Simulation of the fluctuations of energy and charge deposited during *e*-beam exposure

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Energy and charge deposition process's stochastic nature is examined, using a model based on the discrete loss approximation (DLA). Deposited energy deviations computed using continuous slowing down approximation (CSDA) and DLA are compared. It's shown that CSDA underestimates deposited energy fluctuations.

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1. Introduction

Usually in the deposited during *e*-beam irradiation energy analysis one uses the average energy or charge values. However, the usage of highly responsive (few μC/cm^2) resists leads to a relative fluctuation growth, which, in turn, results in surface roughness growth after etching. In the present work, with a help of a program based on discrete (or random) loss approximation, distributions of energy and charge deposited during electron beam interaction with solid are simulated.

The simulation algorithm is described in detail in [1]. The main difference of used method from the widely distributed continuous slowing down approximation is in the interaction randomness taken into account. All significant interaction crossections are taken into account separately. Inner-shell ionazation considered by Grysinski [3] formula, outer shell ionization considered by Meller [4] model; plasmon [5] generation and decay are also taken into account. Elastic interaction was simulated using Mott crossection. For electrons with energies lower then 100 eV a semiempirical scattering model is used [6–8].

2. Simulation results

The results of the simulations in continuous slowing down and discrete looses approximations are compared for 1 μm PMMA film uniformly irradiated by the electron beam. Simulation was performed for dose values between 0.5–35 μC/cm^2, primary electron energy — 20 KeV, beam size — 5×5 nm. Cell size for standard deviation computing was chosen to be $0.05 \times 0.05 \times 1\,\mu$m.

On fig. 1 one can see normalized standard deviation values of the deposited by *e*-beam energy computed using DLA and CSDA together with the primary electrons number deviation. On fig. 2 normalized standard deviation values of the deposited energy and total charge are presented.

The deviation of total charge is higher than that of the energy because in the inelastic interaction some amount of energy is deposited and a unit of charge. So the positive (negative) charge distribution is proportional to the interaction acts density, while the energy distribution is also

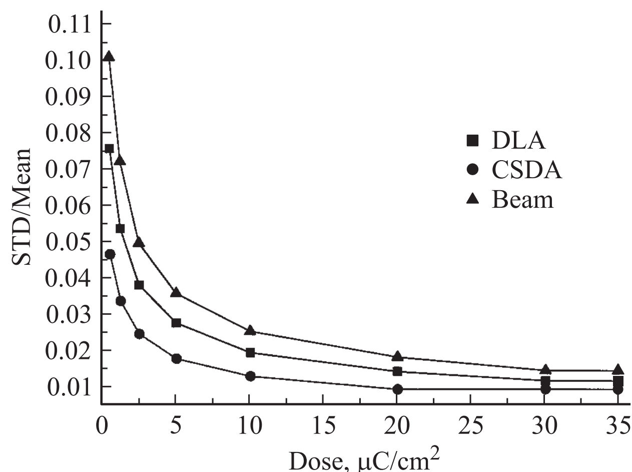

Figure 1. Normalized standard deviation values of the deposited energy computed using DLA and CSDA and primary electrons number deviation.

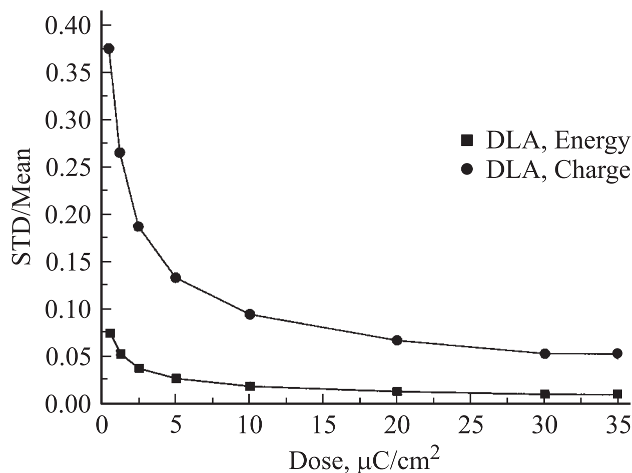

Figure 2. Normalized standard deviation values of the deposited energy and total (positive–negative) charge.

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affected by the loss distribution in single interaction act:

$$D_{\text{charge}} = \sum_i x_i^2 - \left(\sum_i x_i\right)^2,$$

$$D_{\text{energy}} = \sum_i \left(\sum_{j=1}^{x} \xi_j\right)_i^2 - \left(\sum_i \left[\sum_{j=1}^{x} \xi_j\right]_i\right)^2.$$

Here x — number of interactions in cell, ξ — energy deposited in single inelastic interaction event.

3. Discussion

Theoretical analysis of CSDA (where statistical nature of inelastic interactions is neglected) which gives good results when the energy loss deviation is much less than the mean loss value, surprisingly shows that it cannot be applied to the non-relativistic electron scattering process. This can be easily shown by the Landau [2] theory of electrons energy distribution after passage of a thin film of thickness x. Namely the standard deviation σ_Δ to the mean energy loss ΔE ratio (variation coefficient):

$$\frac{\sigma_\Delta}{\Delta E} = \sqrt{\frac{R}{x L_{\text{ion}}}}, \quad L_{\text{ion}} \approx \ln\left(1.16\frac{E_0}{J}\right) \tag{1}$$

is always more than 1. Here R — electron range in medium, J — effective ionization potential (usually 50–500 eV), so the ionization logarithm L_{ion} is about 5. As the distance between the elastic interactions is comparably small ($x \ll R$), Landau formalism can be applied to the analysis of Monte–Carlo algorithms. So it's clear that statistical straggling of energy loss is higher than the mean value and CSDA cannot be applied to the present problem.

From fig. 1 one can see that deviation values given by DLA can be up to 2 times higher than those given by CSDA for the considered case. The reason is that CSDA does not take into consideration energy loss deviation while DLA does. When using DLA the deposited energy distribution deviation is formed not only by trajectories space distribution (like in CSDA) but also by deviations of energy loss in scattering process. As it is known, etching speed V can be estimated using (2), where γ lies between 1 and 6:

$$V/V_0 = (D/D_0)^\gamma. \tag{2}$$

From fig. 1 one can see that for dose values $\sim 1\mu\text{C/cm}^2$ deposited energy fluctuations can be some 10%, which in turn can give the difference of the etching speed $\sim$ 40%.

4. Conclusion

The main result is that discrete loss approximation gives the estimated values of deposited energy fluctuations higher then the continuous loss one. Physical basis of the discrepancy is the fact that at *single* inelastic event a fluctuation of losses is not small in comparison to mean value. The observation of the discrepancy has very serious consequences for nanotechnology performed with e-beam. It should be taken into account as a reason responsible for linear edge roughness (LER), for planar roughness at stamp fabrication for nanoimprint lithography *etc.* Discrete looses approximation is an approximation of higher order than continuous slowing-down approximation. So one can conclude that the continuous slowing-down approximation predicted wrong results for energy fluctuations and for induced roughness after development.

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