Material Representations and Algorithms for Nanometer-Scale Lithography Simulation

E.W. Scheckler, T. Ogawa, S. Shukuri, and E. Takeda
Hitachi Ltd., Central Research Laboratory
1-280 Higashi Koigakubo, Kokubunji, Tokyo 185, JAPAN

Introduction: Lithography simulation has traditionally treated resists as materials with continuously varying inhomogeneous properties (such as local absorbed energy). Additionally, the resist surface is considered smooth before, during and after development [1]. Occasionally, cell-removal algorithms were employed but only as a means to implement dissolution models, with the result sometimes followed by a graphical surface smoothing operation [2]. However, as linewidths decrease below 200nm, exposure fluctuation and resist roughness take on dimensions comparable to feature sizes [3]. A few cell-based simulators have considered exposure induced roughness in X-ray lithography [4] and ion induced roughness in plasma etching [5]. However, a new simulation paradigm is still required to further model nanometer-scale variations in advanced lithography, both as a means to better understand the underlying physical processes and to provide a tool for lithography process design. We present HIACINTH (HItachi's Algorithms for Calculation of IC Nano-process TecHnologies) as a means towards these goals.

Data Structures: An effective material representation must be both detailed enough to support features required by the physical models and compact enough to fit the available computer memory. Also, the data structures must support efficient algorithms. Volume partition methods have proven successful in a variety of applications and our method begins with a 3D array of cubic cells as the top level of a hierarchical data representation. The resists is represented as a collection of overlapping polymer chains, each contained within a sphere of radius proportional to the square root of the number of chain links [6]. The cells are filled with spheres, as shown in Fig 1. Each sphere has a randomly determined size based on the resist molecular weight distribution. Each sphere's location is also determined randomly. The cell size is chosen to be a few times larger than the average molecule diameter, but still small enough to preserve the efficiency of such operations as locating a sphere's nearest neighbors. It is necessary to fully allocate the spheres only for cells in contact with developer. In our implementation, each sphere requires 30 bytes, and each cell requires 4 bytes. A 100nm line comprised of 50,000 molecules in a $100nm^3$ region (10x10x10cells) thus requires about 1 MByte. The hierarchical representation may be continued further, down to the monomer or even atomic level, but this is not necessary for the models presented here.

Algorithms: Two basic resist changes occur in lithography: 1) internal structure change as a result of exposure and bake steps, and 2) external shape change as material is removed during development. In positive electron and x-ray resists, the structure change occurs due to chain scission. For our model, this means that large spheres are cut into smaller spheres, as shown in Fig. 2, with the cut locations given by a Monte Carlo calculation of energy absorption event locations. Alternately, the positive resist may be initially allocated with sphere sizes given by the local molecular weight distribution *after* exposure for a given absorbed dose, following [7]. We have found that both methods result in the same macroscopic molecular weights after exposure, but that the latter method is only applicable if the beam edge sharpness is larger than a typical resist polymer size. Negative resists are rendered insoluble when cross-links form to interconnect the polymer chains. Generally, a post-exposure bake step activates photo-generated acids, which catalyze cross-linking reactions. HIACINTH calculates an average acid random walk step length and number of steps from the kinetic theory of acid generation and consumption following [8]. Model parameters are derived from FTIR measurements. Fig. 3 depicts the PEB model.
An outline of the development algorithm for both resist types is shown in Fig. 4. First, all surface spheres are located. The algorithm proceeds by comparing a random number with the Poisson probability of removing a surface sphere given the time step, sphere size, the number of cross-links, and the degree of developer penetration. A practical method for deriving the Poisson removal rate (number removed of size x per second) for a given sphere is to solve the integral equation equating the mass removal rate according to a macroscopic model with the integral over all possible weights of the Poisson rate times the resist weight distribution. If a sphere is removed, then all neighbor spheres are flagged as being on the new surface. Also, if the removed sphere penetrates an unallocated cell then molecules must be assigned for that cell, with surface spheres appropriately identified. The above algorithm is only appropriate for resists which do not swell appreciably, which are in fact the only resists suitable for nanometer-scale lithography. The program structure also leaves open the possibility of other removal algorithms, for example based on the developer diffusion into the resist rather than the Poisson probability model currently used. The general method may also be extended to multiple-species resists and X-ray or optical exposure sources.

Simulation Examples: The effectiveness of the simulator can be demonstrated by the following examples. PMMA is a well characterized positive electron-beam resist. A sample of Tokyo Ohka OEBR-1000 resist subject to a 100nm wide 50keV beam at $400\mu C/cm^2$ and developed for 120s in 1:3 MIBK:IPA results in the feature shown in Fig. 5. The dimensions and shape agree well with experimental structures. The development simulation required approximately 20 minutes of CPU time on a Sun SPARCStation 2. The resist edge roughness may be estimated by measuring the linewidth at several evenly spaced points along the resist line. The resulting standard deviation is a good estimate of the edge roughness. Altering the incident dose, developer sensitivity and contrast leads to different average molecular weights at the line edge which in turn dramatically affects edge roughness, as plotted in Fig. 6.
Shipley SAL-601-ER7 negative, chemical amplification resist has also been widely studied. The etch rate is related to the number of cross-links attached to the original resin molecule. The post exposure bake effect on the random walk parameters (step size and number of steps) is still under scrutiny, but approximate models (based on [8,9] result in the example of Fig. 7 for a fine line exposed in 20nm thick resist by the Hitachi S-900 SEM, operating at 5kV acceleration voltage, and a line dose of 180pC/cm. The result agrees with [10]. CPU time for this case was 10 minutes on a Sun SPARCStation 2

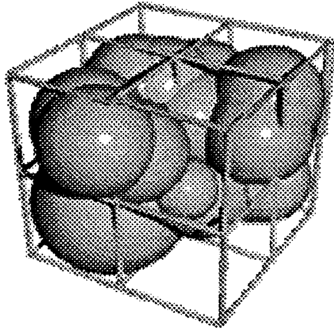

Fig. 1: Spheres representing polymer chains contained within an array of cubic cells.

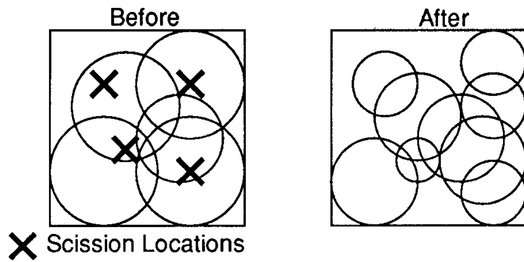

Fig. 2: Chain scission model for splitting spheres.

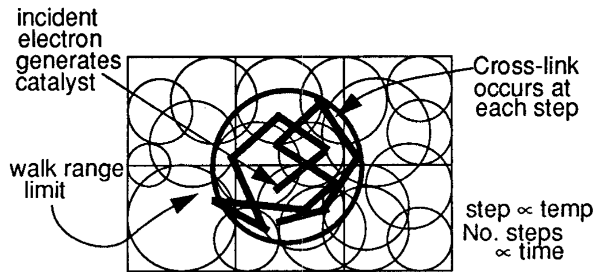

Fig. 3: Depiction of PEB random walk model for cross-linking.

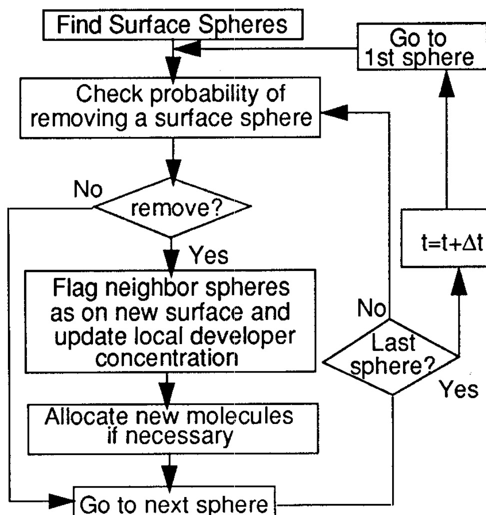

Fig. 4: Development algorithm flow chart.

References

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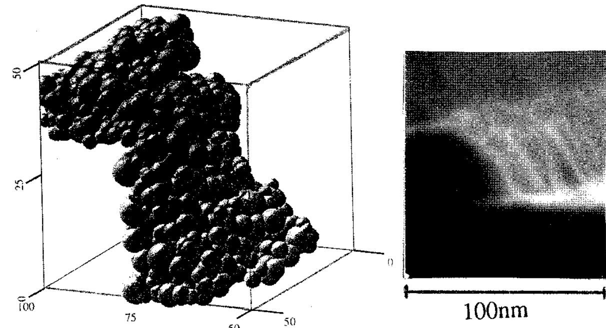

Fig. 5:Half of PMMA line in 100nm thick resist, exposed at 400μC/cm^2, 50keV, and developed for 120s in 1:3 MIBK:IPA. SEM is of similar case with 10nm Au coating.

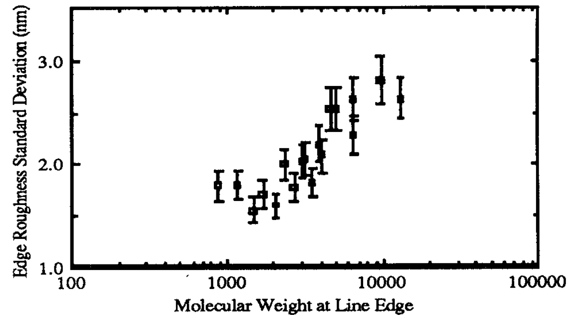

Fig. 6: Standard deviation of edge roughness vs. edge molecular weight, achieved with different initial doses and developers. Error bars give 67% confidence of the std. dev. measurement.

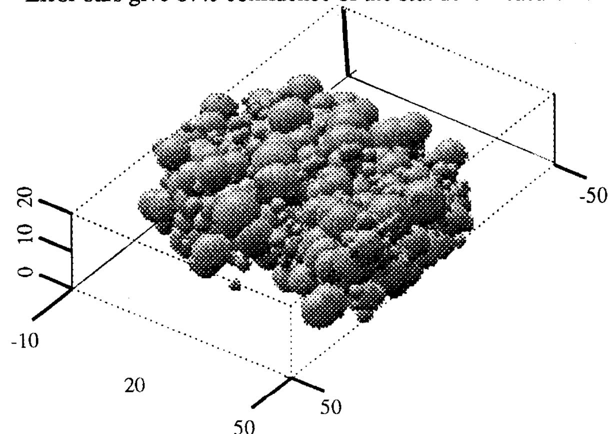

Fig. 7: Line in 20nm thick SAL-601 resists, exposed by Hitachi S-900 at 5keV, 180pC/cm line dose, and developed or 60s in 0.27N MF-312. PEB is at 85°C for 5 minutes.