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나노 패터닝을 위한 이온빔-고체 상호작용 분석

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Analysis of Ion Beam-Solid Interactions for Nano Fabrication

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ABSTRACT

Ion beam processing is one of the key technologies to realize maskless and resistless sub 50nm nano fabrication. Unwanted effects, however, may occur since an energetic ion can interact with a target surface in various ways. Depending on the ion energy, the interaction can be swelling, deposition, sputtering, re-deposition, implantation, damage, backscattering and nuclear reaction. Sputtering is the fundamental mechanism in ion beam induced direct patterning. Re-deposition and backscattering are unwanted mechanisms to avoid. Therefore understanding of ion beam-solid interaction should be advanced for further ion beam related research. In this paper we simulate some important interaction mechanisms between energetic incident ions and solid surfaces and the results are compared with experimental data. The simulation results are agreed well with experimental data.

Key Words : Ion Beam(이온빔), Sputtering(스퍼터링), Re-deposition(재증착), Diffuse Emission(확산방출), Backscattering(후방산란),

1. INTODUCTION

The use of ion beam technologies in the field of mechanical engineering has recently increased, because of the ability to fabricate sub 50nm structures with focused ion beams (FIB). In addition Micro/Nano Electro-Mechanical Systems (MEMS/NEMS) and Micro Opto-Electro Mechanical Systems (MOEMS) are potential promising applications in the fields of mechanics and electronics. Nevertheless, ion beam nano fabrication has some limitations, surface swelling in the low ion dose regime, precipitation of incident ions, damage formation, and re-deposition effect due to sputtered atoms. In recent years, many studies reported that the re-deposition effect is the most outstanding unwanted effect to avoid or control in fabricating micro and nano devices.

In most cases ions that bombard surfaces originate from plasma or an ion beam. Upon bombarding a surface, the incoming ions may be reflected, stick or be adsorbed, scattered, eject or sputter surface atoms, or get buried in subsurface layers (ion implantation). Surface heating, chemical reactions, atom mixing, and alternation of surface topography are other manifestations of ion bombardment. We have developed the 2D FIB simulation software AMADEUS (Advanced Modeling and Design Environment for Sputter Processes), which is capable of simulating sputtering and re-deposition. Sputter yields and sputtered atoms distributions are basic inputs for AMADEUS. Analysis of ion beam-solid interactions gives us a credible sputter yield and sputtered atoms distribution.

During half a century, several efforts have been made to predict ion-solid interactions by computational simulation. One of the Monte Carlo simulation software packages, SRIM (The Stopping and Range of Ions in Matter)[1], has been widely used for predicting the sputtering yield for many different ions at a wide range of energies. IMSIL (Implant Simulator)[2] and TRIDYN (TRIM.SP Dynamical)[3] are other famous software packages. TRIDYN is capable of simulating the dynamical changes of the target during sputtering, while IMSIL may also take the crystal structure of the target into account.

In this work, simulations have been done with TRIDYN, IMSIL and SRIM. The results are compared with experimental data. It is a good solution to understand

and overcome limitations of nano fabrication. Fig. 1 shows simulation typical results of the ion trajectories and recoils.

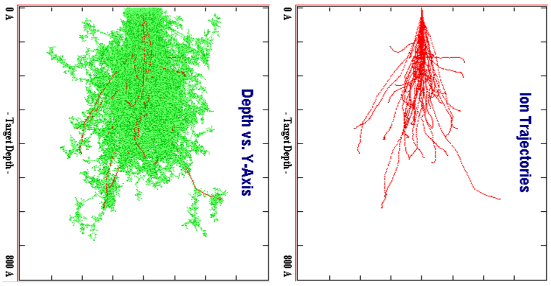

Fig. 1 Recoils (a) and trajectories (b) of 30keV Ga$^+$ ions, incident into silicon substrate (calculated by SRIM).

2. SPUTTERING

2.1 Sputtering Yield

Atomic bombardment of solids leads the removal of atoms from the target into free space. When the ion impact initiates a sequence of collision events in the target that leads to the ejection of a matrix atom, we speak of sputtering. Since sputtering is the result of momentum transfer, Y mainly depends on incidence angle defined between the directions of ion incidence and the target surface normal. It is defined as

$$Y = \text{Sputtered atoms} / \text{Incident ion} \tag{1}$$

The yield is normally a function of many variables, including masses of ions and target atoms, ion energy, direction of incidence to the surface of the target, target temperature and ion flux. The sputtering yield Y is enhanced as the incidence angle increases until a maximum is reached between 70°-80° and dramatically decreases beyond 80° because most of the incident ions are reflected in high incident angle as shown in Fig. 2.

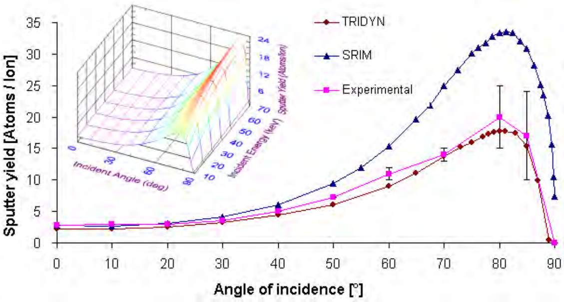

Fig. 2 Comparisons of sputtering yield between SRIM, TRIDYN and experimental data (30keV Ga$^+$ ions into silicon substrate) and sputter yield of silicon according to various incident angles and energies.

The results obtained from TRIDYN are much closer to the experimental data from the SRIM simulation. Generally, it is known that the sputter yield is greatly increased at certain value of energy. And it is as continuously increased as energy is increased, but the increasing rate is decreased. This is due to the increasing of implanted ion percentage. The inset of Fig. 2 shows the sputtering yield change as a function of various incident energies and Angles. The sputter yield for a number of metals and semiconductors as calculated by TRIDYN are entered in Table 1.

Table 1 Sputter yield of several ion species and substrates

Ion (Sub.)	Energy (keV)	Yield	Ion (Sub.)	Energy (keV)	Yield
Ga(Si)	30	2.6	Ga(Au)	40	15.7
Ga(Cr)	30-70	2.3	Kr(Si)	25	3.1
Ga(GaAs)	30	1.2	Kr(Au)	25	20
Ga(Al)	68	4.2	Kr(W)	22	4.1

2.2 Composition Change

The composition of target material at surface region is changed because of ion implantation. And the implanted ion is sputtered away by continuing ion bombardment. This effect is used to mix of two-or multiple-components atoms tend to mix causing both compositional and structural change the effect known as ion mixing. Table 2 shows that substrate composition is changed as the incidence angle is increased.

Table2 Composition changes of various ion and substrates

Ion	Sub.	Energy (keV)	Angle	% of Sub. Component
Ga	Si	30	0	70
			30	75
			60	90
			80	95
	Al	30	0	71
Ga	Ta	30	0	83
Ar	Si	30	0	80

3. EMISSION OF SPUTTERED PARTICLES

As a result of ion bombardment, charged particles (e.g., electrons, ions), neutrals, and photons of varying energies and abundances are emitted from the surface. Contained within them is a rich source of compositional and structural information on surface properties. Rutherford Backscattering (RBS) and secondary ion mass spectroscopy (SIMS) are used to detect and analyze these emitted signals. But in etching and sputtering processes, sputtered atoms are one of the notorious problems, which cause re-deposition in side- and bottom surfaces of groove.

3.1 Angular Distribution of Sputtered Particles

Normally, the angular distribution of emitted atoms modeled by $\cos^n\theta$, known as cosine emission low as is illustrated in Fig. 3.

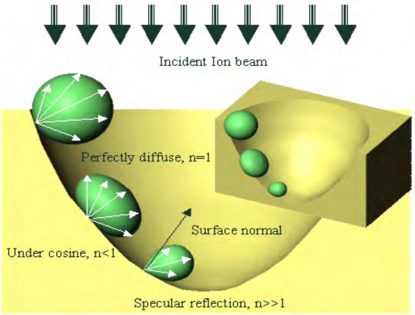

Fig. 3 Illustration of angular distributions of sputtered atoms.

Sputtered atoms often exhibit an ideal, diffuse angular distribution, being sputtered away at many angles centered on the surface normal. The distribution may in fact be more sideways, described by an "under cosine" distribution (where n is less than 1 in a $\cos^n\theta$ distribution), in some cases though they can exhibit a specula distribution, being sputtered at just a few angles near an angle opposite that of the incident angle.

But a large number of experimental observations indicate that the emitted atom distribution cannot be modeled with cosine emission rule but with heart shape distribution function. And according to incident angle θ, the distribution function is not axis (2D) or rotational (3D) symmetrical.

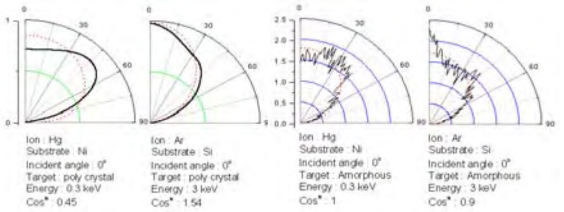

Fig. 4 Polar plot of simulated and experimental sputtered atoms distributions and index n of cosine low, the red dotted lines at each plot indicate the cosine shape according to n. (Left two plots are experimental and right two are simulated data, experimental data are from Ref. [4])

In this work, the sputtered atoms distribution calculations were done mainly with IMSIL because SRIM cannot simulate and predict the specula reflection caused by glancing incident ions and crystallographic effects in sputtered atoms emission. After a series of simulations, results are compared with experimental data only in case of normal incidence. The simulation results are a little bit different in cosine index n, by well matched in shape as shown in Fig. 4. Simulation results are well fitted by $\cos^n\theta$ with optimized index n especially in case of high-energy region, normally 1~50keV, as is used in FIB processing. In this region is normally described by perfect diffuse with n=1 or a little bit higher to 2 as listed in Table 3.

And studies of ion bombarded single crystal reveal that atom emission reflects the lattice symmetry. In case of FCC metal it has been observed that atoms are preferentially ejected along the [110] direction, but ejection in [100] and [111] directions also occurs to lesser extends. For BCC metals [111] is the usual direction for atom ejection. This is the crystallographic effect in sputter process [5].

Table 3 Comparisons of simulated and experimental data of cosine index n (from Ref. [4]).

Ion	Substrate	Energy (keV)	Exp.	Sim.(IMSIL)
Hg	Pt	0.25	0.55	0.9
Hg	Fe	1	0.89	1.3
Hg	Fe	0.75	0.54	1.0
Ar	Au	300	1.49	1.5
Ar	Ag	5	1.23	1.3

3.2 Refraction of sputtered Atom Emission

When sputtered atoms are ejected, they have to overcome the surface binding energy, which is called surface potential and can be assumed isotropic or planar. This potential causes the energy loss during ejection of atoms. In the planar potential model the sputtered atoms also experience refraction. The final emission angle is changed as a result of the planar potential. This effect is more pronounced for low energies and large emission angles of the sputtered atoms [5]. Fig. 5 shows the simulation results. The incidence direction is from the left to the center of plots. At incidence angle of 70°, the distribution is more preferential panels (b) and (d). And in case of (c), comparably rare particles are observed in the center region, it leads to a heart shape distribution of the sputtered atoms. The atoms, which experience the planar potential, change their direction somewhat. As a result of the refraction of the atoms, the distribution is spread wider then before. This can be seen by comparing (a) and (b) with (c) and (d) in Fig. 5.

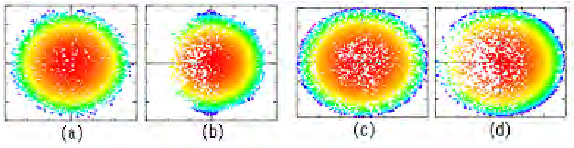

Fig. 5 Top views of simulated sputtered atoms distribution gathered on half sphere. 30keV Ga ion incident into Si substrate. (a) and (c) are normal incident case, (b) and (d) are incident at 70°. The first two((a) and (b)) show the distribution without refraction and (c) and (d) show after the refraction (calculated by IMSIL).

4. BACKSCATTERING

4.1 Reflection Yield and Angular Distribution of Backscattered Particles

When energetic ions are incident into a substrate, some of them are reflected back towards the substrate as neutrals, retaining much of their initial ion energy. And some ions penetrate into substrate until they loose their energy or are scattered backwards.

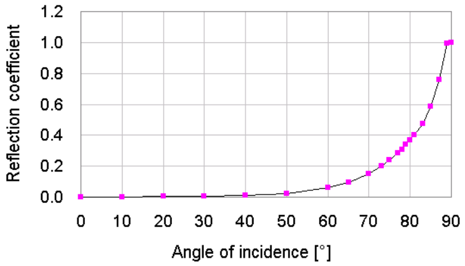

Fig. 6 Reflection coefficients according to the angle of incidence for bombardment of 30keV Ga^+ ions on Si substrate (calculated by IMSIL).

These reflected and backscattered particles cause the 2nd sputtering on opposing surfaces. Therefore, unlike the sputtered particles, which usually have low energies, the reflected and backscattered particles' energy and angular distribution are important. The particle reflection coefficient R_N is defined as:

$$R_N = N_{bs} / N_p \quad (2)$$

where N_p is number of projectiles, N_{bs} is the number of backscattered projectiles. From our simulations we find that most of the reflected ions keep their energy and are reflected or backscattered by specula reflection. The reflection coefficient is greatly increased, as incidence angle is increased. And approaches almost 1 as the incidence angle approaches 90° (in Fig. 6).

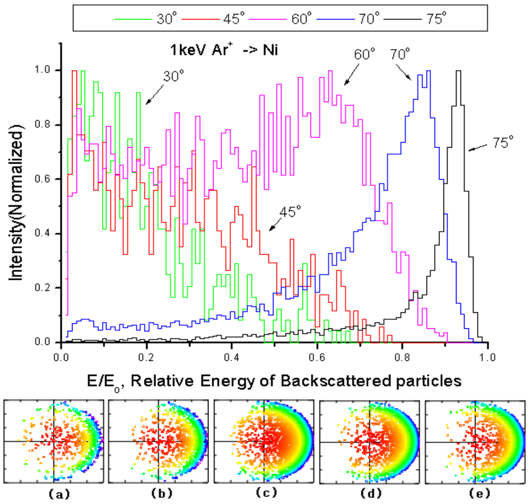

Fig. 7 Calculated data of energy distributions and top view of backscattered particles distributions under various incidence angles, 1keV Ar+ ion into Ni substrate (calculated by IMSIL).

The energy distribution of backscattered particles changes dramatically when the angle of incidence θ is varied. As can be seen in Fig. 7, for a 1 keV Ar bombardment on a Ni substrate, the energy distribution has a maximum at low energy area for $\theta < 45°$, whereas for $\theta > 45°$ a strong peak develops near the incidence energy.

5. CONCLUSION

Understanding of ion-solid interactions is fundamental in ion beam induced micro- /nano fabrication. Also, sputtering and re-deposition are the key mechanism in ion beam direct fabrication. Sputter yield Y, composition change during ion bombardment, distribution of sputtered particles, reflection coefficient R_N, energy and spatial distribution of backscattered particles are simulated and analyzed in this work.

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