# A Mathematical Extension to Knudsen Diffusion Including Direct Flux and Accurate Geometric Description

L. F. Aguinsky[1], P. Manstetten[2], A. Hössinger[3],
S. Selberherr[2], J. Weinbub[1]
[1]*Christian Doppler Laboratory for High Performance TCAD at the*
[2]*Institute for Microelectronics, TU Wien, Gußhausstraße 27-29/E360, 1040 Wien, Austria*
[3]*Silvaco Europe Ltd., Compass Point, St Ives, Cambridge PE27 5JL, United Kingdom*
*aguinsky@iue.tuwien.ac.at*

As device designs become three-dimensional, modern semiconductor manufacturing technology must evolve to enable high aspect ratio (AR) features [1]. One critical challenge in high AR processing is the depletion of neutral species towards the bottom of a feature. In deposition cases, depletion manifests itself as a decline in step coverage [2], while in etching it is linked to AR dependent etching [3]. The defining characteristic of neutral species transport is isotropic reflections on the surface [2], which motivates two common modeling approaches: Radiosity [4] and Knudsen diffusion [2]. Radiosity is the exact formulation of the net exchanges between all surfaces, including a particle source. However, it requires the inversion of a matrix describing these exchanges. Otherwise, the Knudsen diffusion approach rests on physically-motivated approximations to the mass balance to provide a coarser but more insightful description, enabling an intuitive understanding of the effects of the parameters. We propose an extension to the standard Knudsen diffusion approach (Figs.1,2) by including the direct flux from a source and a geometric factor. The direct flux stems from the radiosity approach but avoids the costly matrix inversion by disregarding reflections. The geometric factor is obtained from an integral over the whole geometry performed at each differential cross section. It allows for a more accurate description of the indirect flux due to reflections. We verify this novel approach (Fig.3) against our reference radiosity model for a finite cylinder [4], obtaining good agreement (Fig.4). We show that the infinite cylinder approximation, used in standard Knudsen diffusion [2], fails near the extremities of finite cylinders (Fig.5) and that the hydraulic diameter approximation for rectangular trenches [5] has inadequate asymptotic behavior (Fig.6).

**Acknowledgments.** The financial support by the Austrian Federal Ministry of Science, Research and Economy, and the National Foundation for Research, Technology and Development is gratefully acknowledged.

[1] C.G.N. Lee et al., J. Phys. D: Appl. Phys. **47**, 273001 (2014).
[2] A. Yanguas-Gil, Growth and Transport in Nanostructured Materials (Springer, 2017).
[3] K. Ishikawa et al., Jpn. J. Appl. Phys. **56**, 06HA02 (2017).
[4] P. Manstetten et al., Solid-State Electron. **128**, 141 (2017).
[5] M. Ylilammi et al., J. Appl. Phys. **123**, 205301 (2018).

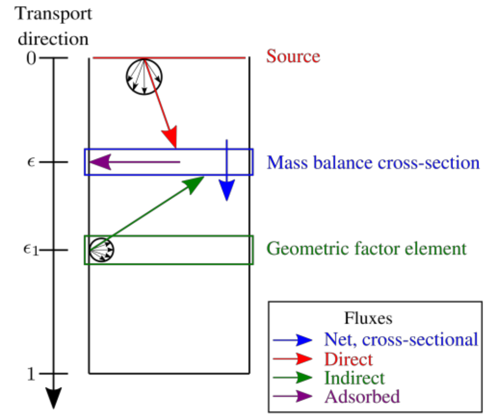


*Fig.1: Schematic representation of the model. The goal is to obtain the net, cross-sectional flux through the mass balance volume (blue) by balancing the direct (red), adsorbed (purple), and indirect (green) fluxes. The complete indirect flux contribution is obtained by integrating over all $\epsilon_1$ (green elements).*

$$\tilde{j}(\epsilon) = \overbrace{F_D(\epsilon) + g(\epsilon) \times \overbrace{\tilde{D}_{Kn} \times \frac{d\psi}{d\epsilon}}^{\text{Standard Knudsen diffusion}}}^{\text{Extended Knudsen diffusion}}$$

$$\frac{d\tilde{j}}{d\epsilon} = k \times \psi(\epsilon)$$

$\tilde{j}$ : Normalized, net, cross-sectional flux
$\psi$ : Normalized concentration
$\epsilon$ : Normalized axial distance
$F_D$ : Direct flux
$g$ : Geometric factor
$\tilde{D}_{Kn}$ : Normalized Knudsen diffusivity
$k$ : Surface adsorption rate

*Fig.2: Schematic representation of the system of ordinary differential equations modeling neutral transport. The colors relate to Fig.1. We note the differences between our model and the standard Knudsen diffusion approach [2]: The presence of direct flux and the geometric factor. The adsorbed flux is modeled by a volumetric sink term, as in [2].*

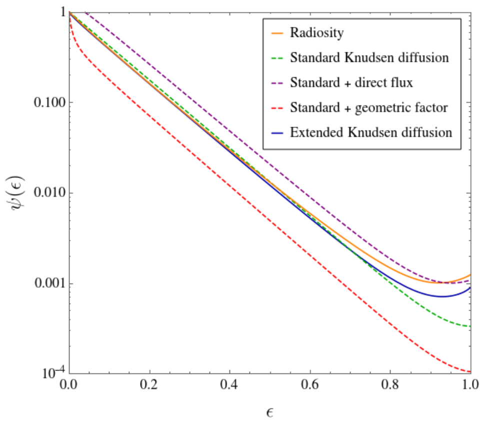


*Fig.3: Comparison of the local concentration between different approaches for a cylinder of AR 50 and sticking 1%. We note that the full extended Knudsen diffusion approach is required for more accurately matching radiosity [4] over most of the feature.*

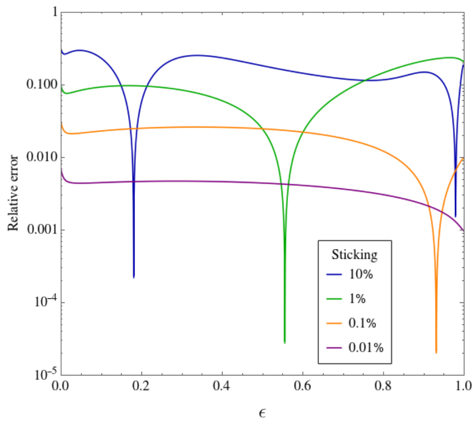


*Fig.4: Local relative error, defined as the relative difference between the extended Knudsen diffusion and radiosity [4] results, for a cylinder of AR 50 and varying sticking. Here, we showcase how our model produces adequate results even in high sticking regimes.*

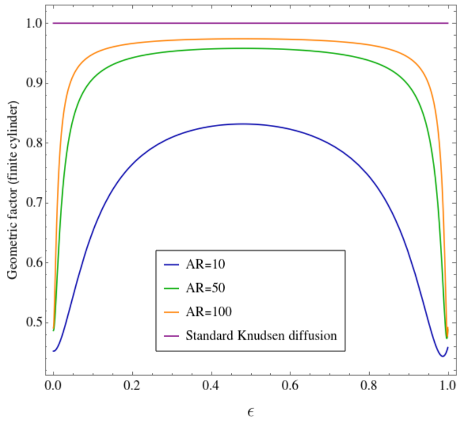


*Fig.5: Geometric factor as a function of axial distance $\epsilon$ for a finite cylinder of sticking 1% and varying ARs. Our model highlights significant discrepancies in the standard approach [2] for the extremities of the cylinder even for high ARs.*

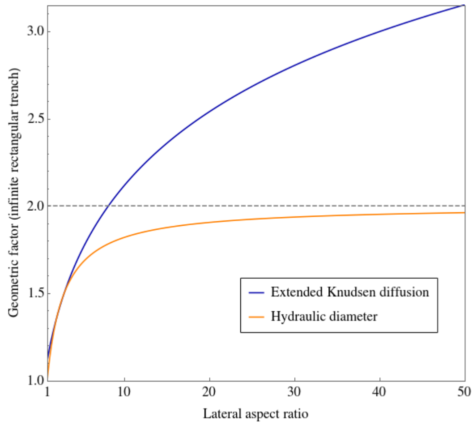


*Fig.6: Geometric factor for a rectangular trench of infinite length, for each lateral AR, given by our model and by the hydraulic diameter approximation [5]. Our model has divergent asymptotic behavior. This is expected, as the problem is intrinsically three-dimensional.*