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CALCULATION OF A TOPOGRAPHIC CONTRAST IN THE SCANNING ELECTRON MICROSCOPE

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Abstract

A direct simulation of electron scattering in solids is developed. Using this simulation, a topographic contrast found in the scanning electron microscope is quantitatively discussed. The surface topography studied here is a rectangular rod pattern and a rectangular groove pattern at an infinite horizontal plane surface of Al. We quantify characteristics of the secondary electron image and of the backscattered electron image at the topography. The intensity profile at the bottom surface of the groove pattern is roughly approximated by an analytical model.

Key Words: Scanning electron microscope, topographic contrast, trench structure, Monte Carlo calculation, direct simulation.

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Introduction

It has been attempted to analyze image contrasts of the scanning electron microscope (SEM) by several methods to get informations about the ultimate resolution,[4,7,10,11] or to derive basic data for a three-dimensional reconstruction of a specimen surface structure from the image.[14,16] The method most commonly adopted for these applications is to use a Monte Carlo simulation of electron trajectories in the specimen. Using the simulation, intensity profiles of secondary electrons (SEs) and back scattered electrons (BSEs) emitted from a topographic pattern can be obtained as a function of various parameters of the electron beam and of the specimen. However, simulations which have been usually performed carried some kind of adjustable parameters, such as the mean ionization energy in the Bethe energy loss equation, or the screening parameter in the screened Rutherford equation. As the result, even if several different simulation models provide similar results for some physical quantities (e.g. secondary or backscattering yield), it does not guarantee that all the simulations give similar values for other quantities.

Recently, several authors have tried to simulate electron trajectory in a direct manner, using each cross section for every major process.[5,9,15] If we consider each collision process separately, it is no use to bother about the application limit of some averaged formula, and it is straightforward to calculate values of e.g., energy loss and angular scattering in each collision. Cailler and Ganachaud made a direct simulation of electron scattering, and they could explain several humps and peaks of experimental energy distributions of emitted electrons.[3,5] Although it was not a simulation, Bindi et al. made a numerical approach considering the major processes which the electrons underwent in a direct manner with the Boltzmann equation.[2] Ding and Shimizu calculated electron trajectories using energy loss functions which were experimentally obtained, and where various energy loss mechanisms were automatically taken into account.[4] Several other authors have been trying to simulate in a hybrid manner, where only one or two substantial processes were simulated in a direct manner and others were averaged to save the com-

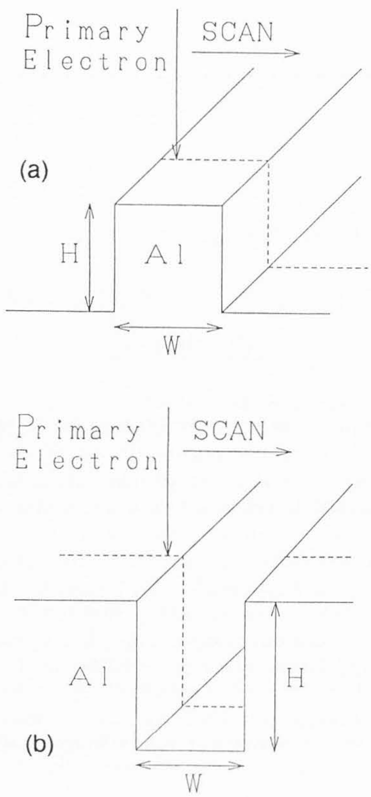

Fig.1. The surface topography studied here: (a) shows a rectangular rod pattern on an infinite horizontal plane surface of Al, and (b) shows a rectangular groove pattern at the same surface. We studied the intensity variation of electrons emitted from the pattern, as a PE beam scans across it along the broken line.

putation time. [1, 6, 8, 12, 13]

Since we are interested in secondary electron signal of the SEM, it is important to calculate slow electron (say $\leq$ 100 eV) trajectories accurately in the specimen. As we mentioned above, the calculation procedure of Cailler and Ganachaud gives quite a good agreement with experimental results, especially for the energy distribution, and it reinforces that the treatment of slow electron behavior in their model is valid enough for the simulation of slow electron scattering processes. This paper presents an application of a direct simulation model, basically the same as their model, to the understanding of SEM signal intensity variations at surface topographic features.

The topographic contrast in the SEM varies depending on several parameters such as (1) the pattern height (or depth) at a specimen surface, (2) the pattern width, (3) the atomic number of the material, (4) the electron beam diameter, (5) the

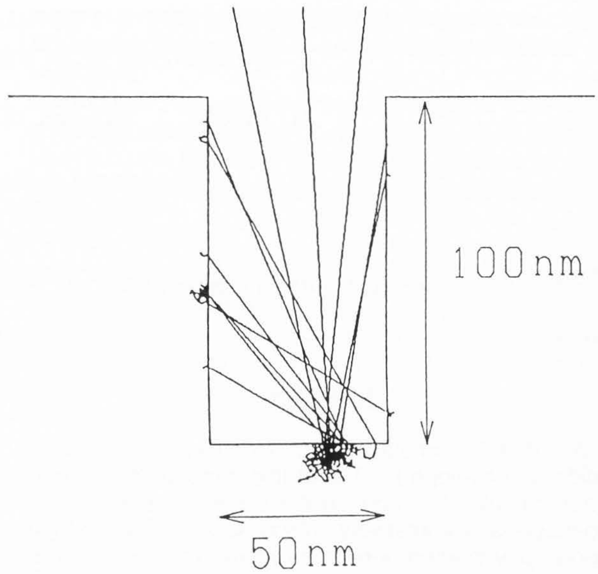

Fig.2. Example of electron trajectories calculated in the specimen by the present simulation. Trajectories of SEs and BSEs in and out the specimen surface excited by six PEs, which are incident normally at the bottom surface of the groove at 0.5 keV. The trajectory of incident PE beam in vacuum is not shown.

electron beam energy, etc. A direct approach, excluding any empirical value, does not exist so far to quantify each of these contributions separately to the final SEM signal intensities. The aim of the present study is to quantify the correlation among those parameters in the SEM signals.

Calculation of SEM Image

The present simulation analyzes secondary electron (SE) and backscattered electron (BSE) images. In the simulation, the following processes are taken into account: (1)cascade multiplication of hot electrons produced via ionizations of inner-shell electrons and conduction band electrons, and plasmon decay, (2)reflection or refraction of electrons at each specimen boundary, (3)reentry of once-emitted electrons from the specimen surface into other parts of the specimen because of the structure of the surface and of the electric field above the surface, (4)electron collection field in a specimen chamber of the SEM produced by its detection system, and (5)electron trajectory toward the detector in the specimen chamber of the SEM. Equations used in the present simulation is in the following: (i)the Mott cross section for elastic scattering of electrons by an atomic potential, (ii)the Gryzinski equation for inner-shell electron ionization, (iii)the Lindhard dielectric function for conduction band electron ionization and bulk plasmon excitation, (iv)the Laplace equation to obtain the potential distribution in the specimen chamber, and (v) the equation of motion to trace

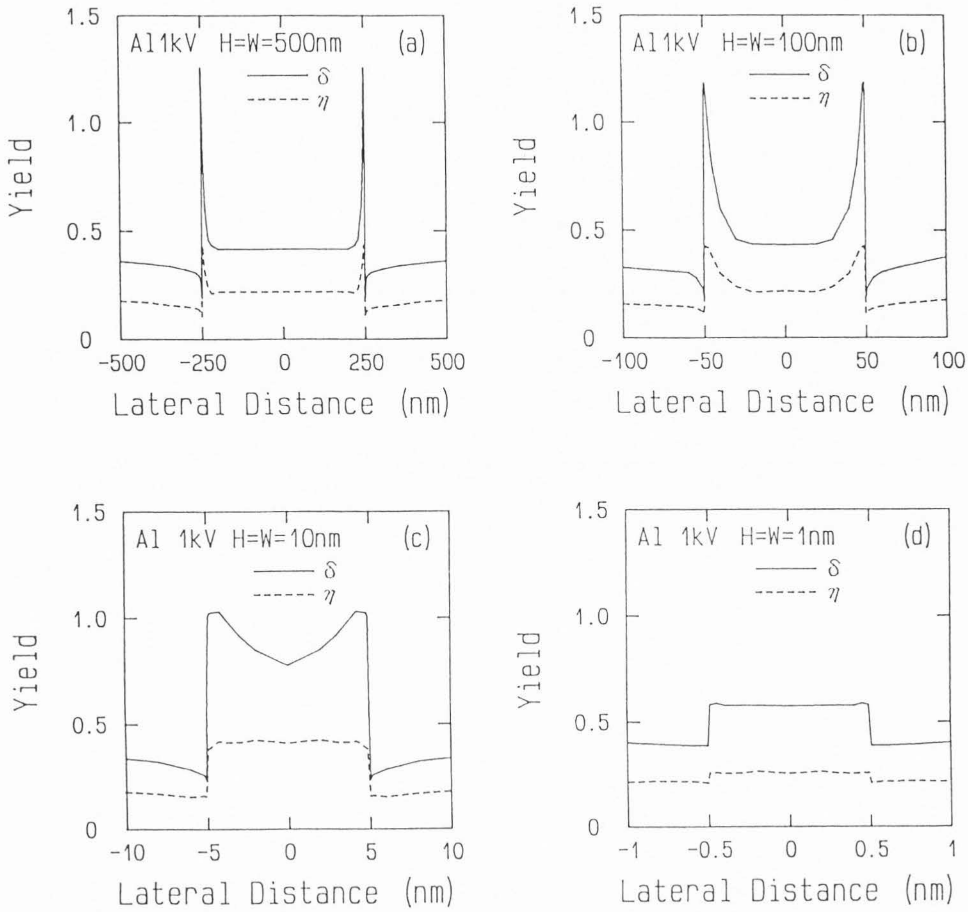

Fig.3. The calculated intensity profile of emitted SEs and BSEs from the rod pattern for 1 keV PEs. δ and η are for SE and BSE signals, respectively. (a)-(d) show the results for the sizes of H=W=500, 100, 10, and 1 nm, respectively.

electron trajectory within this electric field. Depending on the value of each total cross section, we choose one scattering process, and depending on the variation of its differential cross section, the scattering angle or energy loss of one simulating primary electron is determined by the Monte Carlo method. In this simulation every momentum and energy transfer at each electron collision is exactly taken into account, and the energy and the emitting angle of a secondary electron excited at a collision are precisely determined. Details of the model are described in other papers.[9-11] All signal intensities are expressed in terms of the yield, which is the ratio of the number of electrons emitted to the number of incident primary electrons (PEs). Every emitted electron whose energy is greater than 50 eV at the specimen surface is defined as a BSE, irrespective of its direction of motion. If the electron energy is less than 50 eV at the specimen surface, we define it as a SE. The surface topography studied here is a rectangular rod pattern on an infinite horizontal plane surface, and a rectangular groove pattern at the surface as shown in Figs.1(a) and (b), respectively. We study the intensity variation of electrons emitted from the pattern, as a PE beam scans across it along the broken line as illustrated in Fig.1. The specimen is assumed to be made of Al. The height (depth) and the width of the pattern are defined by the variables H and W, respectively.

Results and Discussions

An example of electron trajectories calculated by the present simulation is shown in Fig.2. Trajectories of six PEs incident at 0.5 keV and hot electrons excited by the PEs are simulated. All of the trajectories shown in the figure are either SEs or BSEs excited by PEs, and the trajectory of PEs in vacuum is not shown. It is seen that three electrons are coming out from the groove. The incident point of the PE is around the center of the bottom of the rectangular groove of depth H=100 nm and width W=50 nm. Because of the structure, electrons emitted from the bottom surface may reenter the side wall of the pattern and generate further hot electrons at the wall, then some of them may be reemitted from the wall. In this trajectory simulation, the electron collection field, made by the conventional

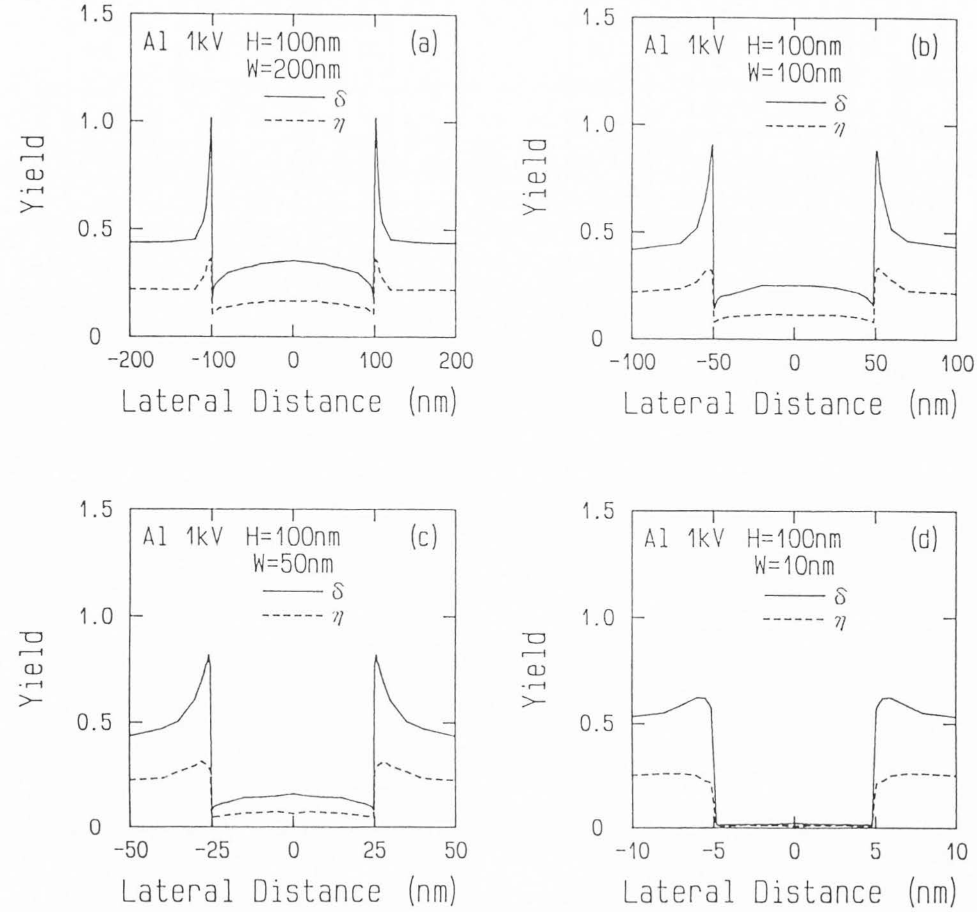

Fig.4. Intensity profile of emitted SEs and BSEs from the groove pattern for 1 keV PEs. δ and η are yields for SE and BSE signals, respectively. (a)-(d) show the results for the sizes of W=200, 100, 50, and 10 nm, respectively at H=100 nm.

Everhart-Thornley detector above the specimen surface, is considered. However, the region plotted here is so small that the curvature of the electron trajectory in the vacuum space of the groove is not obvious. By calculating large number of electron trajectories, we obtain statistical results. Although it is possible to take into account the effect of the detection field in the simulation as described above, since the influence of the field is not so large for a small topographic structure in the SEM, here, we present only intensity profiles of emitted SEs and BSEs from the specimen assuming no electric field is present above the specimen surface.

Intensity profile for the rod pattern

The profiles of emitted SEs and BSEs from the rod pattern are shown in Fig.3 for 1 keV PEs. Figures 3(a)-3(d) show the results for the sizes of H=W=500, 100, 10, and 1 nm, respectively. If the pattern width is large enough, the intensity profile shows a sharp rise at the edge, as is well known for the edge contrast. The intensity profile at the edge shows a wider distribution for the BSE signal than for the SE signal, then it is considered that the resolution of the SE signal is better than that of the BSE signal for 1 keV PEs. As the size H (=W) becomes less than 10 nm, the edge peak of the BSE signal becomes indistinct and shows almost a flat intensity at the top surface. The same situation occurs at H=W=1 nm for the SE signal. The decrease of the maximum intensity is mainly due to the decrease of the height of the pattern, which determines the surface area for the signal emission and a volume for hot electron multiplication.[11] If we look at this edge signal more in detail, there is a displacement of the peak position of the signal from the position of the real edge of the rod. The displacement is around 0.5 nm for SEs and 2 nm for BSEs at 1 keV PEs, and it is 0.5 nm for SEs and 10 nm for BSEs at 3 keV PEs as given in the previous paper.[10] The displacement increases for BSEs with the increase of the PE energy, but it remains constant with the energy for SEs. Although the displacement is large and the profile is broad around its peak for BSEs, there is a very sharp intensity rise almost at the edge. If we amplify the difference between the signals at the top edge and at the bottom edge, to make it much larger than the noise level in the SEM system, it may be possible to get the BSE image with

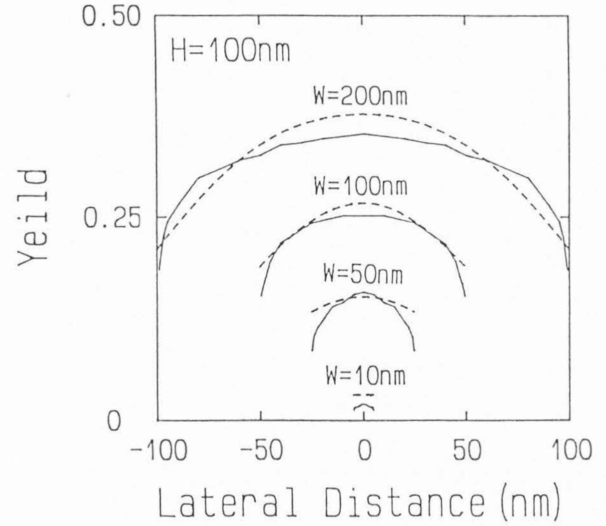

Fig.5. Variation of a signal intensity profile from the bottom surface of the groove pattern. A comparison is made between the results calculated by the direct simulation and those of the analytical model. The solid line is obtained by the direct simulation, and the broken line is obtained by the analytical model.

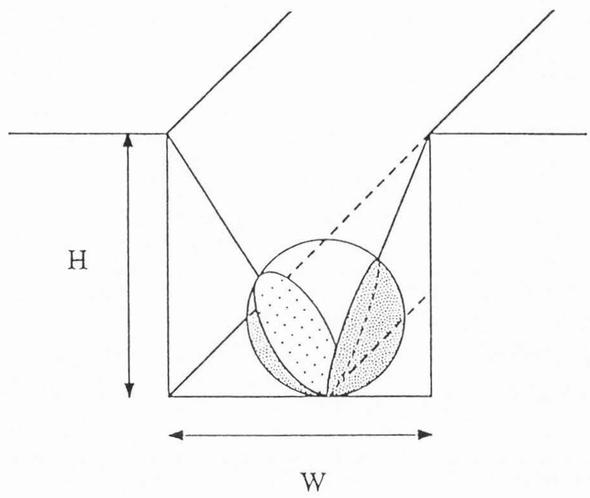

Fig.6. Analytical model introduced in the present study. The volume of the sphere is in proportion to the number of electrons emitted from the surface, and it indicates the signal intensity at the surface. A signal intensity from the groove is in proportion to the non-shaded volume of the sphere.

very high resolution. Then the resolution may be practically comparable with that of SEs. At the same time, since a higher PE energy gives an almost flat profile at the top surface for the BSE signal, it should be possible to observe the BSE image of the rod pattern without large edge effects. The high intensity rise close to the edge, as found in the SE image, frequently hides fine structures around the top edge.

Intensity profile for the groove pattern

Figure 4 shows the intensity profile for the groove pattern. A series of the figures are for different aspect-ratios (H/W). The depth of the groove is 100 nm, and the width varies from 200 nm to 10 nm. As the width decreases, the probability for electrons in the groove to escape through the opening decreases, and the signal that coming from the bottom decreases. Consistent with this fact, the peak height of the signal intensity at the top edge also decreases with the decrease of the width. This kind of groove pattern is frequently called a trench pattern by manufacturers of semiconductor devices. When this pattern is used for making a trench capacitor, the sizes of the width and of the height directly determine the value of the capacitance. It is an important process to measure and to inspect the size and the quality of the groove pattern. Because of its small size, SEM is most commonly used to examine the pattern. Then, the problem is the visibility and the quantification accuracy. As we use the SEM, the question is : (1)is it possible to inspect the surface quality at the bottom and the side wall of the trench?, (2)how can we determine the real top edge and the bottom edge from the intensity profile of the SE and the BSE signals?, (3)is it possible to reconstruct the real structure in 3D from the SEM image?, (4)what determines the resolution limit of the SEM?. It should be quite useful to provide theoretical values for the intensity profile by the simulation.

One interest, in inspecting the groove, is how the signal from the bottom varies with the aspect-ratio (H/W). Figure 5 shows only the variation of the signal intensity profile from the bottom surface. The maximum is found at the center of the bottom surface. This variation may be explained by the acceptance of the signal, and this variation may be obtained by a simpler treatment. Here, we assume a simple analytical model as follows: The angular distribution of electrons emitted from the bottom surface agrees with a cosine law, and electrons which hit the side wall after the emission from the bottom will be absorbed and no reemission occurs. Then, a signal intensity emitted from the groove can be calculated from the volume of the not-shaded-part of the sphere put on the bottom surface, as shown in Fig.6. Here, we intend to apply this model to both SE and BSE signals considering a general aspect of electron behavior. The volume is in proportion to the number of electrons going through the opening of the trench. The whole volume of the sphere is in proportion to the number of electrons emitted from an infinite plane surface, and it indicates the signal intensity far outside the trench. If we normalize the non-shaded volume by the whole volume of the sphere, we obtain the normalized intensity profile at the bottom. The profile calculated here depends only on the aspect-ratio of the trench. A comparison is made between the results of this analytical model and those calculated by the direct simulation, and it is shown in Fig.5. The two profiles show fairly good agreement. If one does not mind this slight difference in an application to the electron beam measurement, it may be sufficient to use this analytical model.

Figure 5 shows that even if the aspect-ratio is 2 (W=50 nm) or 10 (W=10 nm), the SE yield at the center of the bottom surface is 0.145 or 0.021, respectively. If this amount of signal is much larger than the noise level of the signal detection and the subsequent amplification systems, it is possible to find the signal variation at the bottom. If there are further topographic structures at the bottom, the signal intensity is much higher because of the edge peak of each feature. It is possible to estimate roughly its yield from the results obtained above. If we assume that there is a small rod pattern or a groove pattern superimposed on a large groove pattern, the final signal intensity of the edge peak of the small pattern can be calculated by a convolution of the yield of the edge for the small pattern and the yield of the bottom surface of the groove.

Conclusions

A direct simulation is developed considering hot electron generation, its propagation in the specimen, and its emission from the surface. Using this simulation, a topographic contrast found in the SEM is quantitatively discussed. We quantify characteristics of the edge contrast for SEs and BSEs. The intensity profile at the bottom of the groove pattern obtained by the direct simulation can be roughly approximated by a simple analytical model. We discuss the visibility of the bottom of the groove pattern by the SEM. This simulation makes it possible to quantify various parameters in the application of the SEM to the electron beam measurement.

References

1.Adesida I, Shimizu R, Everhart TE (1980). A study of electron penetration in solids using a direct Monte Carlo approach. J. Appl. Phys., 51, 5962-5969.

2.Bindi R, Lante'ri H, Rostaing P. (1980). A new approach and resolution method of the Boltzmann equation applied to secondary electron emission, by reflection from polycrystalline aluminium. J. Phys. D13, 267-280.

3.Cailler M, Ganachaud JP. (1990). Secondary Electron Emission from solids. I. Secondary Electron Spectroscopy. Scanning Microsc. Suppl. 4, 57-80, II. Theoretical Description. Scanning Microsc. Suppl. 4, 81-110.

4.Ding Z-J, Shimizu R. (1989). Theoretical study of the ultimate resolution of SEM. J. Microsc. 154, 193-207.

5.Ganachaud JP, Cailler M. (1979). A Monte-Carlo calculation of the secondary electron emission of normal metals. Surf. Sci. 83, 498-530.

6.Ichimura S, Aratama M, Shimizu R. (1980). Monte Carlo calculation approach to quantitative Auger electron spectroscopy. J. Appl. Phys., 51, 2853-2860.

7.Joy DC. (1984). Beam interactions, contrast and resolution in the SEM. J. Microsc. 136, 241-258.

8.Kotera M. (1989). A Monte Carlo simulation of primary and secondary electron trajectories in a specimen. J. Appl. Phys. 65, 3991-3998.

9.Kotera M, Ijichi R, Suga H, Wittry DB. (1990). A Simulation of Electron Scattering in Metals. Jpn. J. Appl. Phys., 29, 2277-2282.

10.Kotera M, Fujiwara T, Suga H, Wittry DB. (1990). A Simulation of the Topographic Contrast in the SEM. Jpn. J. Appl. Phys., 29, 2312-2316.

11.Kotera M, Fujiwara T, Kanai N, Suga H. (1991). Theoretical Evaluation of a Topographic Contrast of Scanning Electron Microscope Images. Jpn. J. Appl. Phys., 30, 3287-3293.

12.Luo S, Joy DC. (1988). Monte Carlo calculations of secondary electron emission. Scanning Microsc. 2, 1901-1915.

13.Murata K, Kyser DF, Ting CH. (1981). Monte Carlo Simulation of Fast Secondary Electron Production in Electron Beam Resists. J. Appl. Phys., 52, 4396-4405.

14.Reimer L, Stelter D. (1987). Monte Carlo Calculations of Electron Emission at Surface Edges. Scanning Microsc. 1, 951-962.

15.Shimizu R, Kataoka Y, Ikuta T, Koshikawa T, Hashimoto H. (1976). A Monte Carlo approach to the direct simulation of electron penetration in solids. J. Phys. D9, 101-114.

16.Takeuchi S, Nakamura H, Watakabe Y, Mimura R, Aihara R, Thompson WB. (1989). A study of electron beam metrology using computer simulation. J. Vac. Sci. Technol. B7, 73-78.

Discussion with Reviewers

R. Bindi: What is the reason why you keep H=W for the rod pattern?

Authors: One reason is that a big difference between H and W is not realistic for a discussion of the ultimate resolution of the SEM. The other reason is for simplicity.

R. Bindi: How do you explain the displacement of the peak position of the signal ; its variation for BSEs with the PE energy and the fact that it remains constant for SEs?

Authors: The reason of the displacement is discussed in detail in reference 11. Here, we describe it briefly. There are three planes where electrons can emit near the edge, that is, the top surface, the side wall and the bottom surface. Electron signal intensity is obtained by the sum of electrons coming from all these three planes. If PEs are incident at the top surface far away from the edge, electrons can emit only from the top surface. If PEs are incident at the top surface close to the edge, some of the scattered electrons in the specimen can emit from both the side wall and the bottom surface. Accordingly, the number of electrons emitting from the top surface decreases. If PEs are incident at the bottom surface close to the edge, since 3/4 of space is filled by the specimen, only electrons going toward the remaining 1/4 of space can emit from that opening of the specimen. Depending on the PE energy, electron penetration is different, and this dependence modifies the above argument. Summing over the electrons emitted from these three planes, the peak of the intensity is generated.

The reason why the peak position for the BSE signal moves and the one for the SE signal does not, depending on the PE energy, can be explained as follows: As the PE energy increases, the path length of BSEs in the specimen increases, and the peak of the signal appears farther from the edge. On the other hand, the SE energy distribution does not depend on the PE energy, and the path length is independent of the PE energy. Then, the phenomenon pointed out can be attributed to the fact that there are two peaks in energy distribution of emitted electrons from the specimen. That is, one is a peak for BSEs at a high energy region, and the other is a peak for SEs at around 1-2 eV.

L. Balk : To use the analytical model, it is necessary to normalize the volume of a sphere to the number of electrons emitted from the plane surface. How should the size of this sphere be chosen in relation to the height and width of the groove?

Authors : As we can see the difference in Fig.5, the tendency of the two curves is different. In this sense the present normalization in the analytical model is not good enough. We will make it clear the reason of this disagreement quantitatively in future.

S. Ichimura : Can the present results and the simple analytical model be applied to a substrate used for making a trench pattern (SiO_2/Si)?

Authors : Since this analytical model does not depend on a material of the groove but obtained only by its geometry, it is applicable to any system. However, in the system of SiO_2/Si, SiO_2 may charge up during electron irradiation, and this is not intended in the model. It is not intended in the present direct simulation, too. In the present simulation, the material is Al, and if we want to get a result for Si, we have to calculate from the beginning. The charging up of SiO_2 may be treated by some other simulation model.

R. Bindi : Could you comment the effect of the detection field?

L. Balk : The analytical model neglects the electron collection field of the electron detector used in a SEM. Can you estimate up to which width and height this simplification is valid?

Authors : For a rod pattern, almost all emitted SEs from the pattern will be collected by the detector, then, it is not necessary to take account of the field for a SE intensity. Only the problem of this neglect may be in a treatment of emitted electrons from an edge flying toward other surface, but these electrons will not contribute much to the result. Then, incomplete collection of electrons shows some effect of the detection field. For example, for a BSE intensity profile if the detector is set on the right side, BSEs emitted toward the right will be collected more easily than those emitted toward the left. If the detection field is strong, collection of BSEs will be better. For a groove pattern, since we are considering a relatively small pattern, the electric field will not immerse in the groove, and electron trajectories in the groove are not influenced so much. After they emit from the groove, all of them will be detected, and it is not necessary to consider the field.

L. Balk : Is it possible to apply the analytical model to groove patterns with non-vertical walls or have reflections of emitted electrons on the tilted groove walls to be taken into account?

Authors : This is not considered yet. We are producing a simulation program considering groove patterns with non-vertical walls. It will be compared with the results of the analytical model in the near future.

S. Ichimura : Isn't it necessary for quantitative discussion of a topographic contrast to consider a size of a primary electron beam? Are all results the same even if primary beam size is taken into account?

Authors : The influence of the PE beam diameter is discussed in detail in reference 11. Here, we describe it briefly. If PEs are incident at a very wide plane surface, the intensity is not dependent on the beam size. If there are edges or some structures on the surface, each individual intensity profile should be convoluted by an electron density distribution of the PE beam. There is a displacement between peak position of the edge profile and the real edge. The peak position of the signal is always found at the top surface of the edge pattern. The displacement increases with the increase of the beam diameter. The increase of the displacement does not show a monotonical dependence on the PE energy. The dependence for SEs is different from that for BSEs.

S. Ichimura : Your use of term "quantitative" may be incorrect and you mean "qualitative". Since the accuracy of the SE and BSE yield estimated by the calculation is not proven by comparison with experiments.

Authors : Experimental data are always real, but they suffer from all kinds of inaccuracy caused by noise, interference, etc. in their acquisition processes. In this sense, the experiment is not always quantitative. The term which is inherent in the signal production mechanism should be taken into account, but the term which depends on the machine should be useless. Numerical calculation can include quantitatively some particular mechanism of producing the signal, and show clearly the amount of the contribution to the final results. In this sense, the calculation gives us a quantitative idea, and this can help us for a further understanding of the experimental results quantitatively. We have tried to verify our calculated results by an agreement between experiment and our result for several physical quantities (e.g. SE energy distribution [9] and yields of SE and BSE at a semi-infinite plane specimen [3]. We do not think they are enough, and it should be necessary to refine the calculation model in many aspects to see a quantitative agreement with experimental results.

F. Hasselbach : What is the computing time for get-

ting, e.g., the result given in Fig.3 (a)? Is it possible to do these extensive calculations on a PC?
Authors : Figure 3(a) is constituted by about 50 data points. The number of incident PEs calculated in the present simulation is 10,000. It takes about 20 minutes by a big computer (FACOM VP-30E; 220 MFLOPS) to calculate for each point. Assuming that PC has an ability of one MFLOPS, 220 x 20 x 50 =220,000 minutes should be necessary to obtain the figure, and it is not practical to get it by PC.

F. Hasselbach : With a state of the art field emission SEM at least the SE yield curves given in Fig.3(a), (b) and 3(c) could be proven to a high degree of accuracy experimentally. Do you plan to make such tests or do experimental results exist in the meantime?
Authors : It is very meaningful to compare our results with experimental data. However, we have not had a chance to do that, and we would like to do it in the very near future.

J.P. Ganachaud : Could you indicate which kind of improvements the direct simulation method is able to bring compared to simpler models in a theoretical analysis of the surface topography?
Authors : A major difficulty for the simpler model is the treatment of a behavior for low energy electrons. Using a direct simulation, we can trace every trajectory of electrons for all energy ranges in a real space. It is possible for direct simulation to consider some particular mechanism of producing the signal quantitatively, and to show clearly the amount of the contribution to the final results. For example, the direct simulation is more reliable in a discussion of the ultimate resolution of scanning electron microscopy, and also in order to get a data-base for the three dimensional reconstruction of the surface topography from the SEM image contrast. Furthermore, as a future study with the SEM, in order to evaluate a spectroscopic imaging by the SEM, for example, angle resolved or energy resolved imaging of the surface topography, the direct simulation brings much more useful informations than the simpler treatment. We expect that the direct simulation will help us to understand the experimental results quantitatively.