A Two-Dimensional Lorentzian Distribution for an Atomic Force Microscopy Simulator

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Atomic Force Microscopy (AFM), a lithographic technique capable of manufacturing nanometer-sized devices, is a promising alternative to modern lithographic methods. Performing physical simulations to replicate the AFM process is not feasible for large surface simulations, therefore a Monte Carlo approach must be considered. Previous research showed that the physical shape of an oxide dot or wire, generated using AFM, most closely resembles a Lorentzian distribution. Therefore, the goal of this work is to create a Monte Carlo simulator for AFM oxide growth on a silicon substrate. The resulting oxide nanodot or nanowire shall follow a two-dimensional Lorentzian distribution around the AFM needle tip. The simulator must be seamlessly integrated into an existing Level Set simulation environment. The wafer surface and surfaces where different materials intercept (such as the Silicon/Silicon Dioxide interface) are described using the Level Set equation. The equations describing the effects of processing conditions, including bias voltage, process time, wafer orientation, and ambient humidity, on the height and width of oxide nanodots and nanowires are taken from literature. Using the given equations, the final shape of the nanostructure is calculated. In order to generate the structure on the top two Level Set surfaces of the wafer, a Monte Carlo method is implemented. Particles are generated with a Lorentzian distribution, around the AFM needle. Each particle is then accelerated towards the silicon wafer, generating a small "bump" on the surface. This leads to the creation of a Lorentzian-distributed dot or wire, as required. The one-dimensional Lorentzian distribution is well known and a particle which follows the Lorentzian distribution is generated using $r_x = \tan\left[\pi\left(\xi_{r_x} - \frac{1}{2}\right)\right]$, where ξ_{r_x} is evenly distributed between 0 and 1. However, a rotational two-dimensional distribution must be generated, whose diagonal intercept follows a Lorentzian distribution. The attempted algorithms have involved the generation of a Lorentzian-distributed radius, followed by an evenly distributed angle θ between 0 and 2π. The generated particle location is then given by $(\mathrm{x}_0,\mathrm{y}_0) = (\mathrm{r}_x\cos\theta,\mathrm{r}_x\sin\theta)$. The physics-based intuitive algorithms used to generate r_x are:

1. The generation of a two-dimensional even distribution around the needle tip for the variable ξ_{r_x}. This value is then used in order to generate the Lorentzian-distributed radius, r_x.

2. The generation of r_x by integrating the probability distribution, while taking into account both two-dimensional directions: $(\mathrm{dx}_0,\mathrm{dy}_0)$ or $(\mathrm{dr},\mathrm{d}\theta)$. This results in the two-dimensional distribution $\xi_r = \frac{1}{\pi}\int \frac{r}{(1+r^2)}dr \Longrightarrow r_x = \sqrt{e^{2\pi\xi_r} - 1}$. Using an evenly distributed ξ_r, a Lorentzian-distributed r_x is generated, followed by an evenly distributed angle θ between 0 and 2π. The generated point is then $(\mathrm{x}_0,\mathrm{y}_0) = (\mathrm{r}_x\cos\theta,\mathrm{r}_x\sin\theta)$. This proved to be the most applicable method to incorporate the Monte Carlo method for nanodot and nanowire generation in a Level Set environment.