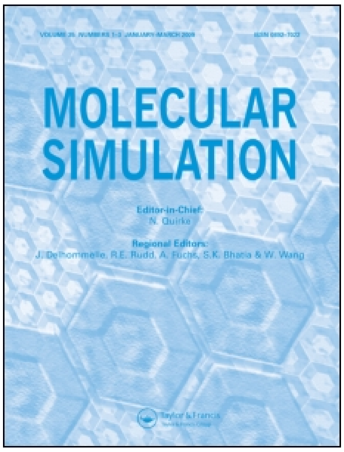

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Vacancy clustering and diffusion in germanium using kinetic lattice Monte Carlo simulations

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To cite this Article Kang, J. W. , Choi, Y. G. , Lee, J. H. , Lee, S. H. and Oh, H. J.(2009) 'Vacancy clustering and diffusion in germanium using kinetic lattice Monte Carlo simulations', Molecular Simulation, 35: 3, 234 — 240
To link to this Article: DOI: 10.1080/08927020802395427
URL: http://dx.doi.org/10.1080/08927020802395427

Molecular Simulation
Vol. 35, No. 3, March 2009, 234–240

Taylor & Francis
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Vacancy clustering and diffusion in germanium using kinetic lattice Monte Carlo simulations

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(*Received 6 April 2008; final version received 31 July 2008*)

We investigated vacancy-assisted self-diffusion in germanium by means of kinetic lattice Monte Carlo (KLMC) simulations below the melting temperature, for a vacancy concentration of $1 \times 10^{18}/\mathrm{cm}^3$. At higher temperatures, fewer clusters formed, but there was less variation in the number of clusters than at lower temperatures as the time increased. Equilibrium diffusivities in the clustering region were 10^2 lower than those of free vacancies in the initial stage of KLMC simulations. They were expressed according to three temperature regimes: $6.5 \times 10^{-4} \exp(-0.35/k_\mathrm{B}T)$ cm^2/s at temperatures above 1100 K, $5.2 \times 10^5 \exp(-2.32/k_\mathrm{B}T)$ cm^2/s at temperatures of 900–1100 K and $6.0 \times 0^{-7} \exp(-0.19/k_\mathrm{B}T)$ cm^2/s at temperatures below 900 K. The effective mean migration energy, 1.1 eV, closely coincided with that of the 1.0–1.2 eV in experiments and was very different from the migration energy of the free vacancy.

Keywords: kinetic lattice Monte Carlo; germanium; diffusion; vacancy

PACS: 61.50.Ah; 61.72.Cc; 61.72.jd

1. Introduction

High intrinsic carrier mobility implies that the germanium-based substrates are a possible alternative to conventional silicon, for applications in advanced nano-electronic devices [1]. There is renewed interest in germanium, because of its superior low-field mobilities, its low dopant activation temperatures and its small band gap that could potentially reduce source/drain parasitic resistance [2]. Thus, 200 and 300 mm germanium substrates recently became commercially viable [1]. Recent developments in process technologies, such as high-*k* gate dielectrics, effectively overcame the technological drawback of integrating germanium in device fabrication, which was limited by the inability to grow the mechanically stable insulating oxide that was comparable to SiO_2 in silicon technology [2]. Czochralski-grown germanium crystals inherently contain lattice defects that can affect the yield and performance of electronic devices built on germanium substrates [3]. A quantitative understanding and subsequent control of the lattice defect formation in germanium crystals is therefore of crucial importance. Lattice defect formation by clustering of intrinsic point defects is mainly governed by their diffusivity and solubility. A well-known problem is the occasional formation of large pits on germanium wafer surfaces. Recently, it was shown that these pits are related to the formation of voids by vacancy clustering during Czochralski crystal growth [4]. In contrast to silicon, these properties are very poorly understood for germanium, mainly due to a lack of reliable experimental data [5].

Vanhellemont et al. [6] have summarised the vacancy of migration energies in germanium obtained from several experiments. From electron-irradiated and low-temperature (25–700 K) annealed oxygen-rich germanium samples, a migration barrier for the single vacancy of about 0.2 eV has been estimated [7]. The diffusivity of vacancies and self-interstitials in the temperature range between 420 and 620 K has also been estimated from photo stimulated electron emission experiments by Ershov et al. [8]. These experiments predicted that the vacancy migration energy is 0.52 ± 0.05 and 0.42 ± 0.04 eV for the uncharged and single negatively charged state, respectively. Recent experiment of Cu and Ni diffusion in germanium [9] showed that, in contrast to silicon, the self-diffusion coefficient in germanium is dominated by vacancy diffusion. The data from self-diffusion experiment leads to a vacancy migration barrier estimation of about 1.0 eV in the temperature range between 973 K and 1173 K [9]. This is, however, in conflict with the above-mentioned low-temperature estimation of 0.2–0.5 eV [7,8]. Van Vechten [10] explained the discrepancy between the low- and high-temperature enthalpy of the vacancy migration by assuming that the transition state of the single-vacancy migration at high temperature is different from that at low

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ISSN 0892-7022 print/ISSN 1029-0435 online

DOI: 10.1080/08927020802395427
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temperature. Pinto [11] suggests that, similar to the silicon vacancy [12], the high-temperature vacancy in germanium differs in properties from the low-temperature one.

In the continuum model, Śpiewak et al. [13] investigated void concentrations using the balance equations which are derived for the discrete and continuous treatment of nucleation phenomena. Continuum models must assume that the behaviour of small vacancy clusters in germanium with respect to their means of aggregation, i.e. whether they diffuse or dissociate [14]. Variation in behaviour over differing ranges of temperature or concentration is not considered in the continuum models [14]. Kinetic lattice Monte Carlo (KLMC) models do not include any assumptions regarding to the behaviour of clusters, since they are based on interactions between individual defects [14]. These models can also simulate much larger systems, over longer times than the molecular dynamics simulations. This work uses a KLMC model to investigate the formation of vacancy clusters and the mechanism by which clusters grow, as a function of the temperature and concentration.

2. Methods

KLMC methods were widely used to simulate atomic scale diffusion processes [14–20]. In this work, we implemented the KLMC method that was used to study the vacancy clustering and diffusion in the silicon by Haley et al. [14]. Lattice defects are randomly examined and if a move to a neighbour site is allowed, each defect is individually moved. Defects can include dopant and native point defects, but in this work are limited to vacancies. Possible movements include vacancies exchanging lattice sites with lattice atoms or other vacancies. After each KLMC step, which randomly examines defects in the system, the simulation time is incremented by a constant time step, that is the time to exchange a vacancy with a germanium lattice atom.

The average rate of movement of defects in solids by the thermal activation can be calculated in the classical rate theory. [21] A migration event is specified by the following two parameters and the hopping rate (ν) can be expressed as:

$$\nu = \nu_0 \exp\left[-\frac{E_\mathrm{m}}{k_\mathrm{B}T}\right], \tag{1}$$

where ν_0 is the attempting frequency as the prefactor and E_m is the migration energy, the free energy needed to change the defect from an initial equilibrium position to a saddle point. Assuming an Arrhenius dependency of diffusivity, the diffusivity is expressed as follows [22]

$$D_\mathrm{V}(T) = D_0 \exp\left[-\frac{E_\mathrm{A}}{k_\mathrm{B}T}\right], \tag{2}$$

where D_0 is the diffusion constant as the pre-exponential factor, E_A is the activation energy, k_B is Boltzmann's constant and T is the absolute temperature. In this work, we used ν_0 calculated with the expression

$$\nu_0 = \frac{8D_0}{a_0^2}, \tag{3}$$

where $D_0 = 1.66 \times 10^{-3}$ cm^2/s and $E_\mathrm{m} = 0.17$ eV by Lauwaert et al. [23] and the lattice constant $a_0 = 5.66$ Å. The V–V binding energy in germanium was only 1.17 eV, which was explained by noting that the Si—Si bonds are stiffer and have higher energy compared to Ge—Ge bonds [2,24].

In KLMC simulations, we can monitor the mean square displacement of vacancies in the cell and evaluate the diffusivity, d_V

$$d_\mathrm{V} = \frac{1}{6}\lim_{t\to\infty}\sum_{i=1}^{N}\frac{|R_i(t) - R_i(0)|^2}{t}. \tag{4}$$

Here, $R_i(t)$ is the position of the ith atom or vacancy at time t.

3. Results and discussion

Considering that the melting temperature of germanium is 1210 K, we performed KLMC simulations for seven different temperatures with concentrations of 1×10^{18}/cm^3 at temperatures below 1300 K. The simulation box was composed of 8×10^6 atomic sites and the periodic boundary condition was applied. Initial vacancies were randomly distributed in the simulation box and defects were randomly examined at each Monte Carlo step. A defect is a member of a cluster if it is a nearest neighbour to at least one and another member of the cluster. The time dependent diffusivity values were obtained from each of the 100 steps using Equation (4).

Figure 1 shows the diffusivity of vacancies as a function of time for various temperatures. The period of the initial constant diffusivity indicates free vacancy diffusion. At temperatures above 1100 K, the diffusivity is always the initial diffusivity, because clusters are not easily formed and most vacancies remain free. At temperatures below 1000 K, as the time increases, diffusivities are decreased in accordance with a power law with an exponent, because clusters form. The time dependency of the diffusivity, D, is expressed as a power of the form;

$$D(t) \sim t^{-\gamma}. \tag{5}$$

In Figure 1, $\gamma = 1.0 \pm 0.2$ is similar to that of silicon. [14]

The diffusivity remains greater at higher temperatures. In general, the power law exponent is greater at lower temperatures. In KLMC simulations, the decreased diffusiv-

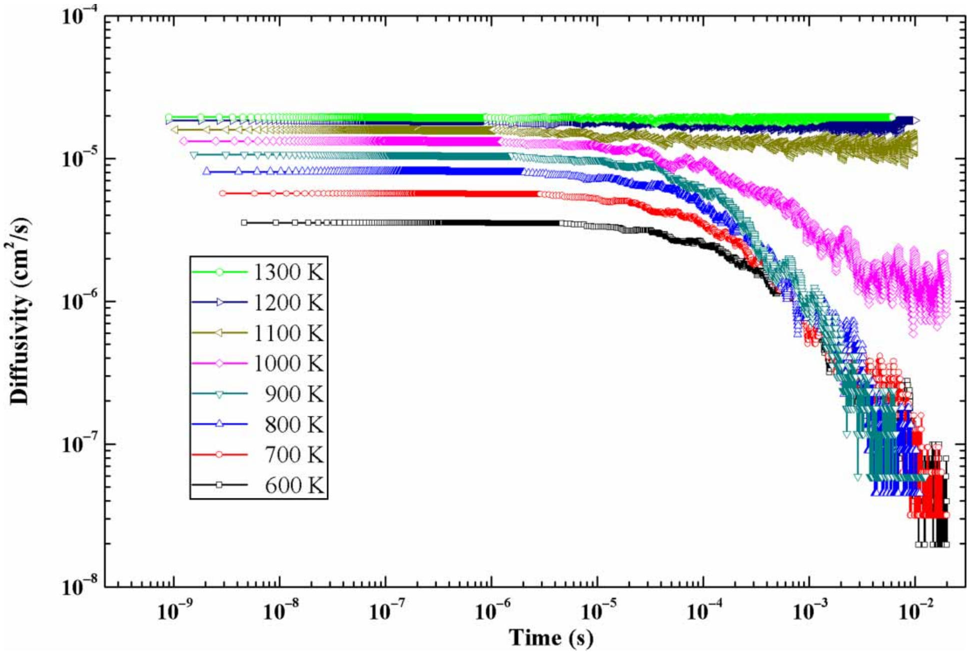

Figure 1. Diffusivity of vacancies as a function of time for various temperatures.

ities are almost constant above 10^{-2} s. The formation of vacancy clusters as a function of time is shown in Figure 2, which shows the fraction of vacancies in clusters as a function of time for various temperatures. As discussed above, at temperatures of both 1100 and 1200 K, the fraction of free vacancies is higher than the others. Figure 2 shows that in KLMC simulations above temperatures of 1100 K, vacancies agglomerate and vacancy clusters grow, then, simultaneously, clusters dissolve. Near the melting temperature of 1200 K, a few vacancies agglomerate in clusters,

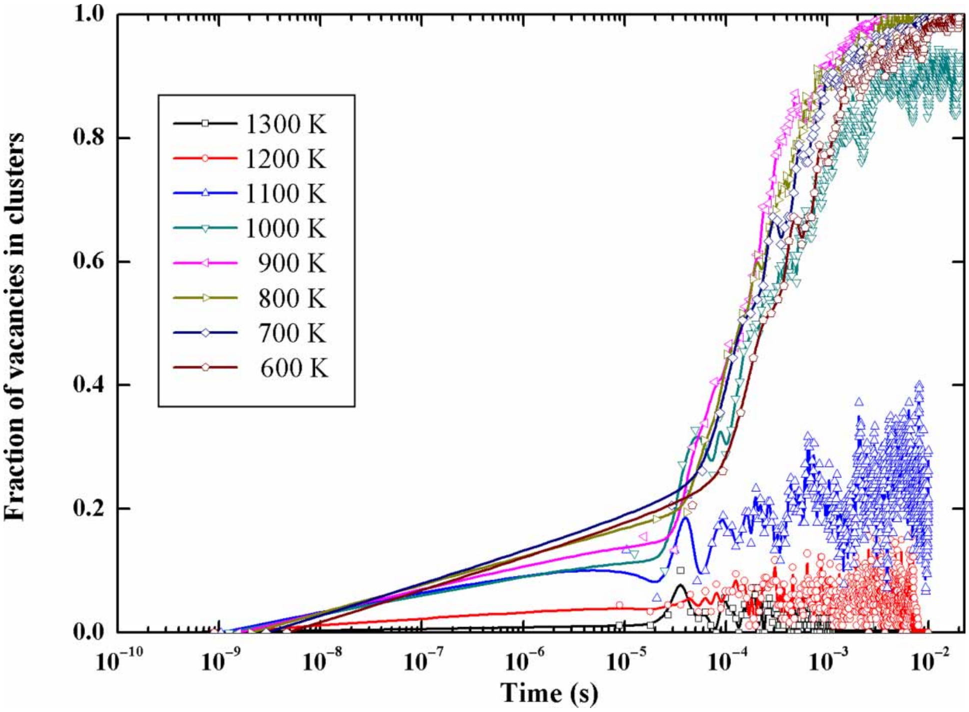

Figure 2. Fraction of vacancies in clusters as a function of time for various temperatures.

but most are immediately dissociated to free vacancies. Since both clustering and dissolving affect vacancy diffusivities, diffusivities of the regime under which clustering phenomena are dominant are $\sim 10^2$ lower than diffusivities of the regime under which dissolving is dominant. For vacancy diffusion in silicon, Haley et al. [14] found that diffusivities of the regime under which clustering phenomena are dominant are $\sim 10^3$ lower than diffusivities of the regime under which dissolving is dominant.

Figure 3 shows the number of clusters as a function of the time, for various temperatures. Below temperatures of 900 K, the number of clusters increases as the time increases. However, the number of clusters is almost constant for temperatures above 1000 K. For the case of a temperature of 1000 K, most vacancies are included in clusters, as shown in Figure 2, but, the number of clusters decreases after reaching its peak, as shown in Figure 3. Figure 4 shows the defect number per cluster, as a function of the time, for given temperatures. At a temperature of 1100 K, the large cluster is found near $t = 0.005$ s and this implies that the clustering effect is dominant at a temperature of 1100 K. At a temperature of 1000 K, the mean size of clusters gradually increases, then remains constant after the peak. However, the mean size of clusters increases very slowly below a temperature of 900 K. The very slow increase of the cluster size at low temperatures was found in the previous work for vacancy diffusion in silicon, investigated by Haley et al. [14]. Figures 2–4 show that vacancy clusters that can grow to large voids can be initiated at a temperature of ~ 1000 K.

Czochralski-grown germanium crystals inherently contain vacancy defects similar to Czochralski-grown silicon crystals and vacancy concentrations in Czochralski-grown germanium crystals are much higher than the equilibrium vacancy concentration [3,13]. So, vacancy clusters can grow to large voids with a size above 100 nm [1,3]. Therefore, effective migration energies for vacancy-assisted diffusions in germanium differ greatly from the migration energy of the free vacancy. The migration energy for the diffusion of a single vacancy was calculated from a known low-density system [14].

Figure 5 shows the calculated vacancy diffusivities in germanium, as well as vacancy diffusivities in silicon obtained from [14]. $T_{\mathrm{m,Si}}$ and $T_{\mathrm{m,Ge}}$ in Figure 5 indicates the melting temperature of silicon and germanium, respectively. Both the initial diffusivities of the vacancy for germanium ($D_{\mathrm{i,Ge}}$) and silicon ($D_{\mathrm{i,Si}}$) are expressed as $9.5 \times 10^{-5} \exp(-0.17/k_{\mathrm{B}}T)$ cm^2/s and $1.89 \times 10^{-5} \exp(-0.1/k_{\mathrm{B}}T)$ cm^2/s, respectively. However, both the stabilised diffusivities after 0.01 s of the vacancy for germanium ($D_{\mathrm{f,Ge}}$) and silicon ($D_{\mathrm{f,Si}}$) are not expressed as a unique equation, but instead expressed as several equations according to the temperature regimes: for germanium, the diffusivities for the three regimes are expressed as $6.5 \times 10^{-4} \exp(-0.35/k_{\mathrm{B}}T)$ cm^2/s at temperatures above 1100 K, $5.2 \times 10^{5} \exp(-2.32/k_{\mathrm{B}}T)$ cm^2/s at temperatures of 900–1100 K and $6.0 \times 10^{-7} \exp(-0.19/k_{\mathrm{B}}T)$ cm^2/s at

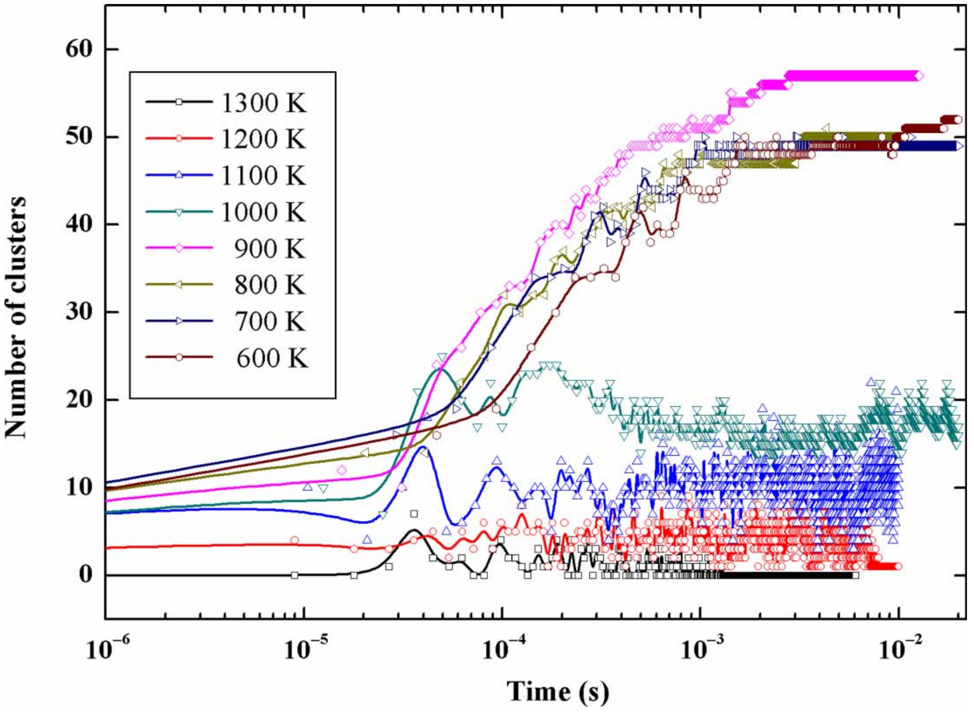

Figure 3. Number of clusters as a function of time for various temperatures.

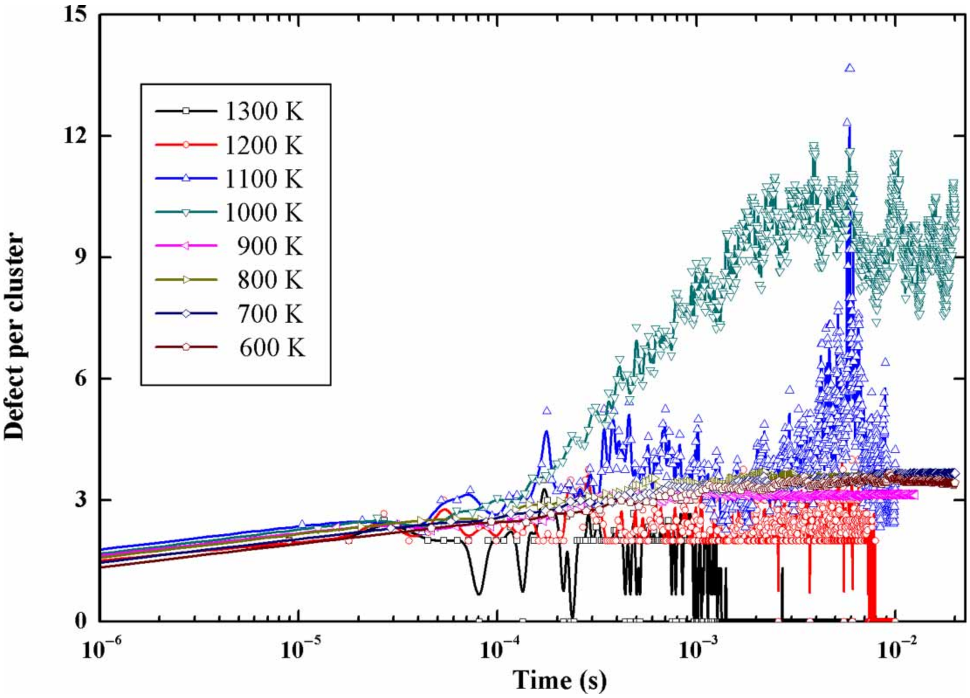

Figure 4. Defect number per cluster as a function of time for various temperatures.

temperatures below 900 K, respectively. In the case of silicon, using the data from [14], the diffusivities for the two regimes are expressed as 2.6×10^{-2} $\exp(-1.35/k_BT)$ cm^2/s at temperatures of 1100–1300 K and 6.5×10^{-4} $\exp(-0.35/k_BT)$ cm^2/s at temperatures below 1100 K, respectively.

For vacancy diffusion in germanium, activation energies strongly depend on diffusion data analysis such

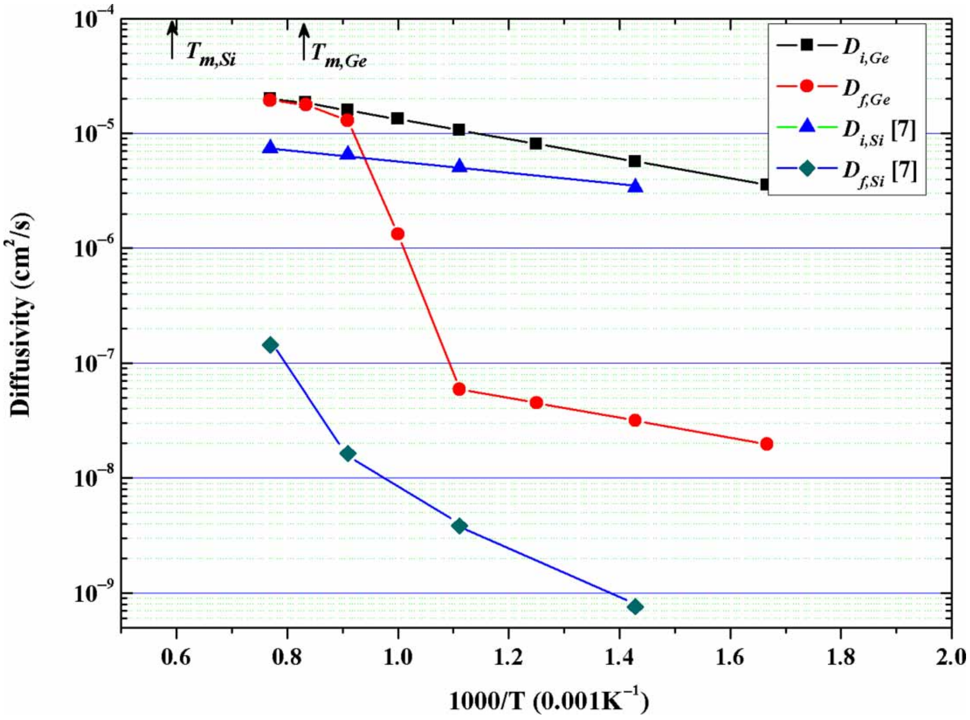

Figure 5. Calculated vacancy diffusivities in germanium as well as vacancy diffusivities in silicon from [7]. $T_{m,Si}$ and $T_{m,Ge}$ indicate the melting temperature of silicon and germanium, respectively.

as 0.2 [11] and 1.0–1.2 eV [9,25–27]. For silicon, the activation energy of vacancy diffusion is still under debate and strongly depends on diffusion data analysis of 0.1–2.0 eV. Recently, Caliste and Pochet [28] showed that the observed temperature dependency for vacancy migration energy was explained by the existence of the three diffusion regimes for vacancies, using KLMC simulations of vacancy-assisted diffusion in silicon. The three effective migration energies of vacancy-assisted diffusion in silicon were 0.46, 1.25 and 2.1 eV under the three temperature regimes and also depended on the vacancy concentration. Their investigation provided a strong explanation for observed temperature variations of vacancy migration energy. We found that the three effective migration energies of vacancy-assisted diffusion for germanium were 0.19, 0.35 and 2.32 eV under the three temperature regimes. This result for germanium is very similar to that of silicon in the previous work by Caliste and Pochet [28].

In Figure 5, effective migration energies for vacancy diffusions at high temperature (above 1000 K) are higher than those at low temperature (below 900 K), thus, the result for germanium is the same as that for silicon, investigated by Caliste and Pochet [28]. They found that the effective migration energy, 2.1 eV of the vacancy diffusion at a temperature of 1273 K was higher than that of 1.25 eV at a temperature of 773 K. However, as the temperature exceeded the melting temperature of silicon 1693 K, the corresponding effective activation energy was found to be 0.46 eV [28]. Since the KLMC simulations were performed below the melting temperature of germanium 1210 K, effective migration energies for germanium at high temperature are higher than those at low temperature, similar to the result for silicon.

In general, the final diffusivities in the cluster region are 10^2 lower than those of free vacancies. Under the temperature regime in which vacancies agglomerate and clusters grow, the effective migration energies for both germanium and silicon are higher than those for other regimes. As shown in Figure 2, below a temperature of 900 K, vacancies are agglomerated into clusters, rather than dissociation of the clusters. Finally, most are included in clusters: a few free vacancies remained under the condition of the low concentration $\sim 10^{16}/\mathrm{cm}^3$, after 0.005 s.

At higher temperatures, fewer clusters are formed, but there is less variation in the number of clusters than at lower temperatures, as the time increases. Clusters which form at higher temperatures tend to be larger on average than those formed at lower temperatures, as shown in Figure 5. The results for vacancies diffusion for germanium are similar to those for silicon [14]. From the results shown in Figures 2–4, the growth of large clusters at lower temperatures operates by different mechanisms than at higher temperatures. At lower temperatures, many small clusters form, mostly vacancy pairs, with most vacancies in the system bound in clusters. Pairs remain bound for relatively long times, during which they aggregate into larger clusters. The rate of aggregation is relatively slow, because diffusion of vacancy pairs is slower than diffusion of free vacancies. At higher temperatures, some vacancy pairs initially form, but many vacancies remain free. Pairs are more likely to dissociate, with constituent vacancies reforming new pairs, thus, at higher temperatures the formation of large clusters involves a combination of aggregation of small clusters and capture of free vacancies. Free vacancies diffuse rapidly, so, larger clusters can form more quickly at higher temperatures. The continuum models of void growth discussed above do not account for this temperature dependency. The difference in vacancy clustering behaviour at lower and higher temperatures could be important when vacancies are used to control diffusion of other species.

Nucleation temperatures of vacancy clustering in silicon are well known as 1300–1370 K [18]. However, the nucleation temperature of vacancy clustering in germanium was never investigated. For our KLMC simulations, the nucleation temperature of vacancy clustering in germanium is estimated as about 900–1000 K. Since the V–V binding energy is higher than the effective migration energy, as the temperature decreases, the hopping rate (or probability) that the vacancy leaves the cluster exponentially decreases; so, diffusivities of clusters are linearly decreased in the log-scale. Considering real-world conditions measured in experiments, final vacancy diffusivities obtained from the work can be considered as the actual diffusivities that were measured. Therefore, when we consider a regression function fitted using final vacancy diffusivities for all temperatures, the mean diffusivity below the melting temperature is estimated by $1\ \exp(-1.1/k_\mathrm{B}T)\ \mathrm{cm}^2/\mathrm{s}$, which closely coincides with the diffusivities obtained from previous experiments, $2\ \exp(-1.2/k_\mathrm{B}T) \sim 4\ \exp(-1.08/k_\mathrm{B}T)\ \mathrm{cm}^2/\mathrm{s}$ [9,26,27]. Especially, the mean effective migration energy, 1.1 eV closely coincides with that of 1.0–1.2 eV in several experiments [9,26,27]. The effective migration energy of 0.19 eV at a low temperatures of below 900 K closely coincides with that of 0.2 eV in the previous experiment [7,25] below 700 K. Considering data between 1000 and 1300 K, the mean diffusivity is estimated by $2.5\ \exp(-1.1/k_\mathrm{B}T)\ \mathrm{cm}^2/\mathrm{s}$ that is in good agreement with $3\ \exp(-1.0/k_\mathrm{B}T)\ \mathrm{cm}^2/\mathrm{s}$ obtained from the previous experiment between 973 and 1173 K [9].

In this work, we investigated various vacancy diffusion regimes for germanium and found that effective activation energies of vacancy diffusions for germanium were dependent on the temperature. This can explain why diffusivities obtained from previous experimental results all differ. The effective migration energy at higher temperatures is higher than that at lower temperatures. The calculated mean effective migration energies of vacancy diffusion for germanium of 1.1 eV, closely coincided with migration energies of 1.0–1.2 eV, obtained from previous experiments [9,24–27]. The trend of temperature dependency of vacancy diffusivity for germanium closely coincided with that for silicon. We considered the nearest interaction between vacancies. Recent work on vacancy-assisted diffusion of silicon considered the 8th neighbour interaction between vacancies [14,18]. Therefore, long neighbour interactions between vacancies in germanium should be included in further work and their binding energies should be obtained from *ab initio* calculations similar to previous work on silicon.

4. Conclusion

We investigated vacancy-assisted self-diffusion in germanium by means of KLMC simulations. Our results provided important information on vacancy diffusion in germanium of below the melting temperature. Equilibrium diffusivities in the cluster region were 10^2 lower than those of free vacancies. Effective migration energies were very different from the migration energy of the free vacancy, which was calculated from a known low-density system. Final diffusivities of the vacancy for germanium were not expressed as a unique equation, but instead expressed as several equations according to the temperature regimes: $6.5 \times 10^{-4} \exp(-0.35/k_B T)$ cm^2/s at temperatures above 1100 K, $5.2 \times 10^5 \exp(-2.32/k_B T)$ cm^2/s at temperatures at 900–1100 K and $6.0 \times 10^{-7} \exp(-0.19/k_B T)$ cm^2/s at temperatures below 900 K. At higher temperatures, fewer clusters formed but there was less variation in the number of clusters than at lower temperatures, as the time increased. The nucleation temperature of vacancy clustering in germanium was estimated as a temperature of about 900–1000 K. The mean migration energy 1.1 eV, closely coincided with that of 1.0–1.2 eV in previous experiments.

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