Anomaly Phase Transition of Silicon: A Molecular Dynamics Study

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Abstract: Silicon shows a very different trend while melting. Melting has remained a challenging subject from a long time. Especially, predicting the melting temperature of any solid substance still exists as a problem in many cases. This work is an attempt to study the mechanism of melting using classical molecular dynamics simulation, to define a set of parameters that could help us predict the behaviors of silicon at any temperature and also its phase transition mechanism. In order to understand the phenomenon, it is important to know the interaction potential governing the silicon system. Stillinger-Weber potential is a good model for Si atoms which takes into account two and three particle interactions. Melting of Silicon atoms is studied using Molecular Dynamics Simulation with the help of LAMMPS software. Heating and quenching processes is implemented on a system of Si atoms. Variations of various parameters like density, volume per atom, potential energy, Lindemann parameter, Non-Gaussian parameter, and coordination number with temperature has been studied. It has been found that melting in Si occurs in three stages. It involves pre-melting, melting and relaxation. Around 1450 k, the Gaussian parameter begins to jump.

At this point, the potential energy and Lindemann parameter appear to be steady, indicating pre-melting. Lindemann index and potential energy (PE) take an upward inflection about 1600 k, and coordination number increases from 4 to 8, indicating diamond structural collapse. At temperatures above 1750 k, the non-Gaussian value drops abruptly, indicating that the solid is completely lost its crystallinity.

Keywords: Molecular Dynamics, LAMMPS, Lindemann Parameter, Non-Gaussian Parameter, Co-ordination number

1. Introduction

Silicon, the fourteenth element of the periodic table, having symbol 'Si', is a brittle and hard solid crystal having bluish grey colour lustre, a tetravalent metalloid that behaves as a semiconductor. This p-block element's electronic configuration in the ground state is $[Ne]3s^23p^2$, the four valence electrons are 2 each from 3s and 3p orbitals. It has an atomic radius of 111 pm. In pure state, at room temperature, its behaviour is that of an insulator, so doping is usually done with a group 13 element to increase its conductivity. Its resistivity drops on increasing temperature. This usually unreactive element has a high chemical affinity for oxygen, due to which it is difficult to be obtained in its pure form. The melting point of silicon is 1414 °C. Silicon boils at 3265 °C, which is the 2nd highest among non-metals, falling just after boron. It is also the 2nd most adequate element in the earth's crust. Silicon's three stable isotopes are ^{28}Si (92.23%), ^{29}Si (4.67%), and ^{30}Si (3.10%).

At standard conditions, its structure is of diamond cubic lattice, giving it strong covalent bonds. To break these covalent bond need lots of energy to break. This is the reason behind a high melting point of silicon. Each unit of silicon consisting of eight atoms, their distribution with reference to Figure is described below.

Silicon is the very important element for the advancement of technology, due to widely used of silicon and its products in various fields of engineering and technology. It has been given/attracts greater attention due to widespread application of silicon in our day-to-day life. It is abundant in earth's crust. Silicon is widely used as semiconductor. Silicon is principal component of synthetic polymers silicones. Versatile use of Silicones is as in the form of sealants, adhesives, lubricants, medicine, cooking utensils, and thermal and electrical insulation. Silicon is mostly found in compound form. It is rarely found in pure form and can be used with little processing of natural minerals. During phase transformation it shows anomalous behaviors compare to conventional elements and compounds. Exact mechanism of phase transformation of silicon becomes a challenging problem and remains unanswered[1-5].

Phase transition is reported for many pure materials including silica and silicon[6-8].Transition point is obtained either pressure swinging or temperature swinging method[8-10]. Transition temperature can also be evaluated using specific heat capacity information[11, 12]. Another robust technique for determination of transition point is calculation of entropy[13, 14]. Conventional methods like density hysteresis plot, Lindemann parameter[5], non-Gaussian parameter[15], radial distribution function, structure factor, orientation order parameter etc are employed to predict the transition point of a material.

Solid to liquid transformation of Lennard-Jones(LJ) system under confinement is reported[16]. Transition point is determined on the basis of density hysteresis plot, Lindemann parameter, non-Gaussian parameter, radial distribution function, structure factor, orientation order parameter[16]. From sudden jump in density, one can determine the transition point. Similar kind of phenomena is also observed in potential energy. However, density changes observed after complete phase transformation. So determined transition point is not accurate. Other parameters are Lindemann parameter and non-Gaussian parameter. From the Lindemann parameter value one can estimate the melting and freezing transition point. For determination of melting transition, Change in first and second co-ordination number is important too[15].

Most of the above-mentioned methods are not accurate to predict the melting transition. Estimated melting temperature is often higher compare to true melting temperature. Melting transition can be predicted more precisely

using the knowledge of free energy. Transition temperature of Lennard-Jones(LJ) and sodium Chloride(NaCl) is reported from free energy information[17]. Free energy is evaluated using thermodynamic integration. The reversible path is constructed using pseudo-supercritical path[17, 18]. Phase transformation from solid to liquid under slit[19, 20] and cylindrical confinement is studied using free energy analyses[21].

Melting in solids has been a difficult problem that has yet to be solved, and predicting melting temperature is difficult. Lindemann and Born proposed two empirical criteria, and recent research reports that the two criteria can estimate the solid-liquid transition point for an ideal crystal without surfaces. A crystalline solid should melt at a particular temperature, but in practice, the technique generally last during little while, which could be attributed to the pre-melting phenomenon. The phenomenon has been thoroughly investigated through studies of surfaces, lattice vibrations, missing atoms, grain boundaries, defects and structure catastrophes, particularly those of Tallon and Cahn.

2. Melting criteria

2.1 Lindemann criteria

.   Lindemann parameter is defined as

$$\delta L = \frac{<RMS>^{1/2}}{a} = \frac{<\Delta r^2>^{1/2}}{a}$$

where δL is the Lindemann parameter, "a" is the nearest neighbor distance. The Lindemann parameter estimate for the melting of bulk face-centered cubic (FCC) solid is 0.22 and for body-centered cubic (BCC) it is 0.18[2, 6, 22, 23]. Lindemann criterion is supported by experimental data both for crystalline materials and for glass-liquid transitions in amorphous materials.

2.2 Non-Gaussian Parameter

In case of non-Gaussian parameter from abrupt jump of the peak transition point is estimated. The Non- Gaussian parameter is very temperature sensitive.

$$I(Q't) = \exp\left(-\frac{(\Delta r^2)(t)Q2}{6} + A(t)[(\langle \Delta r^2 \rangle)(t)]^2 * Q^2_{)/72}\right.$$

In this expression the Gaussian parameter[23], $\alpha_2(t)$ is defined as:

$$\alpha_2(t) = \frac{3\langle \Delta r^4 \rangle}{5\langle \Delta r^2 \rangle^2} - 1$$

$$\Delta r = |r_i(t) - R_i(0)|$$

It explains the highly displaced particles near the melting point, which is a relationship of the second and fourth moments of a 3D distribution of Δr with time t, which is zero for a Gaussian distribution

2.3 Radial distribution function and Co-ordination Number

To analyze the real space correlation and structure, the common practice is based on the pair correlation function or radial distribution function g(r) and coordination number Z(r)

$$g(r) = \frac{1}{N_\rho}\left|\sum_{\substack{i=1 \\ }}^{N}\sum_{\substack{j=1 \\ (i \neq j)}}^{N}\sigma(r - r_{ij})\right|$$

$$Z(r) = 4\pi\rho\int_{r_1}^{r_2}g(r)r^2dr$$

3. Simulation And Software Work

3.1 Molecular Dynamics Simulation:

Molecular dynamics simulation is a technique used to get insights about the movements and properties of a system of atoms and molecules. It is basically a computer simulation where the system of atoms and molecules are given to make interaction among themselves for a certain amount of period. As a result, we can predict the outcome of various real-world systems by computer simulations without the need for experiments. MD helps to do it in different length and time scales. It is said to bridge the gap between theory and experiments. Various parameters involving in a system's interaction is calculated in molecular dynamics simulation by solving the Newton's equations of motion for the particular simulated system. The trajectory of the interacting particles can be predicted by the above-mentioned method. In addition, the force that cause the movements of the particles in the system is determined by the interatomic potential acting between the particles. It is generally the solution to the classical motion equations in a system of atoms or molecules.

The estimates of MD simulations are exact that is because, due to the constraints of our machine budget, they can be as precise as we want. At the same time, it is possible to expose the secret information behind bulk measures. Molecular dynamics simulations help in giving numerical solutions when the analytical solutions cannot be found. Due to the fact that a large number of particles usually comprising molecular structures, it is not feasible to analytically determine the properties of these complex systems; MD simulation by computational methods circumvents this challenge. However, lengthy MD simulations, which can be reduced by selecting algorithms and parameter correctly, create accumulated errors in computational integration that cannot be avoided completely.

3.2 Lammps Software

LAMMPS- Large-scale Atomic/Molecular Massively Parallel Simulator is an open source molecular dynamics software[24]. It uses Message Passing Interface (MPI) for parallel communication. Sandia National Laboratories and Temple University researchers maintain and distribute it. It was created as part of a Cooperative Research and Development Agreement among laboratories from the US Department of Energy and few other private sector laboratories[24].

3.3 Atomic Potential Used

Stillinger-Weber Potential is a good model for Si. It considers both two-particle and three-particle interactions. The values of following parameters in metal units have been used.

3.4 Simulation Details and Potential Model

The NPT MD simulations are conducted with the help of LAMMPS [24]. Unit system of the simulation process is metal. The velocity-Verlet algorithm is employed to integrate the equation of motion. Time step (Δt) is 5ps for integration. The temperature and pressure are monitored using a Nose´–Hoover thermostat and barostat with relaxation times of 2000ps and 5000ps for temperature and pressure, respectively. Number of particles are simulated around 400000. The periodic boundary condition is applied in all three directions of the simulation box. We vary the pressure from P = 1atm to P=70atm the density dependence with pressure. During quenching, the initial liquid configurations are taken as ideal diamond structures at 4000k. Cooling process is carried out gradually after each 3000,000 MD time steps. Change of temperature T is 25k for each NPT simulation. Temperature is dropped from 4000k to 500k with a decrement of 25K. At the time of heating process, the last configuration of the quenching simulation initial co-ordinate of the system. Heating is also conducted same way as the quenching. The increment of temperature T is 25K. And for each NPT simulation. Process of heat supply is done until the solid has completely converted into liquid. Temperature range of heating is from 500k to 4000k. lost its crystallinity. The density is determined at every interval. Additionally, we performed two more simulations to estimate the Lindemann parameter(∂L) and Non-Gaussian parameter$(\alpha_2(t))$. The rest of the treatment is remained same as mentioned previously. The Lindemann parameter and non-Gaussian parameter is determined each temperature. Interaction potential of silicon is as follows:

$$E = \sum_i \sum_{j>i} \varphi_2(r_{ij}) + \sum_i \sum_{j \neq i} \sum_{k>j} \varphi_3(r_{ij}, r_{ik}, \theta_{ijk})$$

$$\varphi_2(r_{ij}) = A_{ij}\epsilon_{ij}\left[B_{ij}\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{p_{ij}} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{q_{ij}}\right]exp\left(\frac{\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}}\right)$$

$$\varphi_3(r_{ij}, r_{ik}, \theta_{ijk}) = \lambda_{ijk}\epsilon_{ijk}[cos\theta_{ijk} - cos\theta_{0ijk}]^2 exp\left(\frac{\gamma_{ij}\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}}\right)exp\left(\frac{\gamma_{ik}\sigma_{ik}}{r_{ik} - a_{ik}\sigma_{ik}}\right)$$

Where φ_2 represents two body interaction term. While φ_3 presents three body interaction function. The summation in the formulae are overall neighbors J and K of atom I within a cutoff distance a[24].

The A, B, p, and q parameters are used only for two-body interactions. The λ and $cos\theta_0$ parameters are used only for three-body interactions. The ϵ, σ and a *parameters* are employed for both two-body and three-body interactions. γ is applied only in the three-body interactions. However, it is explained for pairs of atoms. The non-annotated parameters are unitless[24].

Table 1: Values of parameters used in SW potential(in metals unit)

A	B	P	Q	tol	A	Cos(θ)	Λ	γ	ε(eV)	σ(Å)
7.0495562	0.6022245	4	0	0	1.80	-0.3333	21.0	1.20	2.1672	2.0951

4. Results and Discussions

In this section we will discuss the output results of various parameters like density, coordination number, potential energy, Lindemann parameter, and non-Gaussian parameter with the change in temperature. Based on the variation of these parameters, we will try to formulate a basic idea about the melting of Si atoms.

4.1   Density

In this part we describe the nature of density of the Si system as we perform heating and quenching. Sharp density changed is observed for both the heating and quenching case. That indicates first order phase transition. Density of silicon for different temperature is shown in figure 1. In case of density changes after melting or freezing is unlike others common substances. After liquefication density rises whereas during solidification density is dropped. This phenomenon is quite unnatural compare to common substances. Metastable region is observed in middle portion of the hysteresis curve. True melting temperature lies in this hysteresis loop. The following data represents the variation of density with temperature around melting point temperature:
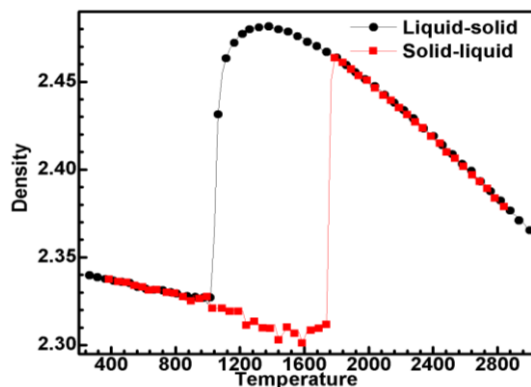

Figure 1: figure represents density as a function of temperature. Filled circle black in color for quenching the system where as filled square for heating the system. quenching and heating curves do not follow the same path which indicates first order transition. Hysteresis loop is clearly observed in density temperature plot. Metastable region is noticed middle of the curve and true transition point lies in this meta stable region.

If we perform the same NPT simulation by varying pressure, we can find a trend of the density as a function of the temperature for different pressure values. Density can be presented using the following equation during the heating processes, where temperature range is $500 \geq T \leq 2000$, other parameter values are presented in Table 2. Regression coefficient(R^2) for fitting polynomial is closed 1.

$$\rho = A * T^3 + B * T^2 + C * T + D$$

Table 2: Before melting the density of silicon can be predicted at different temperature with different constant pressure. R^2 is regression coefficient of the fittings.

Pressure(atm)	A	B	C	D	R^2
1	$-2 * 10^{-12}$	10^{-8}	$-3 * 10^{-5}$	2.3301	0.9999
5	$-2 * 10^{-12}$	10^{-8}	$-4 * 10^{-5}$	2.3302	1.0000
10	$-2 * 10^{-12}$	10^{-8}	$-4 * 10^{-5}$	2.3301	1.0000
30	$-2 * 10^{-12}$	10^{-8}	$-3 * 10^{-5}$	2.3301	1.0000
35	$-2 * 10^{-12}$	10^{-8}	$-4 * 10^{-5}$	2.3303	1.0000
40	$-2 * 10^{-12}$	10^{-8}	$-4 * 10^{-5}$	2.3303	1.0000
45	$-2 * 10^{-12}$	10^{-8}	$-4 * 10^{-5}$	2.3302	1.0000
50	$-2 * 10^{-12}$	10^{-8}	$-4 * 10^{-5}$	2.3303	1.0000

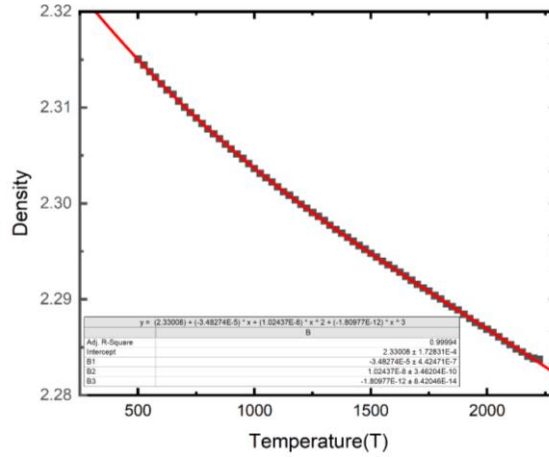| 55 | $-2*10^{-12}$ | 10^{-8} | $-4*10^{-5}$ | 2.3304 | 1.0000 |
60	$-2*10^{-12}$	10^{-8}	$-4*10^{-5}$	2.3305	1.0000
65	$-2*10^{-12}$	10^{-8}	$-4*10^{-5}$	2.3303	1.0000
70	$-2*10^{-12}$	10^{-8}	$-3*10^{-5}$	2.3303	1.0000

Figure 2: Presents the fitting curve before melting.

Similarly, we also predict the density of liquid silicon as a function of temperature for difference pressures. Where temperature range is $2200 \geq T \leq 4000$. Expression for density is

$$\rho = \alpha * T^2 + \beta * T + \gamma$$

Table 3: After melting change of the density as a function of temperature with different constant at different pressure, R^2 is regression coefficient of the fittings. Regression coefficient(R^2) for fitting polynomial is closed 1Others parameters values are given bellow

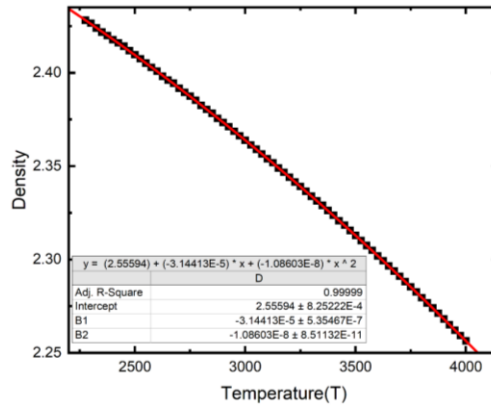| Pressure(atm)	α	β	γ	R^2
1	-10^{-8}	$-3*10^{-5}$	2.5559	1.000
5	-10^{-8}	$-3*10^{-5}$	2.5559	1.0000
10	-10^{-8}	$-3*10^{-5}$	2.5573	1.0000
30	-10^{-8}	$-3*10^{-5}$	2.556 3	1.0000
35	-10^{-8}	$-3*10^{-5}$	2.2556	1.0000
40	-10^{-8}	$-3*10^{-5}$	2.5573	1.0000
45	-10^{-8}	$-3*10^{-5}$	2.5512	0.9999
50	-10^{-8}	$-3*10^{-5}$	2.5568	1.0000
55	-10^{-8}	$-3*10^{-5}$	2.5551	1.0000
60	-10^{-8}	$-3*10^{-5}$	2.5566	1.0000
65	-10^{-8}	$-3*10^{-5}$	2.5569	1.0000
70	-10^{-8}	$-3*10^{-5}$	2.5571	1.0000

Figure:3 Represents fitting curve after melting region

Potential energy also shows the similar kind of behavior which is shown in fig: 4 below. It follows the same nature as density hysteresis plot. The red rectangle represents heating process. The black circle represents quenching process. It can be observed the in the heating process, there is a sudden increase in the density of the system around 1600k. Also, in the quenching process sudden decrease in the density can be seen around 1200k. The plot clearly forms a hysteresis. This is an indication of first order phase change.
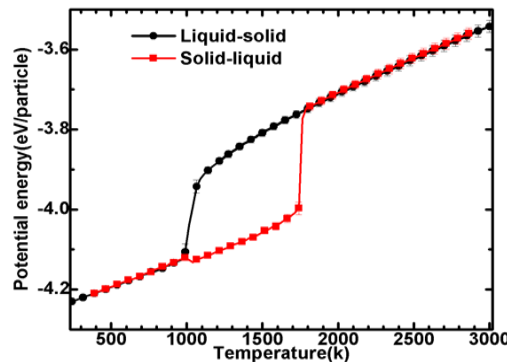
Figure:4 potential energy as a function of temperature similar kind of nature is obtained as density vs. temperature curve

Characteristics of the plot:

The red rectangle represents heating process. The black circle represents quenching process. It can be observed the in the heating process, there is a sudden increase in the potential energy of the silicon around 1600k. Also, in the quenching process sudden decrease in the density can be seen around 1200k. The plot clearly forms a hysteresis just like the density-temperature plot.

4.2 Coordination Number

In this section we illustrate the trend of coordination number of the Si system as we perform heating process. In figure 5 we present radial distribution function. Similarly, in figure 6 presents co-ordination number, which is derived from radial distribution function. The following data represents the variation of coordination number with temperature around melting point temperature:
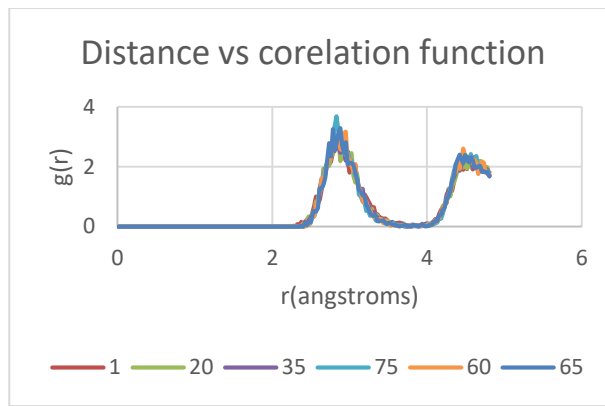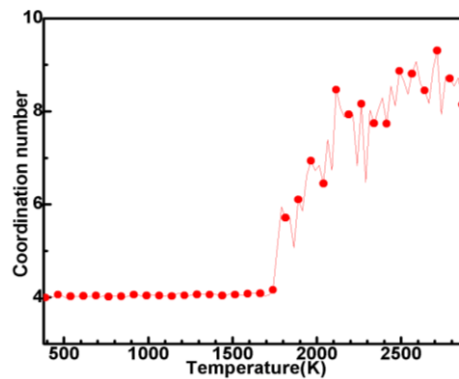
Figure :5 Represents radial distribution function(RDF)

Figure : 6 represents first co-ordination number of silicon as a function of temperature, after melting first co-ordination number sharply rises.

Characteristics of the plot:

From the plot we can see an abrupt rise in the coordination number of the Si system. When, Si is in the diamond lattice form, its coordination number is 4. But due to increase in the temperature of the system, breakdown of the lattice takes place which results in increase of the coordination number.

4.2 **Lindemann Parameter**

In this portion we observe the change of Lindemann parameter as we increase the temperature. It is given by:

$$\delta_L = \sum_{i=1}^{N} \delta_i = \frac{\langle \Delta r_i^2 \rangle^{\frac{1}{2}}}{R}$$
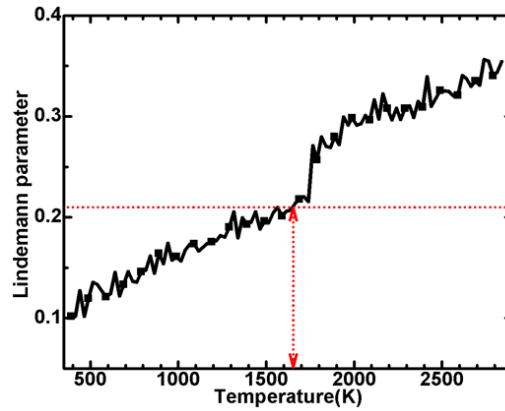
Figure: 7 represents Lindemann parameter as function of temperature, horizontal dotted line indicates critical Lindemann parameter value, while vertical arrow line indicates melting temperature of silicon at critical Lindemann parameter value 0.22.

Characteristics of the plot:

From the plot we can observe an abrupt rise in the Lindemann Parameter of the Si system. This indicates large displacement of the particles from its original position, thus indicating the breakdown of diamond lattice of Si. At melting point, Lindemann parameter is greater than 0.21 for FCC crystal. Vertical red dotted line indication of melting temperature and horizontal dotted line at Lindemann parameter 0.22

4.2 NON-GAUSSIAN PARAMETER:

In this section we observe the change of Non-Gaussian parameter as we increase the temperature. It is given by: $\alpha_2(t) = \frac{3\langle \Delta r^4 \rangle}{5\langle \Delta r^2 \rangle^2} - 1$ *where* $\Delta r = |r_i(t) - R_i(0)|$
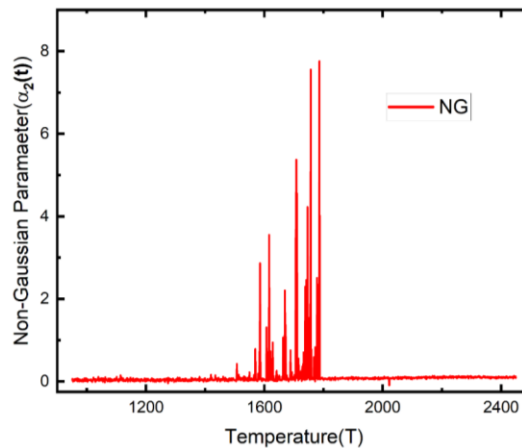

Figure :8 Indicates Non-Gaussian Parameter as a function of temperature, parameter value is very small or close to zero at low temperature however sudden jump is observed due to initiation of melting then drop to zero after completely converted into liquid

Characteristics of the plot:

From the plot we can see that the value of Non-Gaussian Parameter remains low and constant at lower temperatures. This indicates the system is stable and there's no large displacement of particles.

Around 1500 k we see that its value starts to increase and suddenly jumps very high as the temperature further increases. This indicates large displacement of particles, thus suggesting the breakdown of the Si lattice. Lastly, the plot drops and becomes constant indicating the relaxation of the system.

5. Conclusion

Various methods have been employed and we have been successful in observing the phase transition of silicon, depending on various parameters.

The density of silicon in known to be 2.32 g/cc. While simulating with decreasing temperature, this is the value the was noted for density after the melting occurred at approximately 1880 K, which is slightly more than the reported melting point for silicon which is 1687 K.

Also, keeping in mind the traditional meaning of solid to liquid phase transition, the jump in potential energy is also used to indicate the melting stage of any substance. This jump is seen at 1700-1800 K for decreasing temperature and 2400-2500 K for increasing temperature.

For the RDF plots, an atom has a well-defined number of nearest neighbors. On heating there is an increase in the oscillation of atoms about their equilibrium points. On measuring RDF at increasing temperature, as there is a decrease in the number of atoms nearest to it, the peaks slightly change. This is a very clear indication of how the break-down of lattice occurs on heating a substance. The separation and heights of the RDF peaks tells us a lot about the lattice structure of the crystal. Thus basic knowledge about any structural model of any important material can be obtained by doing the RDF analysis it.

We have been successful in showing that there can be various parameters and conditions on which we can predict the melting point of any substance, just by observing the trend of the curves. But we are still not ready with a general rule for any type of substances that could predict the melting point for them. Further, we can work on it and devise a general rule for all particles based on the percentage of Lindemann particles and their transition regions or any other new parameter obtained during study.

7. References

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