Pentacene-OTFTs: Modelling and Parameter Extraction

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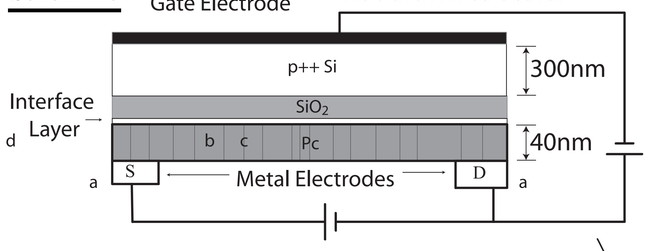
Motivation

To improve understanding of OTFT operation and to test assumptions like presence of extended states and high band mobilty at RT we have developed a quasi-2-dimensional physical model based on the solution of the field equations under steady state conditions allowing for the input of an arbitrary Density of States (DoS) accompanied by an array of parameter extraction methods, motivated by published calculations for polaron bandwidths and mobility[1].

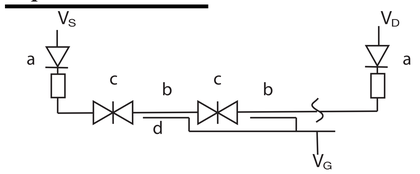
The Device

Schematic



a) Metal to Semiconductor Contacts
b) Crystaline Pentacene
c) Grain Boundary
d) Interface Layer/Self Assembled Monolayer (SAM)

Equivalent Circuit



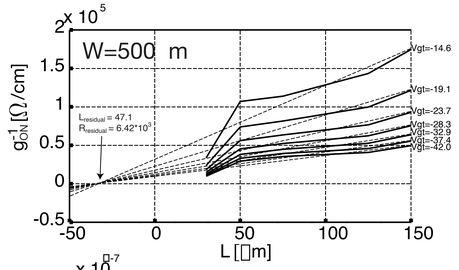
Contact Characteristica

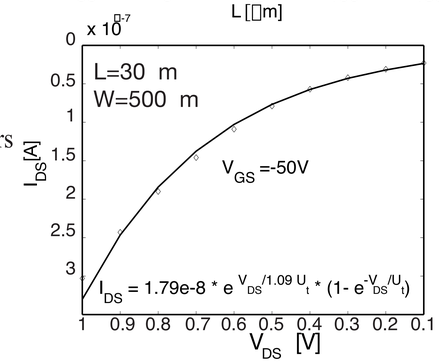
Differnet Kinds of Contacts:

ohmic (evaporated Gold)...

...or...

...non-ideal Schottky-barriers (evaporated Chromium)

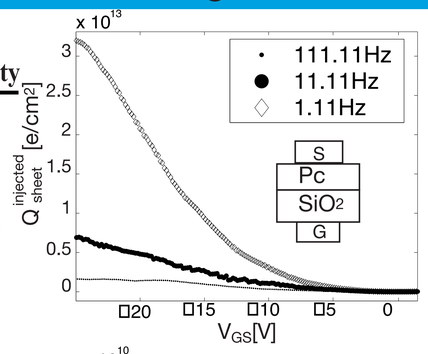




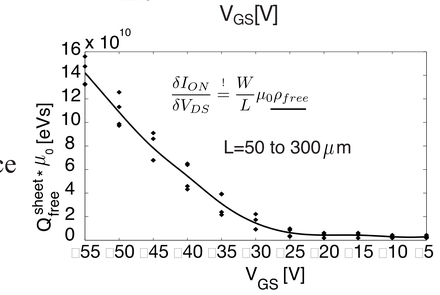
Trapped and Free Charge

Measurement of Charge density

Total charge density from CV-Measurements

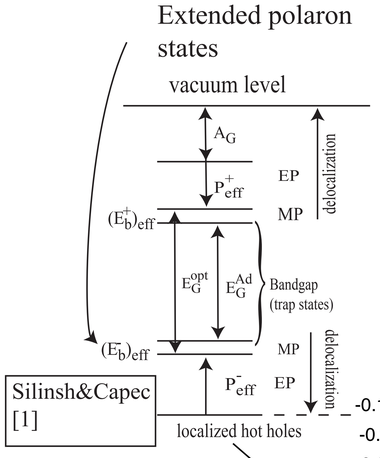


Free charge density from linear region of device chracteristics



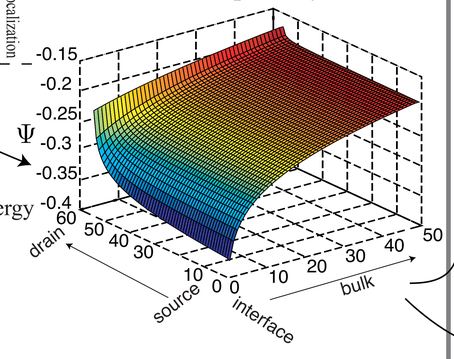
Quasi 2-Dimensional Modeling

Extended polaron states



Silinsh&Capec [1]

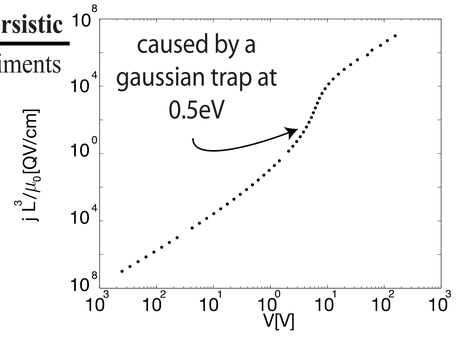
Model Assumptions:
- Channel potential follows surface potential.
- Transverse field bends bands.
- Longitudinal field bends fermi level.
- Current transports by drift.



A_G: Molecular Electron Affinity
$P^{+/-}$: (Electronic) Polarization Energy
$E_b^{+/-}$: Molecular Polaron Binding Energy
E_G^{opt}:Optical Energy Gap
E_G^{Ad}:Adiabatic Energy Gap
MP:Molecular Polaron range
EP: Electronic Polaron Range

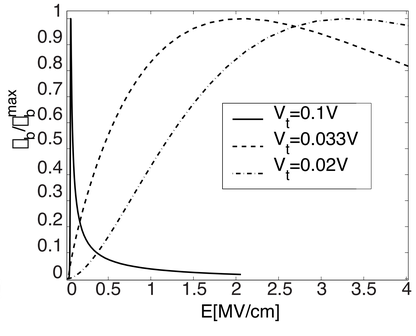
Simulation of Local Substrate Characteristics

SCLC-Characersistic
-resembles experiments
-governs turn-off
-influences saturation behavior



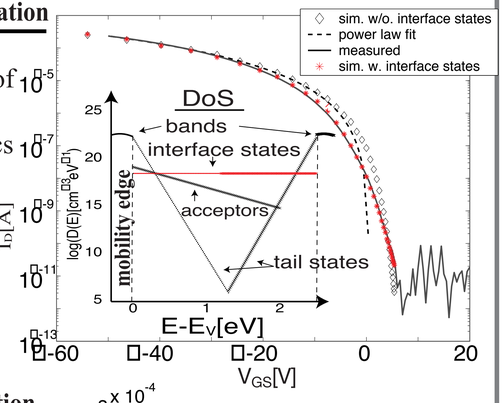
Grain Boundary Barriers

-various field dependencies possible
-did not turn out to govern device dc-characteristics at room temperature!

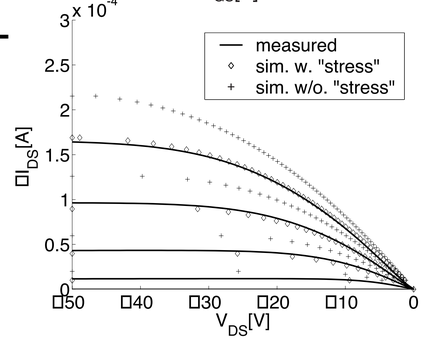


Simulation of Device Characteristics

Transfer-Simulation
-accurate reproduction of subthreshold characersictics and switch-on voltage
-constant band mobility of 16cm²/Vs



Output-Simulation
-97% accuracy after simulating "stress" with increased disorder (tail states)



Acknowledgments

Thanks go to all members of the new materials group (and mark and kathrin)

Conclusion

Simulations show that extended states and thereby drift and not hopping conduction could dominate device characteristics. Band mobilites of >10cm²/Vs seem to be neccesary to explain measurements. Grain Boundaries do not seem to limit the conduction mechanism. Switch-On and sub-threshold characteristcs can be understood in terms of interface states.

References

[1]: Edgar A. Silinsh and Vladislav Capek: "Organic Moledular Crystals", AIP Press '94

[2]: K. Hannewald, V.M. Stojanovic, J.M.T. Schellekens, P.A. Bobbert, G.Kresse and J.Hafner "Theory of polaron bandwidth narrowing in organic molecular crystals", Jan. 2004, Phys. Rev. B (69), pp. 075211 and references therein