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Molecular-Dynamics Study of Amorphous SiO_2 Relaxation

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Abstract. Using Molecular-Dynamics simulation we observed the generation of amorphous SiO_2 target from a randomly distributed Si and O atoms.We applied a sequence of annealing of the target with various temperature and quenching to room temperature. The relaxation time required by the system to form SiO_4 tetrahedral mesh after a relatively long simulation time, is studied. The final amorphous target was analyzed using the radial distribution function method, which can be compared with the available theoretical and experimental data. We found that up to 70% of the target atoms form the tetrahedral SiO_4 molecules. The number of formed tetrahedral increases following the growth function and the rate of SiO_4 formation follows Arrhenius law, depends on the annealing temperature. The local structure of amorphous SiO_2 after this treatment agrees well with those reported in some literatures.

INTRODUCTION

Silicate is the base mineral of the earth crust and its mantle, as well as in other rocky planetary bodies. The mechanical and thermodynamical properties of Silicate is demanding in the studies of earth and planetary systems. Besides its importance in those studies, one type of Silicate, the amourphous SiO_2, is used in wide-spread technological application. Hence, the study of SiO_2 and its crystalline and amorphous phases has attracted interest of researchers for long time.

The perpetually increasing capability of computer has made possible to carry on studies on properties of silicates with a very convincing results. The thermodynamical properties was reported thoroughly by its equation of state, for instance in [1]. Molecular-dynamics method has been used to study the thermodynamics and melting behavior of SiO2 [2]. The information is unquestionably useful, in particular for geophysical researches related to the dynamics of magma and lava flow, and the heating and cooling of magmatic minerals and it consequences to the formation of rocks and planetary crust [3, 4].

Amorphous SiO2 model is usually created from one of well-defined structure, such as α-quartz, and then the disorder is introduced by applying high temperature using NVT ensemble [5]. In this work we simulated an intuitively natural process of amorphous SiO_2, i.e. by starting from the randomly distributed Si and O atoms and performed a sequence of annealing and quenching. The proposed algorithm provide an alternative to generate amorphous target, which is easier to perform and robust. By this initial configuration, we studied the forming of tetrahedral SiO4 and the configurational relaxation process where the amorphous phase was formed from a mesh of tetrahedra. The local structure of amorphous phase was evaluated by calculating the *radial distribution function*, $g(r)$ [6].

METHOD

We consider a cubic periodic cell of simulation box of 108.6 Å side lengths. The volume of the cell is fitted to the density of α-quartz, $0.08/Å^3$. The total amount of 64000 Silicon and Oxygen atoms are put randomly in a

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