Mapping the metastability of Lennard-Jones clusters by the maximum vibrational frequency

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We study the structure-stability relationship of the Lennard-Jones (LJ) clusters from a point of view of vibrations. By assuming the size up to \( N = 1610 \), we demonstrate that the \( N \)-dependence of the maximum vibrational frequency reflects the geometry of the core (the interior of cluster) that will determine the overall geometry of the cluster. This allows us to identify the formation of non-icosahedral structures for \( N \leq 150 \), the vacancy formation at the core for \( N \geq 752 \), and the transition from icosahedral to decahedral structures at \( N = 1034 \). We apply the maximum frequency analysis to classify metastable clusters for \( 19 \leq N \leq 39 \), where transformation pathways between different structures are visualized, and the energy barrier height is estimated simultaneously.

I. INTRODUCTION

Assembly of atoms constitutes nanoclusters, and the structure, thermodynamics, and growth process have been extensively investigated for many elemental systems such as Pb, Ni, Au, and transition metals (see also Ref. [9] for a review). The number of atoms \( N \) plays an important role in understanding the stability of clusters because the total energy at a specific \( N \) is particularly low, compared to that at \( N \pm 1 \). In addition, the cluster geometry can be highly symmetric. For example, the clusters at \( N = 13 \) and 55 can have relatively small energy, which is usually attributed to the icosahedral geometry. On the other hand, for large \( N \), the structure of clusters is determined by several factors (i.e., the volume, surface, edges, and vertices of clusters), and the geometry changes from the icosahedral to decahedral to face-centered cubic (fcc) structures as \( N \) increases. For example, the clusters with the decahedral structure have been recently created for several noble metals, which has attracted attention due to their optical and catalytic properties that are different from those with the icosahedral structure.

The stability and geometry of the Lennard-Jones (LJ) clusters have been extensively studied for many years. It has been known that the \( N = 13 \) icosahedron serves as a seed to generate the lowest energy atomic configurations, that is, the LJ clusters for \( N \geq 13 \) have an icosahedron at the core surrounded by the surface atoms. However, for the cases of \( N = 38, 75-77, 98, \) and \( 102-104 \), the core of the LJ clusters has octahedral, decahedral, tetrahedral, and decahedral structures, respectively. Even when the energetic stability analyses are employed, no significant anomalies have been found at these \( N \)s. In general, the cluster geometry is characterized by studying the local atomic environment in detail, as done by Polak and Patrykiejew and Yang and Tang, where they used four structural motifs (fcc, hcp, icosahedral, and decahedral) to understand the overall and core geometries. Alternatively, we expect that the lattice dynamics calculations might be useful to understand the core geometry because the normal modes at the maximum frequency will involve the vibration of the most rigid part in the system. For example, the sequence of the maximum frequency as a function of \( N \) should identify the difference of the core geometries in the LJ clusters.

In this paper, we study the energetic and vibrational properties of LJ clusters up to \( N = 1610 \). The \( N \)-dependence of the maximum frequency allows us to identify the core geometry that is different from the icosahedral structure. It also enables us to identify the vacancy formation at the core and the structural transition from icosahedra to decahedra for large \( N \). As another application, we construct a metastability map, where the maximum frequency is plotted as the total energy for many metastable structures. For the cases of \( 19 \leq N \leq 39 \), we distinguish the clusters with decahedra from those with icosahedra. In addition, we identify transformation pathways between different structures, and estimate the energy barrier height. The present work will pave the way to understand the structural stability and geometry based on the vibrational frequency.

The vibrational frequency analysis has been recently applied to study the magic numbers in \( N \) charges on a sphere, while finding the lowest energy configurations on a sphere is known as the Thomson problem. The maximum frequency showed relatively small values at \( N = 12, 32, 72, 132, 192, 212, 272, 282, \) and 372. The presence of these magic numbers reflects both the charge configurations on a sphere and the strong degeneracy of the one-particle energies. In contrast, the LJ particles that we study in the present work are free from the boundary condition, and therefore the core geometry of the system influences the vibrational properties. Doye and Calvo have calculated the geometric mean vibrational frequency of the LJ clusters to distinguish the non-icosahedral structures from the icosahedral structure at the selected sizes of \( N = 38, 75, 98, \) and 102. The maximum frequency that we use in the present work is directly related to the vibration of the core around which the interatomic bonding is the strongest in the cluster.
II. THEORY

We study the dynamics of the LJ clusters having \( N \) atoms within the harmonic approximation. The equations of motion can be written as

\[
m \frac{d^2 u_{\alpha i}}{dt^2} = - \sum_{j \beta} D^{ij}_{\alpha \beta} u_{j \beta},
\]

where \( u_{\alpha i} \) is the displacement along \( \alpha \) direction for the particle \( i \) with a mass of \( m \). The force constant matrix \( D^{ij}_{\alpha \beta} \) is defined as

\[
D^{ij}_{\alpha \beta} = \frac{\partial^2 E}{\partial R_{\alpha i} \partial R_{j \beta}} |_{0},
\]

where the derivative is taken at the equilibrium configurations. \( E \) is the total potential energy

\[
E = \sum_{i=1}^{N} \varepsilon_i
\]

with the one-particle energy

\[
\varepsilon_i = \frac{1}{2} \sum_{j \neq i} 4A \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right],
\]

where 1/2 accounts for the double counting of the interaction energy, \( A \) and \( \sigma \) are parameters of the LJ potential, and \( r_{ij} \) is the interparticle distance between the LJ particles \( i \) and \( j \), which can be expressed by

\[
r_{ij}^2 = \sum_{\alpha=x,y,z} (R_{i \alpha} - R_{j \alpha})^2,
\]

where \( R_{i \alpha} \) is the \( \alpha \) component of the position of the particle \( i \). Assuming a stationary solution \( u_{\alpha i}(t) = \varepsilon_{\alpha i} e^{i \omega t} \) with the frequency \( \omega \) and the polarization \( \varepsilon_{\alpha i} \), one obtains the eigenvalue equation

\[
m \omega^2 \varepsilon_{\alpha i} = \sum_{j \beta} D^{ij}_{\alpha \beta} \varepsilon_{j \beta}.
\]

The stable structure with \( N \) particles has \( 3N - 6 \) vibrational modes, where the degrees of freedom for translation and rotation are subtracted. The maximum eigenvalue gives the maximum frequency \( \omega_{\text{max}} \). The units of energy and frequency are \( A \) and \( A^{1/2} \sigma^4 m^{-1/2} \), respectively. Throughout the paper, we set \( A = \sigma = m = 1 \).

To find the lowest energy structures, we referred to two databases: For \( 3 \leq N \leq 150 \), we referred to the Cambridge Cluster Database (CCD) [34], and for large \( N \) up to 1610, we referred to the database provided by Shao et al. [35] (310 to 561 atoms [21], 562 to 1000 atoms [22], and 1001 to 1610 atoms [24]). We used the Broyden-Fletcher-Goldfarb-Shanno algorithm [36] to find the local minimum structures for the cases of \( N = 31, 33, \) and \( 35, 6 \times 10^4 \) initial configurations were needed to obtain the lowest energy structures stored at the CCD [34]. However, we failed to find the lowest energy structure at \( N = 38 \).

To compare the optimized \( E/N \) and \( \omega_{\text{max}} \) with the bulk values (i.e., the case of \( N \to \infty \)), we calculated the total energy and the phonon dispersions of the LJ crystal in the fcc structure. The computational details are the same as those described in Ref. [37], while \( A \) and \( \sigma \) were set to be unity in the present work. We obtained \( E_{\text{fcc}}^N / N = -8.609 \) and \( \omega_{\text{max}}^N = 28.18 \) that corresponds to the longitudinal phonon frequency at the \( X \) point in the Brillouin zone.

III. RESULTS AND DISCUSSION

A. Lowest energy structures

Figure 1(a) shows the \( N \)-dependence of the lowest energy per particle \( E_{\text{min}}/N \). The \( E_{\text{min}} \) decreases with \( N \), while some dips can be observed at \( N = 13 \) and \( N = 55 \). At these \( N \)s complete icosahedral structure can be formed [14, 19]. To emphasize the magic numbers, at which the \( N \) cluster is relatively stable compared to \( N \pm 1 \) clusters, we define the first and second differences in the total energy as

\[
\Delta E = E_{\text{min}}(N - 1) - E_{\text{min}}(N),
\]

\[
\Delta^2 E = E_{\text{min}}(N - 1) + E_{\text{min}}(N + 1) - 2E_{\text{min}}(N).
\]

Figures 1(b) and 1(c) show the \( N \)-dependence of \( \Delta E \) and \( \Delta^2 E \), respectively. Peaks in \( \Delta^2 E \) are observed at several \( N \)s. For example, \( N = 13, 55, \) and 144 are clearly identified as the magic numbers, where \( N = 144 \) cluster has also complete icosahedral structure. The relative stability between different \( N \)s can thus be identified by studying \( \Delta E \) and/or \( \Delta^2 E \).

To shed light on another aspect on the LJ cluster properties, we show the \( N \)-dependence of \( \omega_{\text{max}} \) in Fig. 1(d).
The value of $\omega_{\text{max}}$ increases with $N$. However, an anomalous decrease in $\omega_{\text{max}}$ is observed at $N = 38, 75-77, 98,$ and $102-104$. It should be noted that the lowest energy structures at these $N$s do not have icosahedra at the core [15, 16, 19, 34]. This shows that the atomic displacement of the maximum frequency mode reflects the core geometry: For example, $N = 38$ and $75$ clusters has an octahedron and a decahedron at the core, and the displacement pattern is a breathing of the octahedron for $N = 38$ and asymmetric displacements along the fivefold symmetric axis for $N = 75$, as shown in Fig. 2. The maximum frequency mode for the $N = 76, 77$, and $102-104$ clusters is similar to that for the $N = 75$ cluster: the core at $N = 102-104$ has 19 atoms forming a one-dimensional tube of three decahedra with the fivefold rotational symmetry, and the displacement pattern shows the expansion, contraction, and expansion of the three decahedra. The $N = 98$ cluster has a large core with tetrahedral shape [16], and the displacement localizes to this core in a complicated manner. In this way, the analysis of the $N$-dependence of $\omega_{\text{max}}$ allows us to distinguish the core geometry from icosahedra.

The difference of the core geometry as well as the decrease in $\omega_{\text{max}}$ are related to the distribution of $\varepsilon_i$ in Eq. (4). In general, the $\varepsilon_i$ of the core atom $i$ is lower than that of the surface atoms because the interatomic bonding strength as well as the coordination number will be large around the core. The values of $\varepsilon_i$ are thus scattered as $N$ increases because the core and surface regions are clearly separated for large $N$. The distribution of $\varepsilon_i$ will be modified when the geometry of the core changes. Figure 1(e) shows the standard deviation $\sigma$ of $\varepsilon_i$ as a
As shown in Fig. 1(a), the $E_{\text{min}}/N$ approaches the $E_{\text{min}}^{\text{fcc}}/N$ as $N$ increases. However, the energy difference is still large: $E_{\text{min}}/N = -5.955$ for $N = 150$, and the relative error is more than $30\%$. When $N$ is increased up to 1610, $E_{\text{min}}/N = -7.338$, and the error is reduced to $15\%$. It is interesting to study how the $\omega_{\max}$ approaches the bulk value of $\omega_{\max}^{\text{fcc}}$ because the $N$-dependence of $\omega_{\max}$ is nonmonotonic for small $N$, as shown in Fig. 1(d). In addition, Shao et al. have proposed the vacancy formation at the core for $N \geq 752$ and the structural transition from icosahedra to decahedra at $N = 1034$, which will influence the $N$-dependence of $\omega_{\max}$. Figure 4 shows the $\omega_{\max}$ as a function of $N$ up to 1610: (i) the $\omega_{\max}$ increases from 37 to 43 for $151 \leq N \leq 600$, except for $188 \leq N \leq 192$ and $236 \leq N \leq 238$; (ii) the value of $\omega_{\max}$ decreases to 35 around $N \approx 600$, deviates around 35 for $600 \leq N \leq 800$, and increases from 35 to 36 for $800 \leq N \leq 1034$; and (iii) the $\omega_{\max}$ shows a sudden drop to 29 at $N = 1035$, and almost keeps the constant value of 29 up to $N = 1610$, while the jump within $1367 \leq N \leq 1422$ is observed.

The property (i), an increase in $\omega_{\max}$ with $N$, indicates the hardening of the core in the cluster, which is also observed in small $N$ (see Fig. 1(d)). The property (ii), an significant decrease in $\omega_{\max}$ from 43 to 35, reflects the vacancy formation at the core: for $N \geq 752$ the icosahedral structures with the central vacancy are more stable except for $N = 923$. We consider that some of the peaks around $600 \leq N \leq 800$ and $N = 923$ will be a reminiscence of the behavior for $N \leq 600$. The property (iii) indicates the transition from the icosahedral to decahedral structures. The jump of $\omega_{\max}$ within $1367 \leq N \leq 1422$ is also consistent with the formation of the icosahedral structure with the central vacancy at $N = 1402$. In this sense, the anomalous decreases around $188 \leq N \leq 192$, $236 \leq N \leq 238$, $650 \leq N \leq 664$, $682 \leq N \leq 689$, $755 \leq N \leq 762$, and $815 \leq N \leq 823$ can be attributed to the formation of the decahedral structure. The decahedral and icosahedral structures for the selected $N$s are shown in Fig. 4.

It should be noted that the $N$-dependence of $\omega_{\max}$ is strongly correlated with that of the fcc motif concentration. Yang and Tang studied how many structural motifs are there in the LJ cluster for each $N$ by considering four types of motifs in the fcc, hcp, icosahedral, and decahedral structures with 13 atoms, and showed that the fcc motif concentration is relatively large when $N = 38, 75-78, 102-104, 188-192, 236-238$, and $N \approx 1030$. They attributed such an enhancement to the formation of the Marks decahedron rather than the Mackay icosahedron, which is consistent with our characterization in geometry.
FIG. 4. The $N$-dependence of $\omega_{\text{max}}$ for the lowest energy structures: $151 \leq N \leq 1610$. The dot-dashed line indicates the $\omega_{\text{fcc}}$. The four clusters with the decahedral structure (colored red) are shown. The $N = 1402$ cluster with the icosahedral structure is also shown, where the central vacancy is colored blue and the interatomic bonding is illustrated for $r_{ij} \leq 1.05\sigma$.

FIG. 5. (left) The distribution of $\omega_{\text{max}}$ versus the total energy of $E$ for the 2000 lowest energy structures with $N = 19$. The plotted points are classed into seven groups, where the group 6 includes three points. (right) The illustration of metastable structures of groups 1-7, where the group 6 structures have a decahedron (colored red). The arrows indicate the atomic movements from the group 1 structure.

B. Metastable structures

We next apply the $\omega_{\text{max}}$-based analysis to a classification of the metastable structures with $N$ fixed. Figure 5 shows the distribution of $\omega_{\text{max}}$ as a function of $E$ for the case of $N = 19$, where the 2000 lowest energy structures are plotted. Data points form an island in the $E$-$\omega_{\text{max}}$ plane, which enables us to classify metastable structures into some groups. The lowest energy structure (group 1) is a barrel-shaped double icosahedron, where four atoms form the symmetry axis along which three pentagons are stacked with twisted angle of $\pi/5$. The structures of other groups are basically derived from the group 1 structure (see Fig. 5): in the second lowest energy structure (group 2), the vertex located on the symmetry axis moves to another facet; in the group 3 and 4 structures, the vertex on the first (or third) and second layer of the pentagon moves to another facet, respectively; and in the group 5 structures, two vertices move to other facets. As one approaches the continent (i.e., densely plotted region for
FIG. 6. The distribution of $\omega_{\text{max}}$ versus the total energy of $E$ for the 2000 lowest energy structures with $N = 20-39$. The data of the lowest energy structure is indicated by a large circle (colored red). The dashed line indicates the $\omega_{\text{fcc}}$.

$E \geq -69$, the structures with more complex geometry are observed.

One can find three anomalous structures, which are apart from the continent, with $-70 \leq E \leq -69$ and relatively small values of $\omega_{\text{max}} (\simeq 20.8)$. As depicted in Fig. 5, those metastable structures (group 6) have a decahedron at the core. This result also confirms that the clusters with non-icosahedra can have relatively small $\omega_{\text{max}}$.

We also found that some of the structures have a decahedron: For example, those structures have $(E, \omega_{\text{max}}) = (-68.9578, 20.81)$ and $(-68.6245, 20.92)$. Among the 2000 structures generated in the present calculations, the 142th structure ($E = -68.8976$) has the lowest maximum frequency of $\omega_{\text{max}} = 19.77$, but has neither a decahedron nor an icosahedron at the core region (see group 7 in Fig. 5).

The $E$-$\omega_{\text{max}}$ map gives a rough estimation of the energy barrier height between different structures. For example, the transformation from the group 1 to group 2 can be possible when the energy about $2 \AA$ is added. On the other hand, to obtain the clusters with the decahedral structures, the structure in the group 1 must first move to the continent around $E \geq -68$, and next moves to the island of the group 6, implying that more than $5 \AA$ (rather than $3 \AA$) is needed. This view is consistent with that obtained by the disconnectivity graph calculations.

It is interesting that when the metastable structures differ strongly in geometry, those are located at different region in the $E$-$\omega_{\text{max}}$ plane, as shown in Fig. 5. This gives us the information of the energy barrier height between different structures.

For $N = 19$, the lowest energy structure has a relatively high value of $\omega_{\text{max}}$, while some metastable structures have relatively small values of $\omega_{\text{max}} \simeq 22$. This view is consistent with that obtained by the disconnectivity graph calculations.

For $N = 38$, the lowest energy structure is constructed from a decahedron surrounded by five decahedra, whereas the second lowest energy structure ($\omega_{\text{max}} = 23.5$) is constructed by adding an atom to the $N = 38$ octahedral structure. The en-
nergy barrier height between them is estimated to be more than 5.4 rather than 2.4. In this way, the construction of the $E$-$\omega_{\text{max}}$ map is a useful method to understand the transformation between metastable structures, which will be alternative to the disconnectivity graph constructions [17].

The structural transition from the icosahedral to decahedral structures has been discussed in the literature. Deaven et al. identified a significant change in the one-particle energy distribution [14]: The peak of the lowest one-particle energy shifts dramatically from $\varepsilon_i \simeq -6.5$ at $N = 30$ to $\varepsilon_i \simeq -7$ at $N = 31$. On the other hand, Raoult et al. [12] and Shao et al. [24] showed that the structural transition to the decahedral structure occurs at $N > 1000$ by performing the the total energy calculations. The present calculations suggest that the profile of the $\omega_{\text{max}}$ distribution is quite different across $N = 31$. We expect that the systematic calculations of the $\omega_{\text{max}}$ distribution for large $N$ enable us to understand the structural transitions (from the icosahedral to decahedral, and from the decahedral to fcc structures as well).

IV. CONCLUSION

In conclusion, we studied the $N$-dependence of the total energy $E$ and the maximum frequency $\omega_{\text{max}}$ of the LJ clusters with the size up to $N = 1610$. The $\omega_{\text{max}}$ reflects the atomic vibrations localized at the core region, and the magnitude of $\omega_{\text{max}}$ is significantly small when the core geometry is different from an icosahedron (e.g., $N = 38$, 75–77, 98, and 102–104). The $\omega_{\text{max}}$ also reflects the vacancy formation at the core and the structural transition from icosahedra to decahedra for large $N$. Based on the relationship between the $E$ and $\omega_{\text{max}}$ for the cases of $19 \leq N \leq 39$, we created the metastability map that can provide both transformation pathways between different structures and an estimation of the energy barrier height.

We hope that the $\omega_{\text{max}}$-based approach is applied to study the metastability of more realistic systems including metallic and semiconducting clusters by using accurate potentials. On the other hand, the allotropes of fullerene molecules will show different $N$-dependence of $\omega_{\text{max}}$ because of the hollow spherical structures.

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