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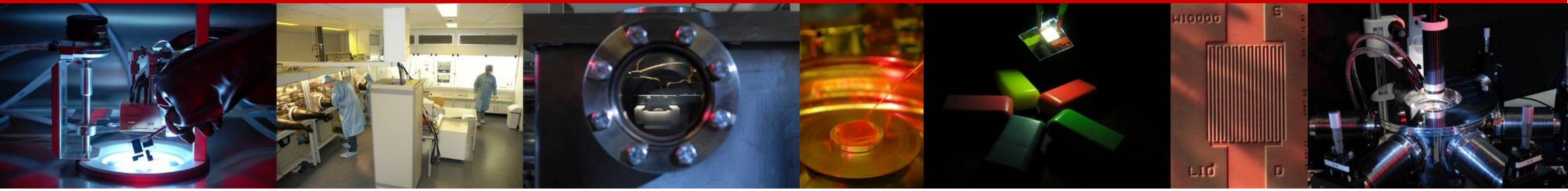
Injection in SIMsalabim: including roughness



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Outline

- **Injection model:**
  - image-force-lowering
  - Scott&Malliaras
- **Effect of roughness**
  - enhanced field
  - enhanced injection
- **SIMsalabim:**
  - implementation

Injection model

- Many different models exist...
- Use a simple one: Scott & Malliaras*
- Due to image force lowering, the carrier density at (close really) the electrode equals (eq. 11 in paper):

$$n_0 = 4\psi^2 N_c \exp\left(-\frac{\phi_b + \sqrt{f}}{kT}\right)$$

- where: $f = qFr_c/kT$
- S&M also give a formula for the current, but we don't need it as we can only use 1 formula (either for n or J).

*Scott&Malliaras, Chem. Phys. Lett. **199**, 115 (1999)
see also: Di Carlo *et al.*, Org. Elec. **15**, 1557 (2014).

Roughness

- George has shown that roughness at the electrode can enhance injection (the field, really)*
- Injection current is exponential in the field => to get the average current, we need cannot simply insert the average field in the S&M formula.
- George's formula for Schottky emission reads:

$$J_s c = A_S T^2 \exp\left(-\frac{\phi_b - \beta\sqrt{F}}{kT}\right)$$

- Note: very similar to S&M's formula for n (previous slide)

*G. Palasantzas *et al.*, Phys. Rev. B **60**, 9157 (1999)

Roughness

- Enhanced injection current (Schottky emission) due to roughness:

$$\frac{J_{sc}}{J_{sc}^{0}} = \exp\left(\frac{\beta\sqrt{F_0}}{2kT}\frac{F_2}{F_0}\right)$$

- F2 is the second-order term in the Taylor series that George uses. We will calculate it later
- This means that the carrier density in the S&M model is given by:

$$\frac{n_0^{\mathrm{rough}}}{n_0} = \exp\left(\frac{\beta\sqrt{F_0}}{2kT}\frac{F_2}{F_0}\right)$$

- where we assume that ψ does not change due to roughness.

G. Palasantzas *et al.*, Phys. Rev. B **60**, 9157 (1999)

Roughness: calculating the field

- Use George's eq. 31:

$$\frac{F_2}{F_0} = \Delta^2 L^2 \int_0^{q_c} \frac{q^2 \coth q}{(1 + aL^2 q^2)^{1+\alpha}} dq$$

- Δ=w/h0. w=rms roughness, h0=film thickness
- a=0.5 approximately. This is calculated from the roughness parameters (i.e. input from Solmaz)
- L=ξ/h0. ξ=lateral correlation length, ~100 nm.
- α=0.5-0.7: roughness exponent. Lower value means more spiky surface.

G. Palasantzas *et al.*, Phys. Rev. B **60**, 9157 (1999)

SIMsalabim: implementation

- There are two effects (formulae shown in previous slides)
  - image-force lowering
  - roughness which enhances injection
- The S&M equation (w or w/o roughness) for n0 (carrier density at electrode) means that we can calculate the barrier lowering by assuming Boltzmann statistics.
- Note: we need Boltzmann statistics at the contacts (V,n,p) to ensure that J=0 if V=0.
- So: in every iteration, we adjust V(0) and n(0), p(0).
  - so use law of mass action to get minority density
- Note: F2/F0 is constant during the simulation, so it can be computed externally.

SIMsalabim: implementation

- What about the sign of F0?
- lowering term only used if it really *lowers* the barrier, otherwise just use phi_b (=input value).