Fast Volume Evaluation on Sparse Level Sets

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Implicit surface representations such as the level set method, as often applied in process simulations [1], usually only represent the interfaces between materials, rather than the full volume of a material itself. This limits the accurate representation of diffusion and the effects of chemical reactions taking place inside a material. Therefore, diffusive processes cannot be modelled directly, but demand regular conversions to a volume representation, requiring computationally costly algorithms. As an alternative, we propose a fast ray tracing algorithm to evaluate the effective volume of a material layer directly on the implicit surface with sub-grid resolution, eliminating the need for a costly volume conversion. Our algorithm is implemented in ViennaTS [2], a level set powered topography simulator. As a relevant application, a polymer stabilisation step, a so-called N_2 flash, performed during gate stack etching [3], was simulated. This fabrication step reduces the volume of a thin layer proportionally to the initial layer volume [4]. Therefore, the volume of the material to be reduced must be known to model this process accurately. Diffusion processes simulated by ray tracing, monitor the path each incoming particle takes through the volume of a material. This is computationally costly due to the large number of rays needed to describe the process. A bottom-up approach [5], where rays are reversely followed from the bottom interface and counted on the top interface, can be used instead, which is shown in Fig. 1. The combination of the path length and distribution of rays on the top interface provides an approximation of the volume accessible to particles diffusing from the top surface. Normalising the length of the rays, as shown in Fig. 2, gives an approximation of the effective volume of the material below each surface point. The effect of the normalisation for the trench geometry shown in Fig. 3, can be seen in Fig. 4, which highlights the discrepancy between pure ray counts per surface element and the effective volume. The simulation of the N_2 stabilisation process step, using the three test geometries, shown in Fig. 3 and Fig. 5, is able to adequately describe the etch process. The developed method can also be applied to a variety of diffusive and volume-dependent processes, such as ion implantation or oxidation without the need for compute-expensive volume extraction. The results of the simulation of a diffusion limited deposition process are shown in Fig. 6.

[1] S. Osher and J. A. Sethian, J. Comput. Phys., **79**(1), p. 12-49, (1988).

[2] ViennaTS. [Online]. Available: http://www.iue.tuwien.ac.at/software/viennats

[3] X. Klemenschits, S. Selberherr, and L. Filipovic, in Proc. EUROSOI-ULIS, pp.1-4, 2018.

[4] O. R. Bengoetxea, Ph.D. dissertation, Université Grenoble Alpes, 2016.

[5] P. L. Manstetten, Ph.D. dissertation, Technische Universität Wien, 2018.

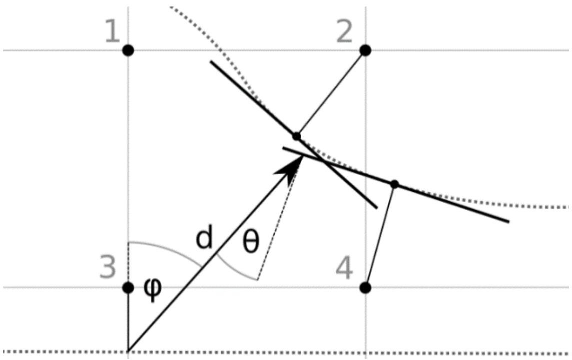

Fig.1: Ray tracing on an implicit surface by approximating the surface using discs [2] shifted from each grid point to the surface by the level set value in the direction of the normal vector. A ray with start and intersection angles of φ and θ, respectively, travels a distance d. The number of rays and their properties are stored in the data structure for each grid point of the top level set.

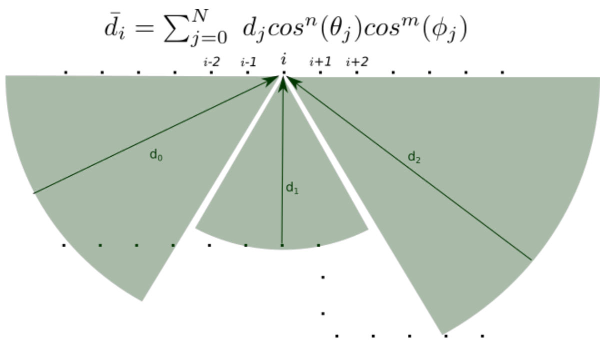

Fig.2: Normalisation of ray distances via power cosine distributions of the start and intersection angle. The powers were chosen as n=m=2 for minimum simulation time while still providing reliable results. The dots correspond to the active level set points, used to define the location of the surface when sparse level set methods are used.

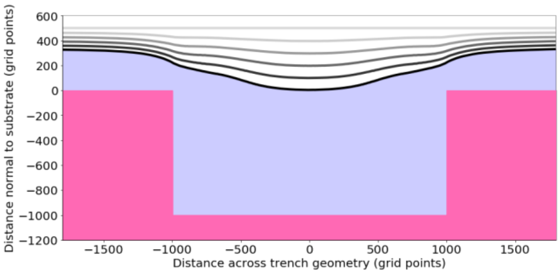

Fig.3: Surface evolution of a thin passivation layer during an N_2 flash process step, obtained from volume dependent etch models. The evolution of the top level set above a trench geometry is shown from light grey as the initial surface to dark grey for the final profile. The substrate and the thin layer are shown in pink and blue respectively.

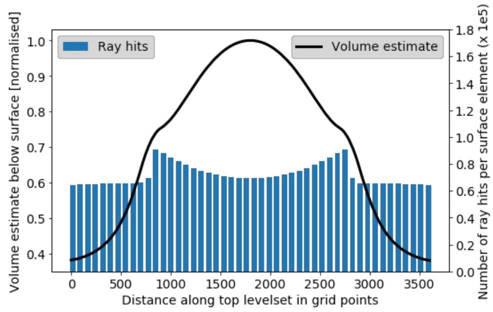

Fig.4: Volume estimate of a trench geometry underneath a plane, given in Fig. 3. The estimated volume (black line) is shown in comparison to the number of rays incident on the surface (blue bars), highlighting the strong effect of the angle dependence on the final profile, which adequately balances the abrupt increase of ray hits due to the sharp edge in the geometry.

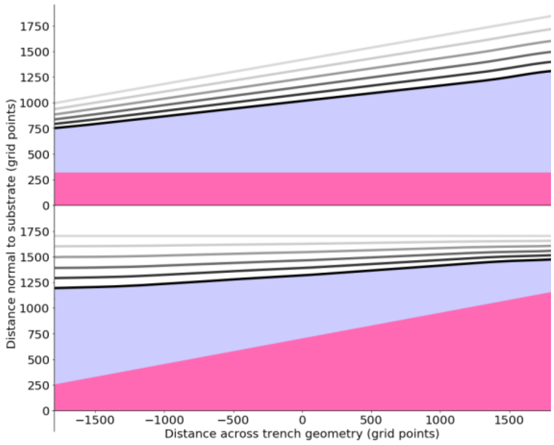

Fig.5: Comparison of two thin layers (blue) on a substrate (purple) during the N_2 flash process, with linearly increasing thickness. Areas with higher volume reduce quicker than those with less volume. The evolution of the top layers' locations over time is shown from light grey for the initial surface to dark grey for the final profile.

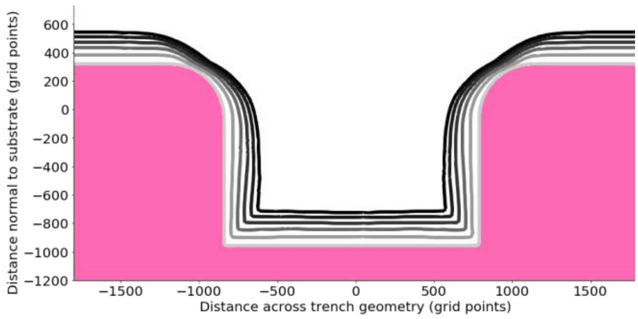

Fig.6: Surface evolution of diffusion limited growth, achieved by considering the volume particles have to diffuse through, in order to react with the surface below. The reacting substrate is shown in purple while the time evolution of the material growing above is shown from light grey to dark grey for the final profile.