MOSFET Gate Dielectric Simulation and Characteristics Analysis

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1 Introduction

In this work we want to investigate the effect of cooling rate of gate dielectric in MOSFET devices. Gate dielectric is made up of amorphous silica. We assume a dry thermal oxidation process was used to grow the gate oxide and therefore we designed our simulations accordingly. We used the LAMMPS molecular dynamics software [1] and reaxff [2] forcefield to drive our results.

One major factor in NBTI aging[3] is the diffusion of surface Hydrogen atoms and/or molecules into the gate dielectric. We speculate that there is a relation between thermal oxidation cooling rate and hydrogen diffusion coefficient. In order to investigate such assumption we have prepared Silica blocks at four different cooling rates:$10^{13}\frac{k}{s}$, $2\times10^{13}\frac{k}{s}$, $5\times10^{13}\frac{k}{s}$, $10^{14}\frac{k}{s}$. The Silica slabs were constructed based on the method explained in [4] with some modifications. Therefore, we prepared boxes with dimensions of $21.76\times21.76\times40.00\mathring{A}^3$ and we filled them by randomly placing 618 SiO_2 molecules in the box. This resulted in a very dense slab of $3.2\frac{g}{cm^3}$. This choice of density gives us a density between Stishovite and low pressure forms of quartz. As in contrast with [4], we were hoping to achieve a higher density of final amorphous silica (i.e. high quality and denser oxide which happens as a result of dry thermal oxidation and is used for gate dielectric). The density for such oxide is around $2.27\frac{g}{cm^3}$ which we were also able to achieve. We prepared two different silica slabs for each cooling rate and averaged our results on the two. The simulation process was as follows:

- We initiated the system at $4000K$ and cooled it down to $300K$ using NVT[1] ensemble for $150ps$ (750000 steps of $0.2fs$). Note that with our choice of density it seems that the cooling rate at this step doesn't matter very much because I obtained very similar results with $15ps$.

- We again warmed the system up to $4000K$ using an NPT[2] ensemble for $1ps$ (10000 steps of $0.1fs$).

- We kept the system at $4000K$ using an NPT ensemble for $75ps$ (750000 steps of $0.1fs$).

[1]This is a formal statistical mechanics designation for a system with constant Number of particles, Volume, and Temperature. Note that temperature is regulated via a Nose-Hoover thermostat

[2]This is similar to NVT but with constant pressure and variable Volume. Note that the pressure in all of the NPT ensembles are fixed at 1 atm.

- We cooled the system down back to $300K$ using an NPT ensemble for three different cooling rates (with time steps of $0.1fs$).
- We let the system relax at $300K$ using an NPT ensemble for $1ps$ (10000 steps of $0.1fs$).

Here we analyze the following five major criteria of SiO_2 glass characteristics:

- Density.
- Charge distribution: This parameter shows the distribution of charges on the Si and O atoms.
- $Si-O$ bond length.
- $O-Si-O$ and $Si-O-Si$ angle.
- Radial Distribution Function (RDF) for $O-O$,$Si-O$ and, $Si-Si$: Radial Distribution Function ($g(r)_{x-y}$) is the probability of finding a y atom in distance r from the x atom.
- Guttman's ring statistics: Ring statistics is a criteria used for characterizing glass silica. It was first introduced in [5] and further definitions for rings were developed later. One such definition is Guttman's definition for a ring [6]. According to this definition a ring is the shortest path from a node(atom) which comes back to that node. Note that in this work we only studied rings that start from an Si atom and have a $Si-O-Si-O-...$ pattern. A simple example of a Guttman ring can be observed in Figure. 1.

2 Density

The material density that we achieved for our three samples are given in Table 1. The results show that we were able to achieve a density very close to that of dry thermal oxidation process. The experimental results according to [8] say that density is 2.20 $\frac{gr}{cm^3}$.

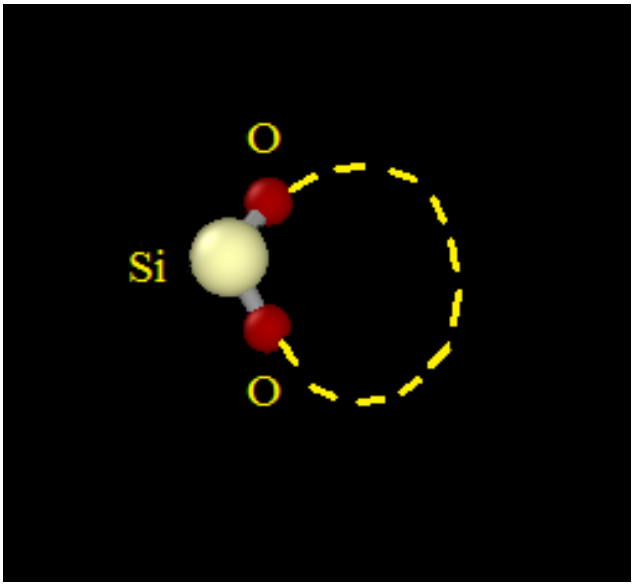

Figure 1: A simple example of a Guttman ring. The length is calculated by counting the number of atoms in the shortest path from Si which comes back to Si from a neighboring O.

3 Charge distribution

The atomic charge distribution of samples (for three different cooling rates) are depicted in Fig. 2. The Charge distributions for the three cooling rates are very similar and therefore this is not a distinguishing characteristic for the cooling rates.

4 $Si-O$ Bond length

As one can observe in Fig. 3, the bond lengths for $Si-O$ bonds have a peak around $1.61\mathring{A}$. To be more precise the exact $Si-O$ distances are given in Table 1. These numbers are close to the experimental results for silica ($1.608 \pm 0.004\mathring{A}$) [7].

5 Angles

Fig. 4 and Fig. 5 show the $O-Si-O$ and $Si-O-Si$ angles for three different cooling rates. The average angle for each cooling rate is given in Table 1. The experimental values for the above angles according to [8] are 144 for $Si-O-Si$ and 109.5 for $O-Si-O$. Our results seem to be a few percent different than the actual values and also than those obtained by other Reaxff simulations as given in Table 1. One reason for this difference is perhaps the

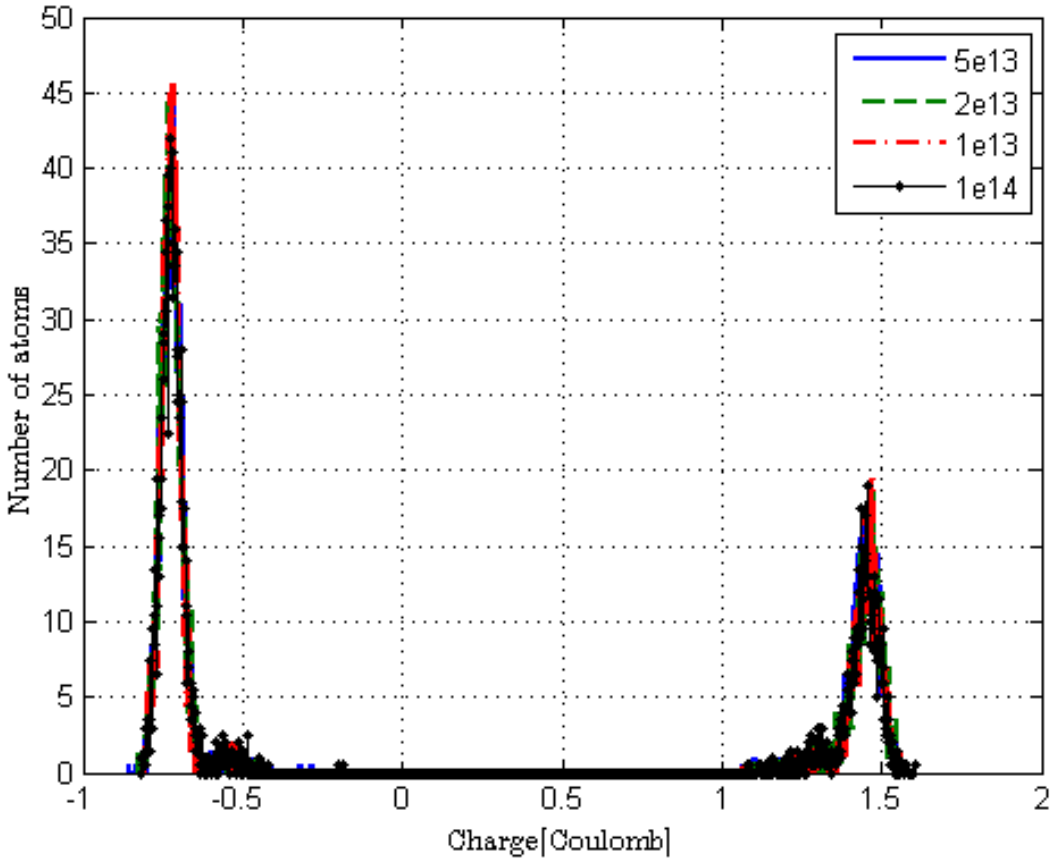

Figure 2: Charge distribution for three different cooling rates.

initial higher density.

6 RDF

We have obtained the $O-O$, $Si-O$ and $Si-Si$ RDF for three different cooling rates as can be observed in Fig. 6, 7 and, 8. The results are very similar for all of the three cooling rates and they seem not to be quite distinguishable based on this criteria.

7 Guttman's Ring statistics

Fig. 9 shows the non-zero diagonal elements of the General Connectivity matrix. This shows how connected the amorphous ring network is. Fig. 10 shows the number of rings per sample for non-zero ring lengths. Note that by ring length we are referring to the number of atoms

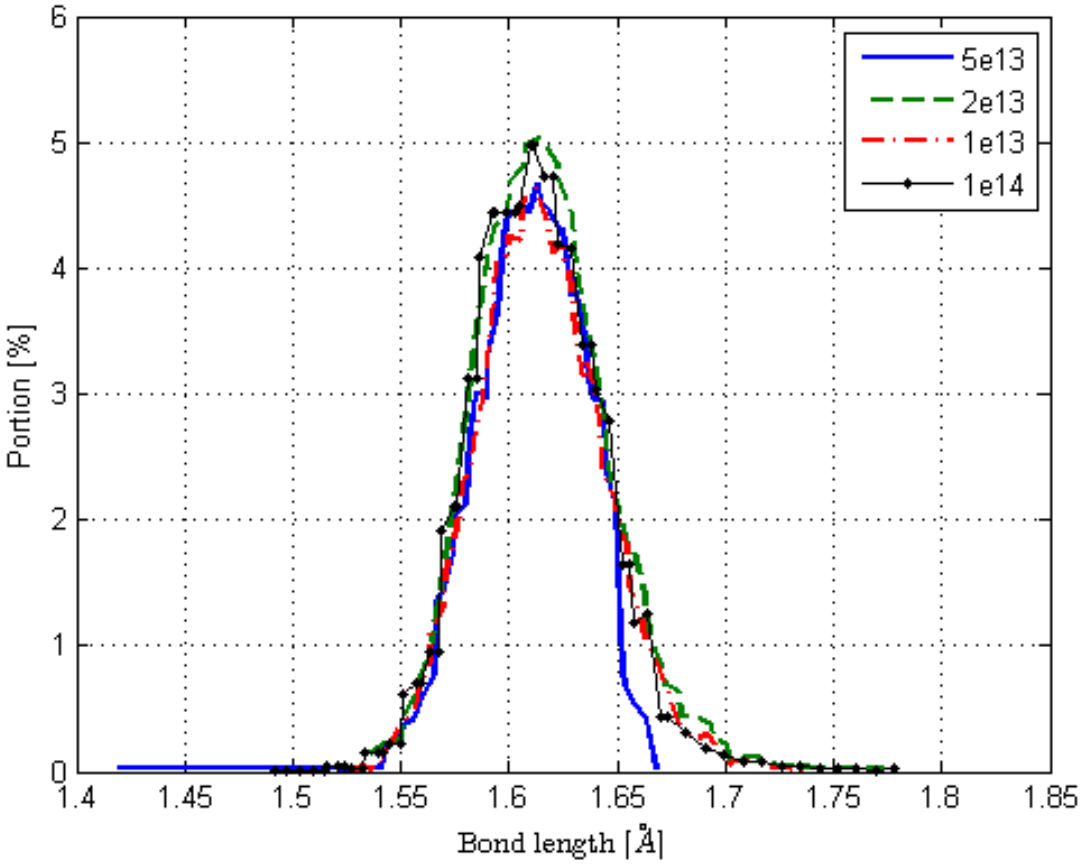

Figure 3: Si-O

present in a ring. These numbers are divided by the total number of nodes (i.e. atoms). As it can be observed the ring characteristics vary a lot for different cooling rates. The length of rings are centered at ten atoms (five tetrahedrons). One can observe that by increasing the cooling rate, the portion of larger rings in the structure are going to increase. [9] has also confirmed similar results but with a slightly different definition for rings and with their most probable ring length being six tetrahedrals(i.e. 12 atoms). This intuitively means that larger empty holes appear in the slab. Further analysis is necessary to relate the ring length and Hydrogen diffusion coefficient.

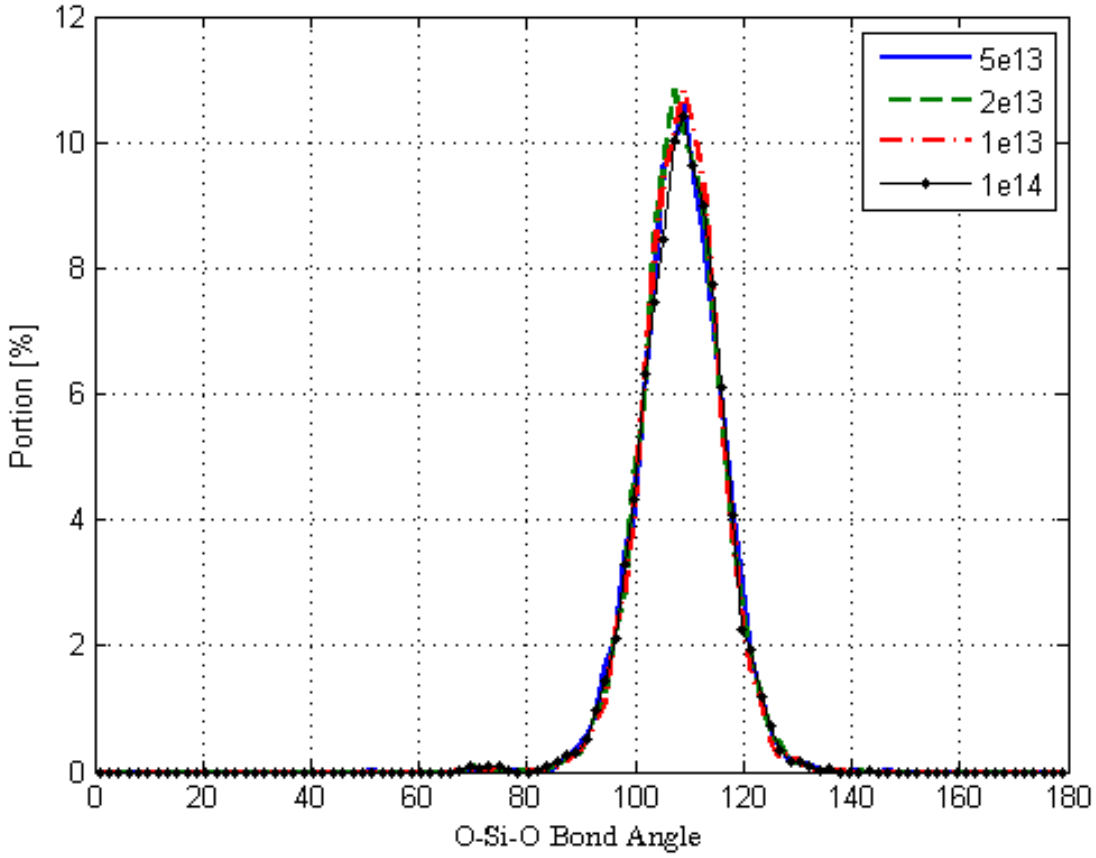

Figure 4: O-Si-O

Silica Type	$10^{13}\frac{k}{s}$	$2\times10^{13}\frac{k}{s}$	$5\times10^{13}\frac{k}{s}$	$\times10^{14}\frac{k}{s}$	Real Glass	Reaxff[4]	MD[9]
Density($\frac{gr}{cm^3}$)	2.28	2.29	2.29	2.29	2.18-2.27 (dry)	2.14	2.27-2.38
Si-O bond length ($\AA$)	1.615 ± 0.029	1.616 ± 0.031	1.609 ± 0.025	1.612 ± 0.076	1.608 ± 0.004	1.59 ± 0.07	-
Si-O-Si Angle (x°)	139.8	139.5	140.3	139.9	144	150	141-152
O-Si-O Angle (x°)	108.3	108.4	108.4	108.4	109.5	109.2	108.3
RDF_{O-O} first peak ($\AA$)	2.52	2.57	2.57	2.52	2.65	2.53	2.590
RDF_{Si-O} first peak ($\AA$)	1.632	1.635	1.665	1.632	1.620	1.56	1.595
RDF_{Si-Si} first peak ($\AA$)	3.12	3.09	3.11	3.08	3.12	3.06	3.155
Average O-Coordination	2.01	2.01	2.01	2.01	-	-	-
	98% =2	97% =2	97% =2	97% =2	-	-	-
Average Si-Coordination	3.99	3.97	3.97	3.96	-	-	-
	97% =4	96% =4	94% =4	95% =4	-	-	-

Table 1: Comparisson of analyzed data with real glass, other reaxff(the forcefield that we use) simulations, other molecular dynamics (MD) simulations.

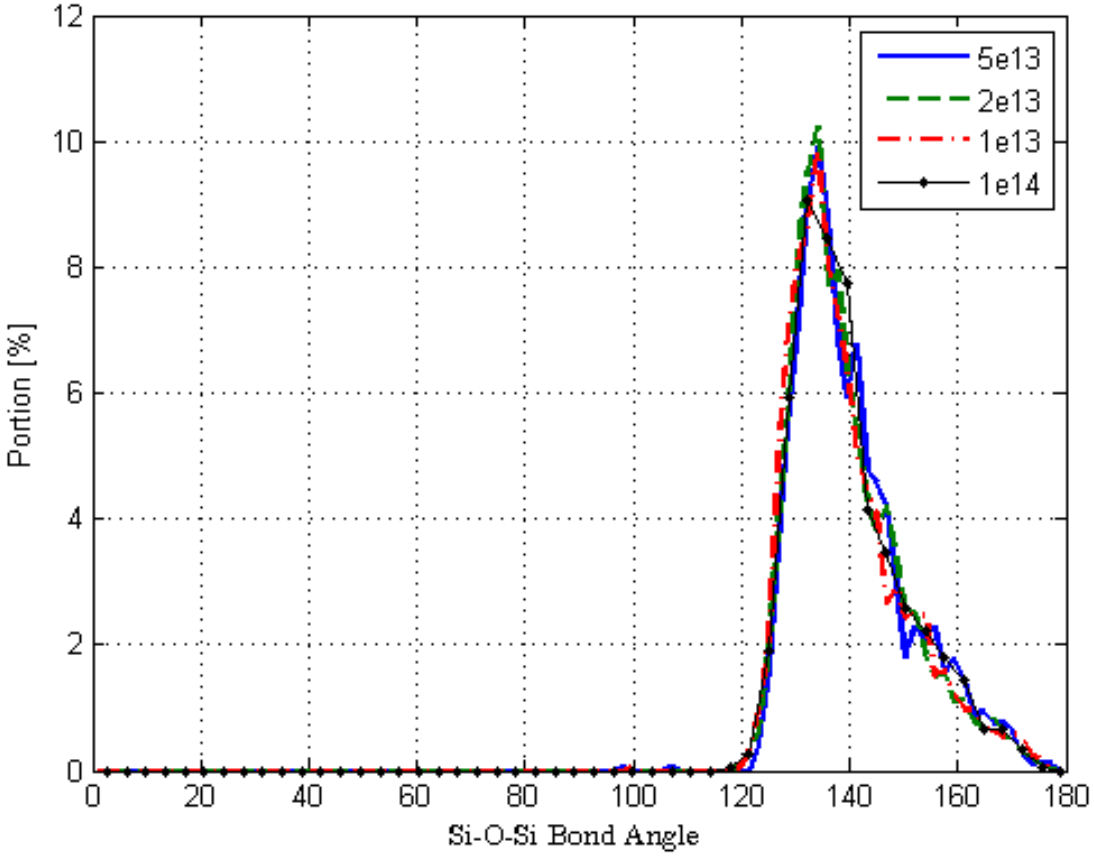

Figure 5: Si-O-Si

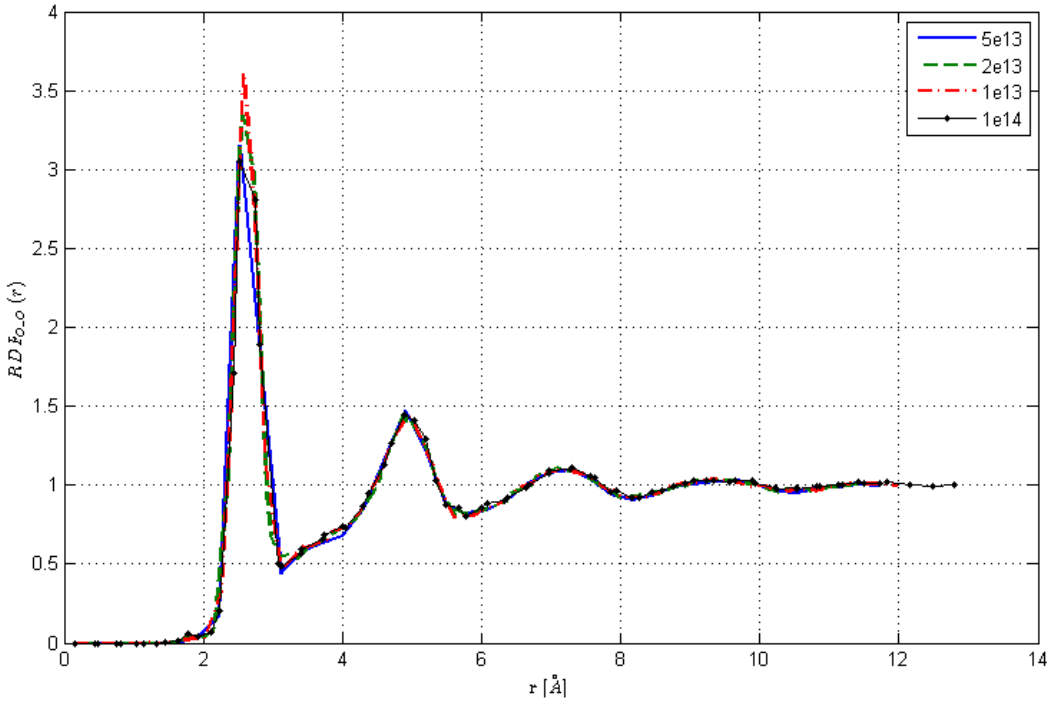

Figure 6: RDF O-O

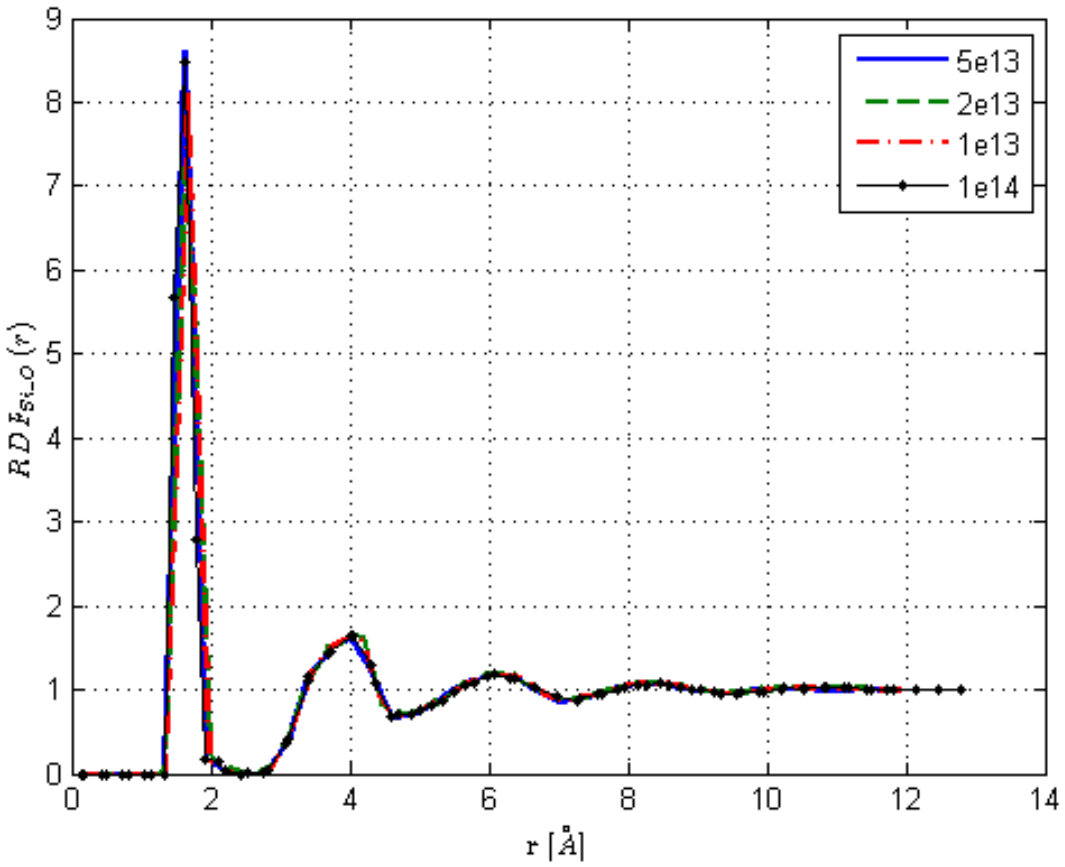

Figure 7: RDF Si-O

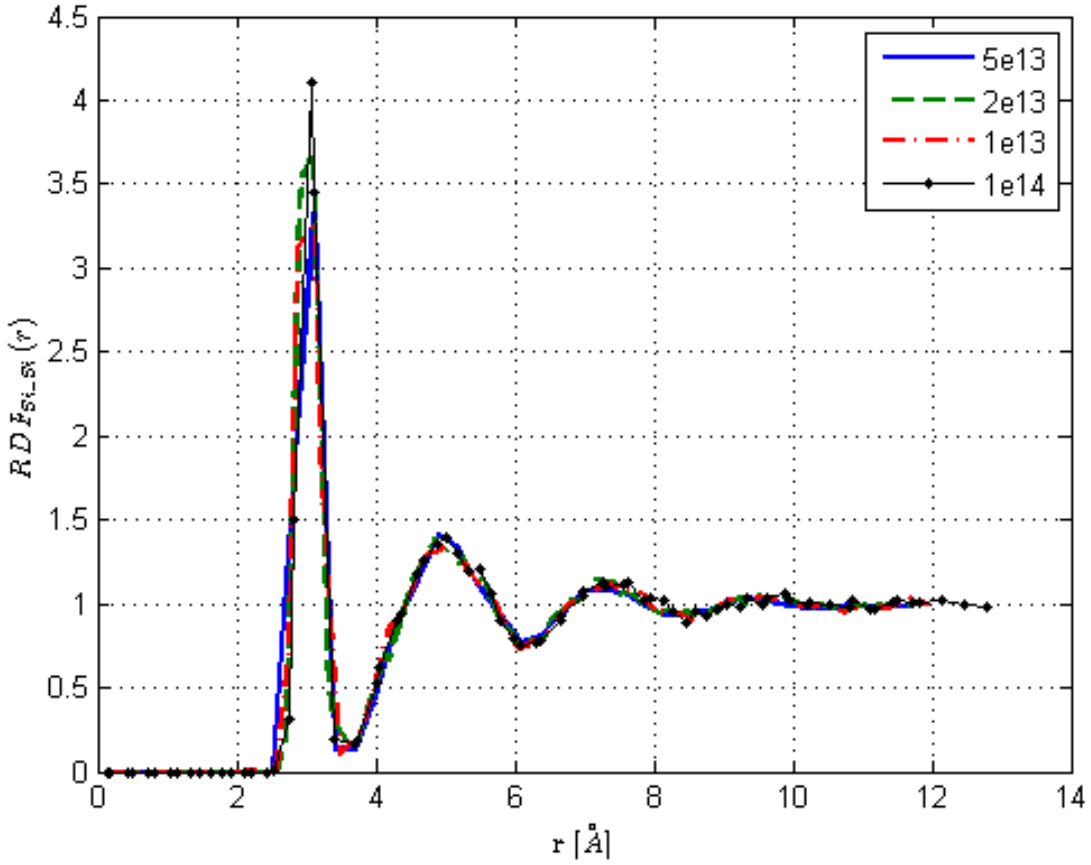

Figure 8: RDF Si-Si

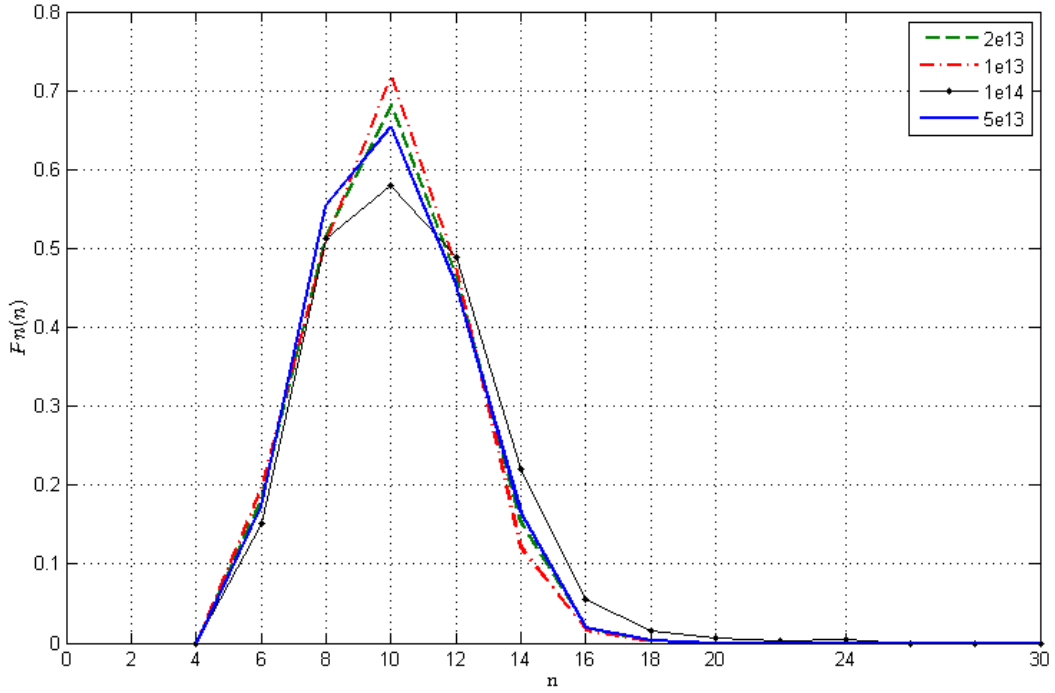

Figure 9: Guttman's Pn(n): The n'th diagonal element of the General Connectivity matrix where n is the ring's length.

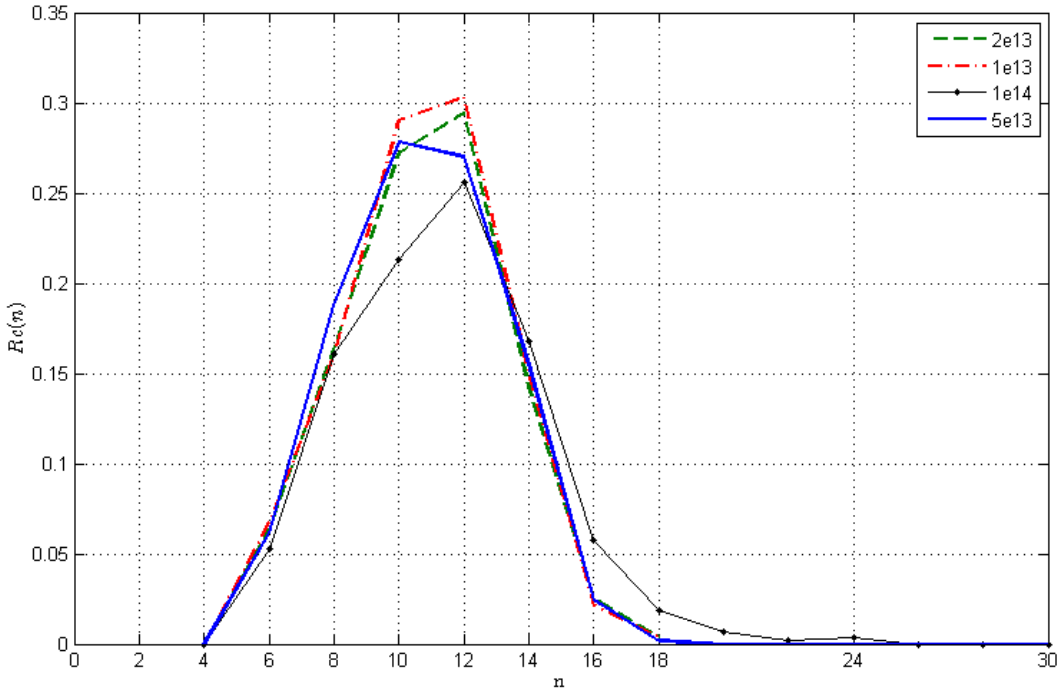

Figure 10: Guttman's Rc(n): The number of rings of length n devided by the total number of atoms. n is the length of the ring

8 Conclusion

We conclude this report by mentioning that basic analysis of the samples at different cooling rates suggest that they are very similar to real silica and therefore they can be used for further investigation and simulation of MOSFET gate dielectric characteristics. We were able to construct dry thermal oxide(high density dielectric oxide) by choosing a higher initial silica density than what has been previously used in the simulations. We also observed that by increasing the cooling rate larger rings are going to appear in the structure. We speculate that this will alter the Hydrogen diffusion characteristics of the sample. Our recommendation for the next step of this research is to analysis the hydrogen diffusion coefficient for different cooling rates and to investigate whether or not a relation between the cooling rate and diffusion coefficient can be established. We included the results of our comparisons with real glass data and similar reax forcefield molecular dynamics simulations in Table 1.

References

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