# Scaled 1D NEGF model for 3D Oxide Barriers and Resonant Tunneling Diodes

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## ABSTRACT

We apply a novel scaling algorithm that projects the full 3D NEGF steady state formalism to a scaled 1D formulation (S-NEGF) that permits the study of the current through realistic 3D structures with appropriate symmetry. Our results for oxide barriers are compared with the well-known Fowler-Nordheim expression and a more general expression using WKB. The impact of trapped holes and the effect of temperature are being considered. The method is also applied to a resonant tunneling diode, where the results agree with previous 3D calculations of R. Lake and S. Datta (L&D) using a more accurate formulation. Using a simple 1D Einstein phonon model we are able to accurately predict the peak-valley current of L&D. The S-NEGF results reproduces 3D NEGF ballistic results for space invariant systems. Scattering is introduced phenomenologically, but it is current conserving.

## MODEL AND SIMULATIONS

Wide band gap materials such as SiC used in vertical power MOSFETs operate at high voltages (high fields) that cause stresses in the gate oxide, shortening its lifetime. The estimation of the lifetime is done by projecting high temperature measurements to room temperature. This projection depends on the model and field considered. High fields are beneficial as the channel resistance is reduced and therefore the power dissipation, however this implies shorter lifetimes. The estimation of this trade-off requires accurate identification of tunnelling current and dielectric breakdown mechanisms. Fowler-Nordheim (FN)[1] tunnelling is widely used to describe tunneling in dielectrics at high fields. A more general model is the Sommerfeld-Bethe (SB) model that considers temperature. We compare S-NEGF [2] with the above models. Fig. 1 and fig. 2 show the current at 300K and 450K respectively, assuming $0.4m_e$ ($m_e$ is the electron mass) in the oxide [3]. The formation of hole traps in the oxide are one of the mechanisms contributing to the dielectric breakdown [4]. These traps can form resonant paths to induce breakdown [4]. Fig. 3 shows the current at 450K and $m_e$=0.65me including two different types of trapped hole (wider and thinner). In addition, at low temperatures and small Fermi energies the FN is not accurate. We have developed an expression (denoted FNG as Fowler-Nordheim Generalized), which agrees with SB and S-NEGF but is analytical. Fig. 4 shows the current, comparing FN, SB and FNG at different Fermi energies, showing the agreement between SB and FNG. Finally, we have used our methodology to reproduce NEGF simulation of a 3D double barrier resonant tunnelling diode presented in [5]. In the ballistic regime the two simulations agree. When considering scattering our results reproduce the peak/valley current quantitatively, by using similar Einstein phonons as in [5].

## CONCLUSION

The S-NEGF methodology presented in [2] has been successfully validated by reproducing 3D NEGF results [5] including complex resonances. We conclude that for triangular barriers FN is a good approximation at relative low temperature, however at small Fermi energies it is not accurate. The S-NEGF method is applicable to very general barrier profiles likely to occur in highly stressed dielectrics. Trapped holes can lead to sufficient enhancement of the current to cause dielectric breakdown. Prohibitive "3D NEGF" large computations for realistic structures can now be circumvented using the S-NEGF formalism that uses recursive algorithms.

## REFERENCES

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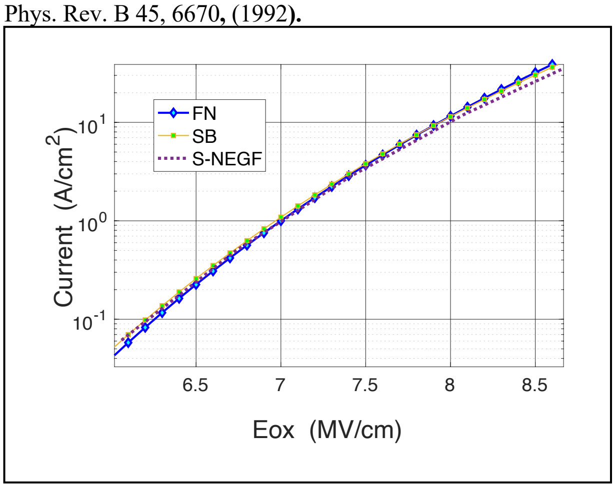


Fig. **1**. Current vs field through an oxide dielectric using different models at 300K; the mass of the carrier in the oxide is 0.40 times the electron mass.

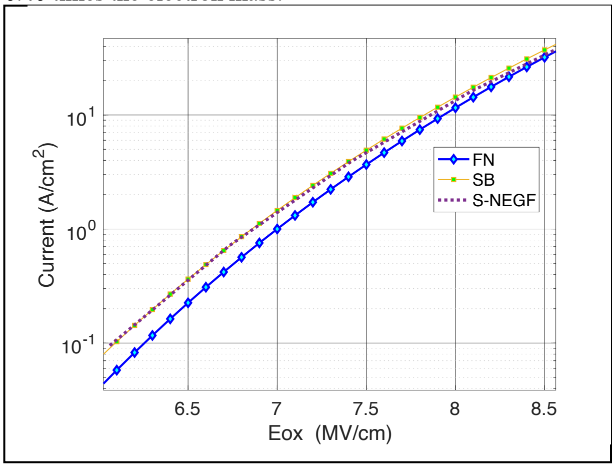


Fig. 2. Current through a triangular barrier at 450K; the mass of the carrier in the oxide is 0.40 times the electron mass.

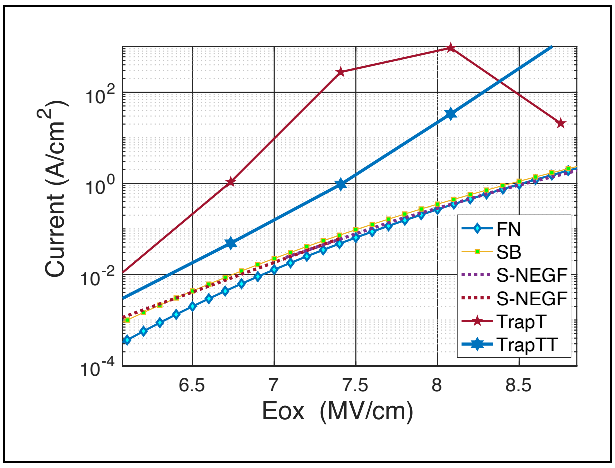


Fig. 3. Current vs Electric field for different models, FN, SB and NEGF with oxide mass of 0.65me and 450K. S-NEGF calculations with a wide Trap width, W and thinner Trap width, T, inside the oxide are also depicted. Note the resonant characteristic for the wide trap current.

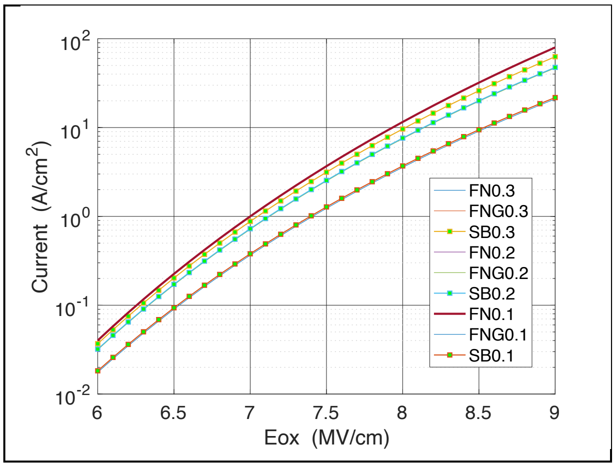


Fig. 4. Currents from FN, FNG and SB for different Fermi energies: 0.3eV, 0.2eV, 0.1eV. The SB and FNG agree as expected. The FN is not accurate for low Fermi energy values.

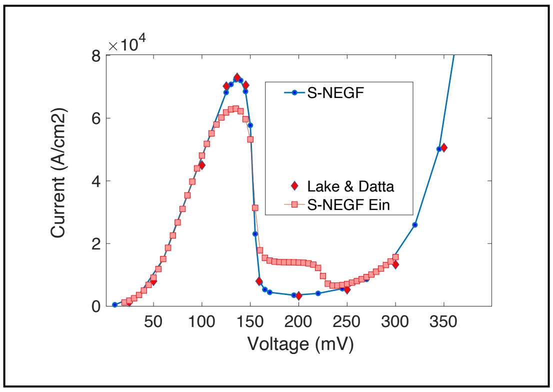


Fig. 5. Current vs voltage for the resonant tunnelling diode of ref. 4 (Lake & Datta). S-NEGF and S-NEGF Ein (Einstein phonons) denoted the calculations of this work.