MOLECULAR DYNAMICS SIMULATION ON EXCIMER LASER ANNEALING PROCESS FOR ULTRA SHALLOW JUNCTION FORMATION

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ABSTRACT

The molecular dynamics method is employed for a very thin film system of which the thickness is within 100 nm under excimer laser irradiation in order to study the optimal pulse duration and shape of the laser as well as to know the dominant physical parameters of the excimer laser annealing process. For the laser energy absorption, the potential energy between atoms is assumed to change according to the laser intensity profile of the excimer laser pulse. The melted depths related to the pulse duration showed to be similar to the junction depth related to the duration time of laser pulse in the experimental results. The laser energy density exceeded the lowest light intensity of melting is one of the dominant physical parameters which affect on the melted depths in the simulation results. The number of lattice defects at constant region is discussed on the laser pulse characteristics such as laser duration time and energy density.

INTRODUCTION

Laser annealing process combined with low energy ion implantation has been studied for electronic devices having ultra shallow junction depth as well as low sheet resistance [1-3]. The junction leakage caused by residual defects and difficulties in integrating process of device fabrication still remain as problems to be solved for its practical uses. Previously it is noted that the sheet resistance and junction depth are affected by laser pulse duration [1,2]. The irradiation time and shape of laser pulses are important factors to control the heating and cooling rates for the annealing process. In such laser annealing process, the computational simulation is one of the most useful tools to predict the optimal laser-pulse duration and shape for ultra shallow junction formation. It is not sure that the Lambert-Beer's law and Fourier's law can be applicable for such a thin layer material within 100 nm thickness. Moreover, since the scale of residual defects in the thin film corresponds to the size of molecules, it is very difficult to know such information in molecular scale from continuous equations. On the other hand, the molecular dynamics method can be applied to various thermal and heat transfer phenomena from molecular to nanometer scales [4,5,6,7,8]. As for the interaction between light and matter, the quantum molecular dynamics method should be applied for understanding the thermal energy absorption by light irradiation [7,8]. Calculations of the quantum molecular dynamics simulation shows that the light energy absorption in visible and ultraviolet ranges should be associated with changes in the potential energy between atoms [7,8]. In the present study, the molecular dynamics method is employed for a very thin film system of which the thickness is within 100 nm under excimer laser irradiation in order to study the optimal pulse duration and shape of the laser as well as to know the dominant physical parameters of the excimer laser annealing process. For the laser energy absorption, the potential energy between atoms is assumed to be changeable according to the laser intensity profile of the excimer laser pulse.

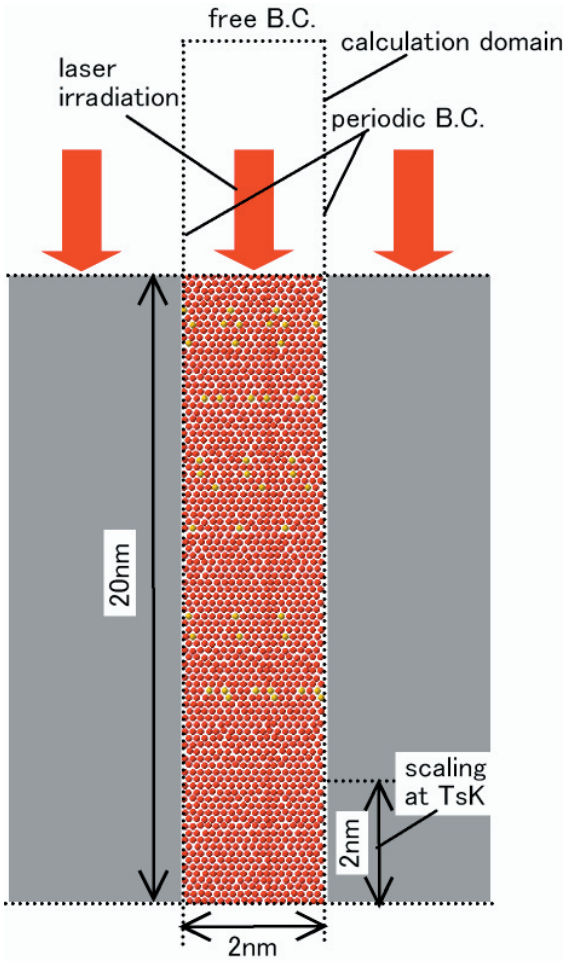


Fig.1 Calculation system for molecular dynamics simulations of laser annealing process.

NUMERICAL METHOD

Molecular Dynamics Simulations

Figure 1 shows a two-dimension calculation system and boundary conditions employed in the present study. The size of calculation domain is about 2 nm width and 20 nm depth in the horizontal and vertical directions. The periodic boundary condition is employed so as to simulate a semi-infinite thin film system in the horizontal direction. Temperature in a lower region within 2 nm distance from the bottom is scaled at T_s K during laser annealing simulations. The calculation system in a unit cell is composed of 900 atoms of which physical parameters correspond to silicon and phosphorus atoms shown in Table 1. 25 phosphorus atoms are included in a unit cell as impurity atoms. Newton's equations of all atoms in a unit cell are integrated numerically with an interval time of 2.5 fs. Lennard-Jones 12-6 potential functions and Lorentz-Berthelot combination rules are used as interatomic potential for the purpose of qualitative understanding atomic behavior under excimer laser annealing process. The temperature of the whole calculation system is scaled at T_s K during several nanoseconds as an initial condition. Total calculation time for laser annealing simulations is from 12.5 to 50.0 nanoseconds.

Modeling of Laser Pulse Absorption

Wavelength of KrF excimer laser beam used in the experiments [1,2] is 248 nm in ultraviolet ray range. Electrons of atoms in a thin film should be excited by excimer laser irradiation and energy absorption. By the energy absorption of ultraviolet laser beam, the potential energy functions between atoms in a thin film should be changeable according to the laser intensity profile of the excimer laser pulse. Moreover, the laser light should be attenuated through the thin film. In the present study, energy parameters in Lennard-Jones interatomic potential functions are assumed to be changed according to the laser intensity profiles. The magnitude of light excitation intensity is assumed as a linear function of the depth of thin film. Magnitude of the light attenuation and potential energy change between atoms in thin films are determined by the experimental results of the junction depth which is assumed to correspond to the melted depths of the molecular dynamics simulations. Simple triangle pulses shown in Fig.2 are employed as the laser pulse shape. These triangle laser pulses are modified as the transient waveform of laser beams observed in the experimental results [1,2]. The laser pulses have two important parameters of the duration time t_B and peak intensity I_A. t_A is defined at the peak of laser intensity and kept as 7ns in the present study. Energy density E_1 of a laser pulse can be calculated by the area of the triangle in Fig.2. Full-width half-maximum (FWHM) of a laser pulse corresponds to the half value of the duration time t_B. Table 2 shows FWHM, I_A and E_1 employed in the present study.

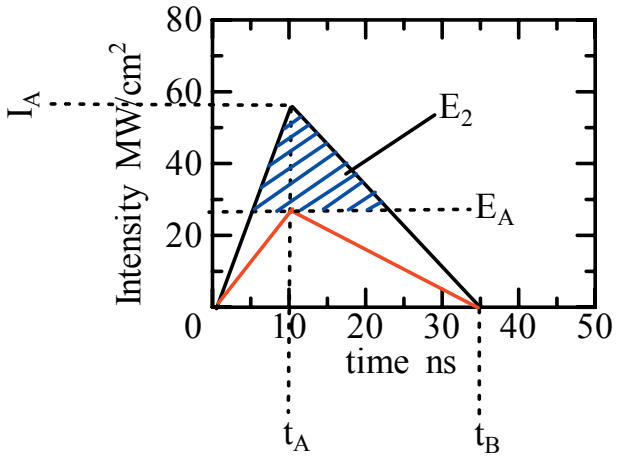


Fig.2 Triangle laser pulse model and physical parameters employed in the present study.

	m 10^{-26}kg	σ A	ε 10^{-20} J
Si	4.664	2.0936	1.6250
P	5.143	1.9689	1.0465

Table 1 12-6 Lennard-Jones potential parameters.

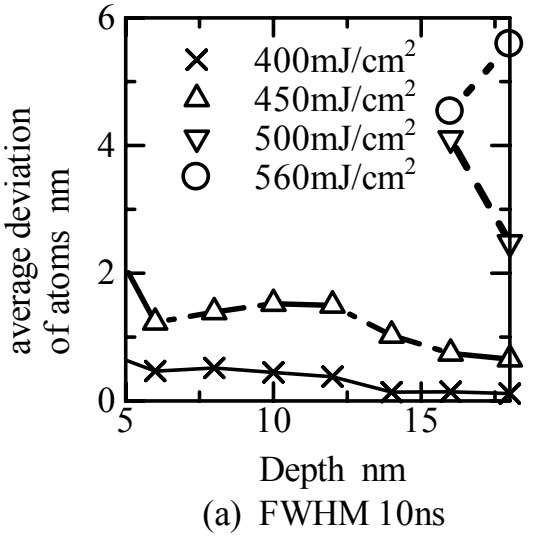
cases	FWHM ns	I_A MW/cm^2	E_1 mJ/cm^2
a-1	10	40	400
a-2	10	45	450
a-3	10	50	500
a-4	10	55	560
b-1	18	30	540
b-2	18	35	630
b-3	18	40	720
b-4	18	45	810
b-5	18	50	900
b-6	18	55	990
c-1	33	50	1650

Table 2 FWHM time, peak intensity I_A and energy density of laser pulses employed in the molecular dynamics simulations.

RESULTS AND DISCUSSIONS

Atomic Motions in Thin Films

Figure 3(a) shows the effects of laser energy density E_1 on the average deviation of atoms in thin films in the case of FWHM 10 ns. The average deviation of atoms is calculated by trajectories of neighboring 100 atoms in depth during 12.5 ns. The average deviation of atoms increases with the increase of laser energy density at the same position in depth. In the case of the same energy density, the average deviation of atoms deceases at deeper positions due to light energy decay. When the laser energy density is 500 and 560 mJ/cm^2,



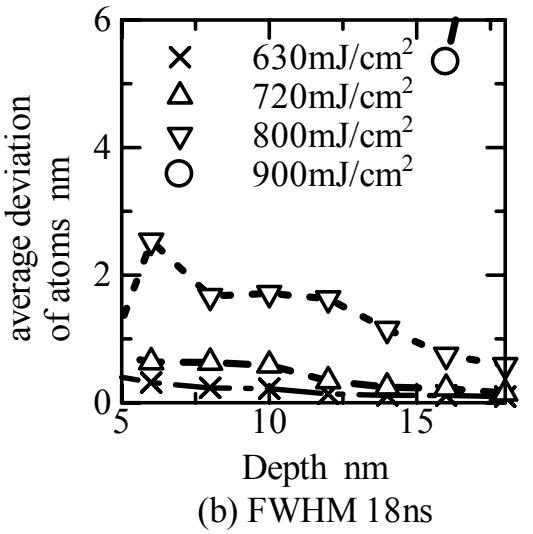


Fig.3 Averaged atomic deviation at film depth points in the cases of FWHM 10 ns and 18 ns with various laser energies.

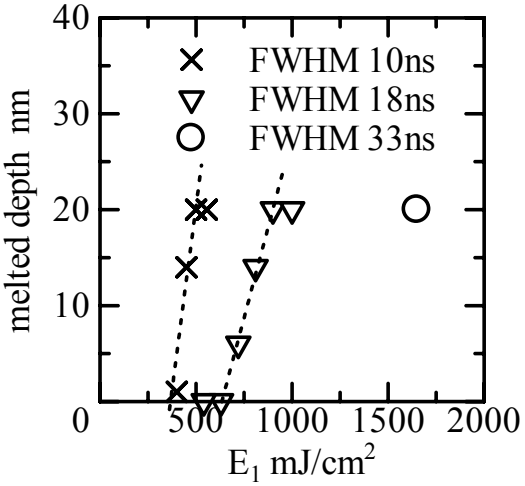


Fig.4 Melted depths in thin films with various laser energy density E_1 and FWHM of laser pulses.

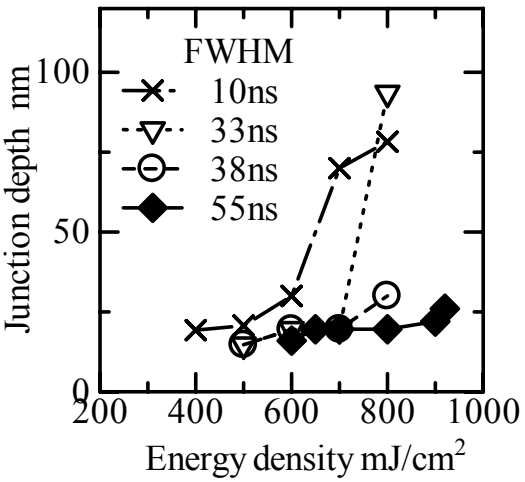


Fig.5 Junction depths in experimental results with various laser energy density and FWHM of laser pulses.

evaporation of atoms are observed in the vicinity of the film surface. Figure 3(b) shows effects of laser energy density E_1 on the average deviation of atoms in thin films in the case of FWHM 18 ns. Large energy density is necessary for melting of thin films in the case of FWHM 18 ns compared with the case of FWHM 10 ns. In Fig.3(b), evaporation of atoms is observed when light energy density is more than 800 mJ/cm^2. These relationships between atomic deviations and laser pulse such as energy density and FWHM of laser pulses are similar to the experimental results of the concentration of boron atoms in depth and laser pulse characteristics [1,2]. Hence, diffusion of impurity atoms into thin films will be related with the average deviation of atoms predicted by the molecular dynamics simulations. The melted depths depending on laser pulse characteristics can be estimated from the averaged deviation of atoms in depth in Fig.3.

Melted Depths of Thin Films

Figure 4 shows the melted depths of thin films with laser pulse characteristics. Because of a limitation of calculation domain in Fig.1, the maximum value of melted depths was 20 nm even when the thin films have melted completely or all atoms in thin films have evaporated. A thin film has melted in deeper regions with increase of the light energy density and decrease of FWHM of laser pulses. When the energy density of laser pulses are less than 400 mJ/cm^2 and 630 mJ/cm^2 in the cases of FWHM 10 ns and 18 ns, respectively, no melting of thin films was observed under laser pulse irradiation. E_A is defined as the maximum energy density when melting of thin films cannot be observed. Larger energy density is necessary for melting of thin films when FWHM of laser pulses are larger. Figure 5

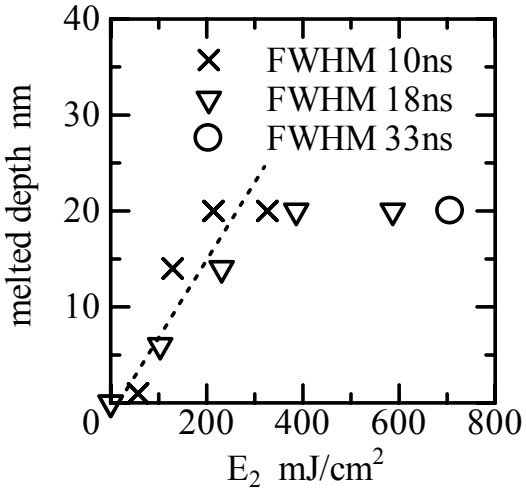


Fig.6 Melted depths in thin films with various laser energy density E_2 and FWHM of laser pulses.

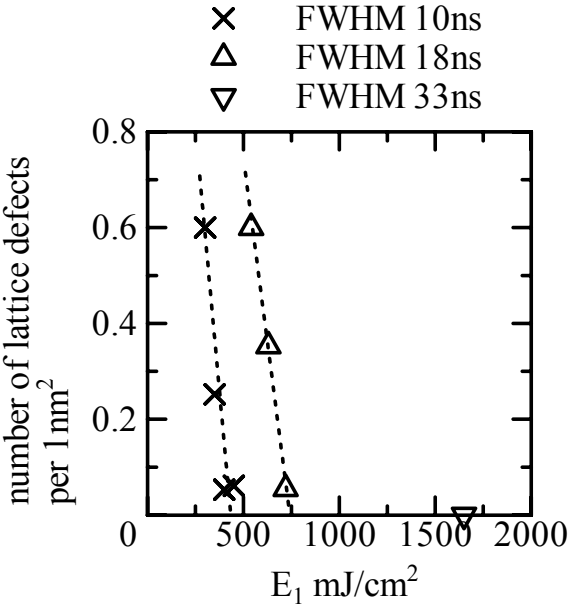


Fig.7 Number of lattice defects per 1 nm^2 with various laser energy density E_1 and FWHM of laser pulses.

shows effects of laser energy density and FWHM of laser pulses on junction depths in experimental results [1,2]. The samples were boron ion implanted Si (100) wafers irradiated with excimer laser under various conditions. The junction depths were evaluated from boron depth profiles measured by secondary ion mass spectrometry (SIMS). The melted depths related to the pulse duration in molecular dynamics simulations showed to be similar to the experimental results between the junction depths and the duration time of laser pulses qualitatively.

In order to evaluate a versatile physical parameter of laser pulses on melted depths, E_2 is defined as the laser energy density that exceeds minimum energy density for melting (E_A) as shown in Fig.2. Figure 6 shows how the magnitude of E_2 and FWHM of laser pulses affect on the melted depths in thin films. The melted depths were almost proportional to E_2 within a limitation of calculation domain 20 nm. The laser energy density exceeded the lowest light intensity in melting is one of the important parameters which dominate the melted depths in the simulation results.

Lattice Defects Formation in Thin Films

Figure 7 shows effects of energy density E_1 and FWHM of laser pulses on the number of lattice defects per 1nm^2 averaged over the whole calculation domain in Fig.1. The average number of lattice defects decreases with increase of laser energy density E_1 and the decrease of FWHM. These relationships between the density of lattice defects and light energy density are similar to those between sheet resistance and light energy density in experimental results [1,2] although the relationships between lattice defect density and sheet resistance is not obviously understood from physical point of view.

CONCLUSIONS

In the present study, the molecular dynamics method is employed for a very thin film system of which the thickness is within 100 nm under excimer laser irradiation in order to study the optimal pulse duration and shape of the laser as well as to know the dominant physical parameters of the excimer laser annealing process. For the laser energy absorption, the potential energy between atoms is assumed to be changeable according to the laser intensity profile of the excimer laser pulse. The light attenuation and potential energy change between atoms in the thin film are determined by the experimental results of the junction depth which is assumed to correspond to the melting depth of the molecular dynamics simulations. The melting depths related to the pulse duration showed the similar relationships to those between the junction depth and the duration time of laser pulse in experimental results. The laser energy density exceeded the lowest light intensity in melting is one of the significant factors dominating the melted depths in the simulation results.

NOMENCLATURE

I_A peak intensity of a laser pulse, MW/cm^2
E_1 energy density of a laser pulse, mJ/cm^2
E_2 laser energy density exceeded E_A, mJ/cm^2
E_A the lowest laser energy density in melting, mJ/cm^2
t_A time at peak maximum of laser intensity, ns
t_B duration time of a laser pulse, ns

REFERENCES

1. Kagawa, K., et al., Extended Abstracts of the Third International Workshop on Junction Technology IWJT2002 (2002), 31-34.
2. Matsuno, A., et al., International Semiconductor Technology Conference ISTC 2002, **2002-17**(2002), 148-152.

3. Shibahara, K., et al., Extended Abstracts of the 2001 International Conference on Solid State Devices and Materials, (2001)236-237.
4. Kotake, S. and Kuroki, M., *9th International Heat Transfer Conference*, **4**(1990), 277-282.
5. Kotake, S. and Kuroki, M., *International Journal of Heat and Mass Transfer*, **36-8** (1993), 2061-2067.
6. Ezato, K., et al., *ASME HTD*, **323**(1996),171-178.
7. Shibahara, M. and Kotake, S., *International Journal of Heat and Mass Transfer*, **40-13**(1997), 3209-3222.
8. Kunugi, T. and Shibahara M., *Molecular Dynamics Simulations, "Femtosecond Beam Science",* Uesaka, M., Ed., Imperial College Press, in press.