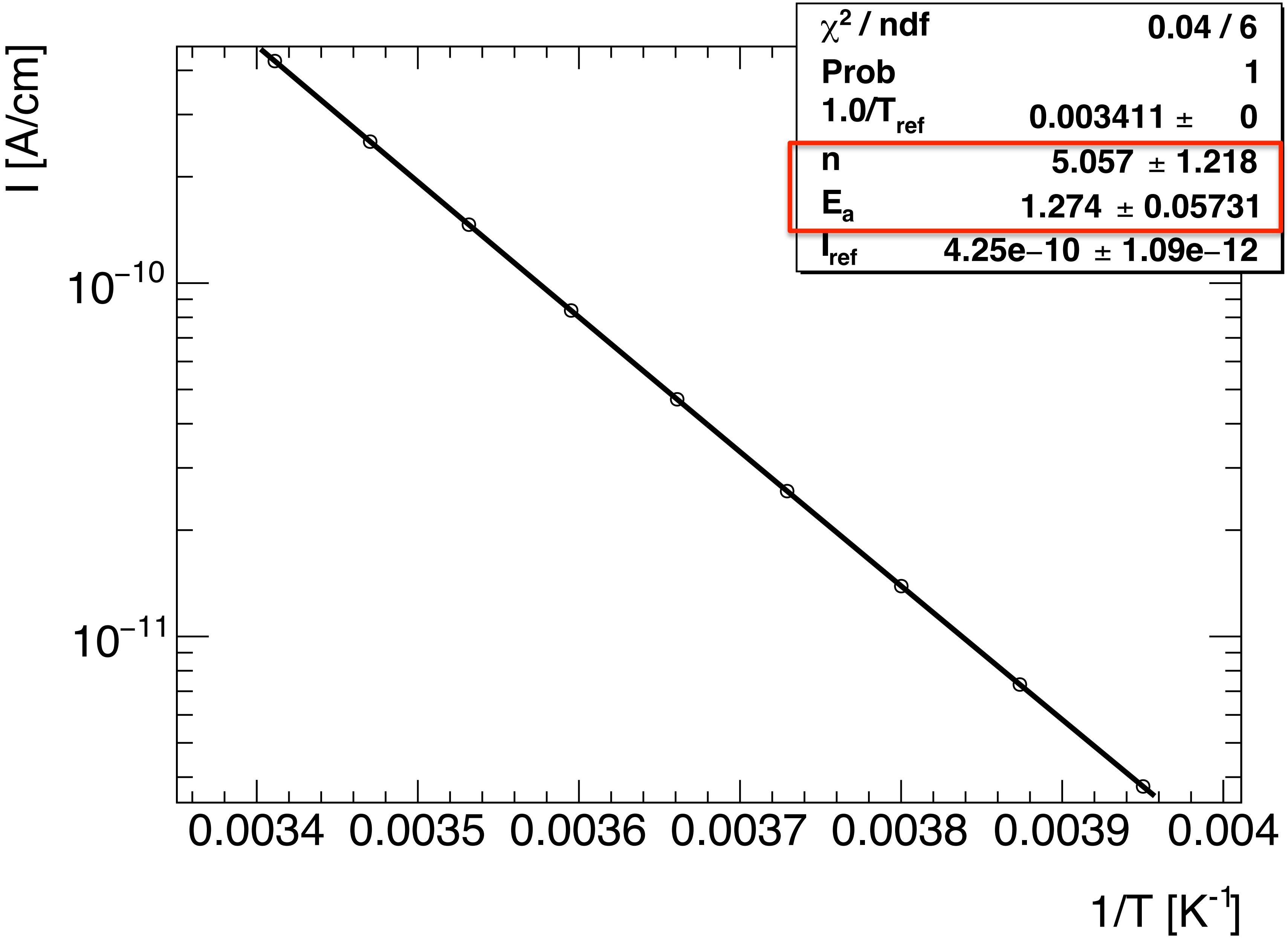
- It was pointed out that Silvaco thermal velocities values are different froms Synopsys ones



Forward current after irradiation, E_g = 1.08 EeV



Perugia 2017, $\Phi = 1x10^{15}\ n_{eq}/cm^2$ – n free par.



Perugia 2017, $\Phi = 3 \times 10^{15}\ n_{eq}/cm^2$ – n free par.