First Principles Analysis on Mechanical Properties of SiO_2 and GeO_2

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1 Introduction

Large scale integration (LSI) has been developed to be higher performance with downsizing. For the insulator thin film, a lot of studies were performed to SiO_2 which is currently a component of a transistor. On the other hand, Ge thin film is considered to be used on the Si substrate as the carrier mobility is higher than that in Si crystal [1]. However, there are few studies on GeO_2. In this study, the mechanical properties of GeO_2 were analyzed by first principles calculation, and the results were compared with SiO_2.

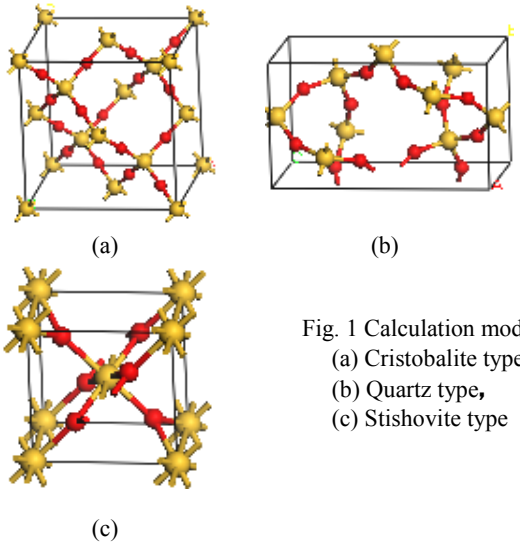
It is quite difficult to analyze the amorphous structure of actual SiO_2 and GeO_2 by first principles calculation. Therefore, in this study, we considered the Cristobalite type, the Quartz type, and the Stishovite type for SiO_2 and GeO_2.

2 Calculation Details

The calculation method is the first principles calculation, in which the ground state of the system is found by solving the Kohn-Sham equation that is a rule equation of the electronic system for a given atomic configuration. The program package used in this study is CASTEP [2]. In this calculation, the Kohn-Sham equation is solved self-consisyently in order to obtain the ground state of the system for given atomic configurations [3].

Wave function is expanded by plane-waves, and ultrasoft pseudopotential [4] is used to reduce a number of plane waves.The cut-off energy for the plane-wave expansion was 340 eV. The expression proposed by Perdew et al. [5] was used for the generalized gradient approximation (GGA) for the exchange-correlation term. The density mixing method [6] and BFGS geometry optimization method [7] are used to optimize the electronic structure and configurations, respectively.

The atomic configurations of Cristobalite type, Quartz type, and Stishovite type for SiO_2 and GeO_2 are shown in Fig. 1(a) to 1(c). In this figure, a yellow ball is Si (Ge) atom and a red ball is O atom.



(a) (b) (c)

Fig. 1 Calculation model of
(a) Cristobalite type,
(b) Quartz type,
(c) Stishovite type

3 Results and discussion

The calculated total energies of SiO_2 of Cristobalite type, Quartz type, and Stishovite type per unit structure (one SiO_2 molecule) are shown in Fig. 2.

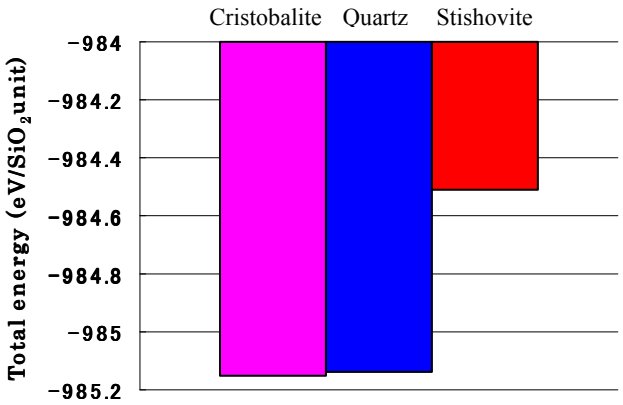


Fig. 2 Total energy of SiO_2 model

This result indicates that Cristobalite type is the most stable for SiO_2. The obtained densities are 2.18 g/cm^3 (Cristobalite type), 2.65 g/cm^3 (Quartz type) and 4.18 g/cm^3 (Stishovite type).

The calculated total energies of GeO_2 of Cristobalite type, Quartz type, and Stishovite type per unit structure (one GeO_2 molecule) are shown in Fig. 3.

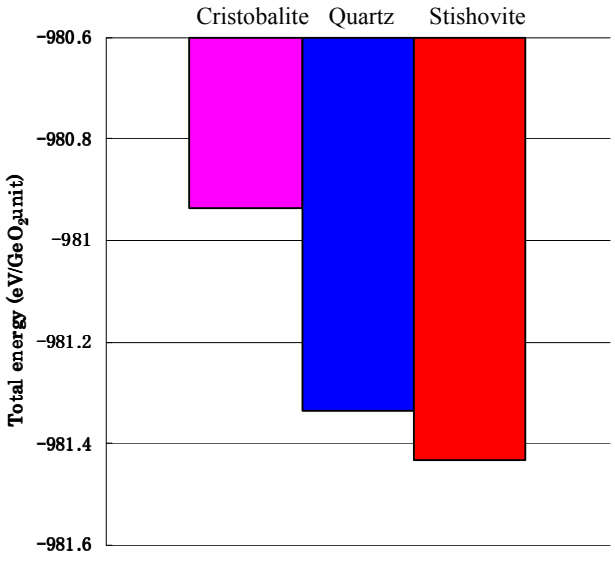


Fig. 3 Total energy of GeO_2 model

It was found that, for GeO_2, Stishovite type is the most stable. The obtained densities are 13.8 g/cm^3 (Cristobalite type), 3.99 g/cm^3 (Quartz type) and 2.24 g/cm^3 (Stishovite type).

Next, the relationship between the total energy and the isotropic strain between -5% and 5% for SiO_2 is shown in Fig. 4.

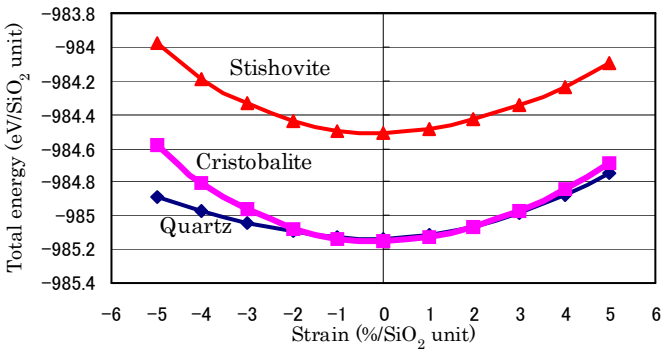


Fig. 4 Total energy-strain diagram of SiO_2 model

It was found that the change of total energy of Quartz type is smaller than other models. So Quartz type can deform easier than Cristobalite type and Stishovite type. When the strain with ±3% is applied to SiO_2, the most stable structure shifts from Cristobalite type to Quartz type.

The relationship between the total energy and the isotropic strain between -5% and 5% for GeO_2 is shown in Fig. 5.

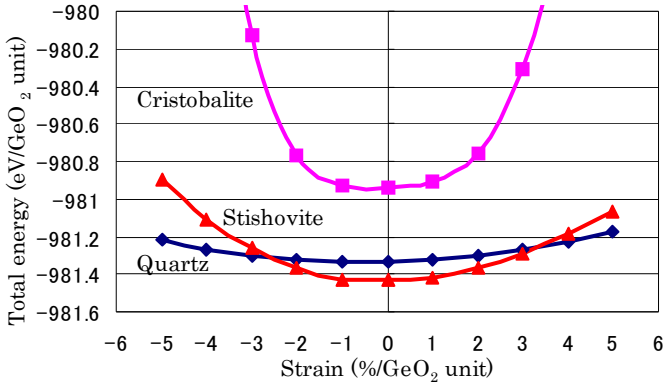


Fig. 5 Total energy-strain diagram of GeO_2 model

It was found that the change of total energy of Quartz type is smaller than other models. So Quartz type can deform easier than Cristobalite type and Stishovite type. When the strain with ±4% is applied to GeO_2, the most stable structure shifts from Stishovite type to Quartz type.

The calculated bulk modulus of SiO_2 and GeO_2 is summarized in Table. 1.

Table 1 Calculated bulk modulus of SiO_2 and GeO_2.

	SiO_2 (GPa)	GeO_2 (GPa)
Cristobalite	165.8	157.0
Quartz	135.0	54.2
Stishovite	170.3	129.5

It was found that the bulk modulus of SiO_2 is larger than GeO_2 in each structure.

The results obtained in this study indicates that GeO_2 crystal is softer than SiO_2 crystal.

4 Conclusion

Mechanical properties of SiO_2 and GeO_2 crystals were analysed by the first principles calculation. It was found that, in SiO_2 model, Cristobalite type is the most stable structure. On the other hand, in GeO_2 model, Stishovite type is the most stable structure.

The calculated result of bulk modulus indicates that GeO_2 crystal is softer than SiO_2 crystal.

References

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