Transverse excitations in liquid metals

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Abstract. The transverse acoustic excitation modes were detected by inelastic x-ray scattering in liquid Ga, Cu and Fe in the Q range around 10 nm^{-1} using a third-generation synchrotron radiation facility, SPring-8, although these liquid metals are mostly described by a simple hard-sphere liquid. *Ab initio* molecular dynamics simulations clearly support this finding for liquid Ga. From the detailed analyses for the $S(Q,\omega)$ spectra with good statistic qualities, the lifetime of less than 1 ps and the propagating length of less than 1 nm can be estimated for the transverse acoustic phonon modes, which correspond to the lifetime and size of cages formed instantaneously in these liquid metals. The microscopic Poisson's ratio estimated from the dynamic velocities of sound is 0.42 for liquid Ga and about –0.2 for liquid transition metals, indicating a rubber-like soft and extremely hard elastic properties of the cage clusters, respectively. The origin of these microscopic elastic properties is discussed in detail.

INTRODUCTION

Lattice modes, or collective modes, are modes of vibration of the entire systems. In the long wavelength limit, they can be described by the classical theory of elasticity in which the system is treated as a continuum possessing macroscopic elastic constants as shown in Fig. 1(a). As the wavelength becomes shorter, approaching the distance between atoms, the microscopic structure of the system, and the forces between individual pairs of atoms, describe the dominant features in determining the nature of the modes of vibration as illustrated in Fig. 1(b).

In simple liquids, longitudinal acoustic phonon modes are always observed by ultrasonic, optical, or inelastic scattering experiments because the density fluctuations can occur due to a strong repulsive force between the atoms when they approach each other. However, transverse phonon modes usually cannot be detected in liquids by ultrasonic or optical measurements because the shear force in the long spatial range is very weak if the liquid has no long-range network such as covalent glass-forming materials.

When the atomic vibration wavelength in a liquid approaches the atomic nearest neighbor distance, i.e., in the terahertz frequency region, the situation changes. There may be a solid-like cage effect on the nanometer scale that acts as a restoring force for acoustic transverse modes. If the above speculation is correct, transverse acoustic modes could be realized experimentally

(a) sound, light

continuum
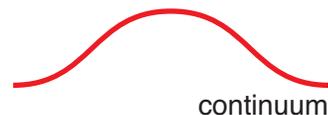
(b) x-ray, neutron
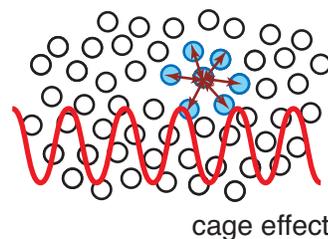
cage effect

FIGURE 1. (Color online.) Various wavelength of waves and cage effect in liquids. (a) sound or light, (b) x-ray or neutron.

even in liquid metals in dynamic structure factor $S(Q,\omega)$ measurements by inelastic x-ray or neutron scattering (IXS or INS) which covers the terahertz and nanometer ranges.

The transverse acoustic modes in simple liquids have been discussed theoretically for more than thirty years. Levesque and coworkers [1] performed a molecular dy-

namic (MD) simulation using a Lenard-Jones potential, which revealed the existence of the transverse acoustic modes in simple liquids. Hansen et al. [2] presented a MD work of time-dependent correlation functions of a classical one-component plasma, and pointed out the existence of high-frequency transverse modes for large Q values. This has been reviewed in several textbooks on simple liquids [3, 4, 5].

Shimojo et al. [6] and Kahl and Kambayashi [7] performed MD simulations using more realistic potentials for liquid Na and Rb, respectively. However, the contribution of the transverse acoustic modes to $S(Q,\omega)$ was negligible since their magnitudes are relatively small and they are highly damped. Thus, the transverse modes in liquid alkali metals may have been masked by the strong and broad longitudinal acoustic excitations and/or quasielastic peaks.

In a previous IXS study on liquid Ga, narrow longitudinal acoustic phonon modes were observed, indicating a positive deviation from the hydrodynamic velocity of sound by about 13% [8]. In addition, subpicosecond (0.39 ps) correlations between the neighboring atoms or short-living covalent bonds were found in the feature of qusielastic lines at the first structure factor $S(Q)$ maximum [9].

Of particular interest was that indications of transverse-like low-energy excitations were observed as shoulders of the quasielastic peak in liquid Ga [9]. This finding may be related to the appearance of the short-living covalent bonds. However, the fit results were scattered as a function of Q due to the insufficient statistics, and it was impossible to discuss the dynamical properties of the transverse-like excitations in detail.

In order to confirm the existence of the transverse acoustic modes, we have precisely measured IXS on liquid Ga [10, 11], Cu, and Fe. In this paper, we present the experimental proof of transverse modes in these liquid metals and discuss the longitudinal and transverse elastic properties in detail.

EXPERIMENTAL PROCEDURE

The liquid metal sample was contained in a single-crystal sapphire cell, which is the so-called Tamura-type cell [12]. The cell and the compact heating system used for liquid metals with a melting temperature lower than 1000°C, Ga, are illustrated in Fig. 2(a), and the sample part is shown in Fig. 2(b) on an enlarged scale. The figures are taken from Ref. [12, 13]. The liquid metal sample was sandwitched between the thin walls (0.25 mm) of the single crystal sapphire. The manufacturing process of the cell and the filling procedure with the sample are in detail given elsewhere [12]. The high x-ray absorption of liquid metals was handled by reducing the sample
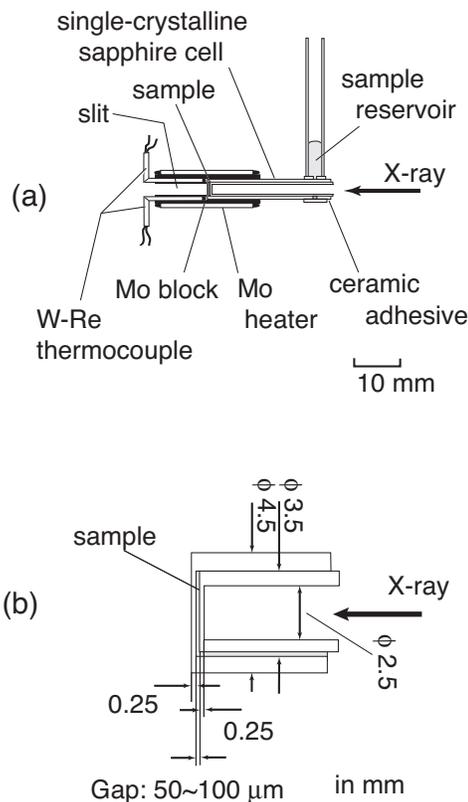
FIGURE 2. (a) The single-crystalline sapphire cell and the heating system used for the present IXS experiment on liquid metals with a melting temperature lower than 1000°C. (b) The sample part shown on an enlarged scale. After Ref. [12, 13].

thickness to 50–100 μm. The purity of the samples was 99.9999%.

Figure 3 shows the cell used for liquid metals with a high melting temperature higher than 1000°C, Cu and Fe. The figure is taken from Ref. [13]. Since the melting point of liquid metal is higher than the softening temperature of the ceramic adhesive, a reservoir-less cell was designed for the high-melting temperature liquid metals. It was inserted in the same heating system shown in Fig. 2(a).

The cell was placed in a vessel [14] equipped with single-crystal Si thin windows capable of covering the scattering angles between 0° and 25°. It was applied with 1.5 bar of high purity grade He gas. The temperature beyond the melting points of liquid metals was achieved by using a Mo resistant heater, and monitored and controlled with two W-5%Re/W-26%Re thermocouples. The IXS measurements were carried out between about $Q = 7$ and 12 nm^{-1} over ω of ± 40 meV. The liquid phase of the sample was confirmed by measuring $S(Q,0)$ spectra dur-
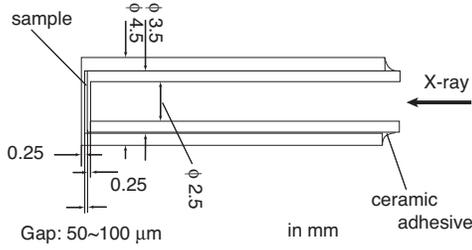
FIGURE 3. The single-crystalline sapphire cell used for the present IXS experiment on liquid metals with a melting temperature higher than 1000°C. After Ref. [13].

FIGURE 4. (Color online.) Inelastic x-ray scattering spectra of liquid Ga [10, 11], Cu, and Fe (from top to bottom) at $Q = 10.6 \sim 12.0$ nm^{-1}.

ing the experiment.

The IXS experiments were performed at the beamline BL35XU in the SPring-8 using a high energy-resolution IXS spectrometer [15]. A monochromatized beam of 3.5×10^9 photons/s was obtained from a cryogenically cooled Si(111) double crystal followed by a Si (11 11 11) monochromator operating in extremely backscattering geometry (89.975°, 21.75 keV). The same backscattering geometry of twelve two-dimensionally curved Si analyzers was used for the energy analysis of the scattered X-ray photons. The energy resolution was determined by the scattering from a Plexiglas sample and values of 1.6-1.9 meV (FWHM) were found for the detecting systems depending on the analyzer crystals. The Q resolution was set to be about ± 0.30 nm^{-1}.

RESULTS

Figure 4 shows the selected results of IXS intensity at $Q = 10.6 \sim 12.0$ nm^{-1} for liquid Ga [10, 11], Cu, and Fe. At these Q values, longitudinal acoustic excitations are clearly seen as peaks at about 18 meV for liquid Ga, 23 meV for liquid Cu, and 28 meV for liquid Fe, depending on the velocities of longitudinal acoustic sound in these liquid metals.

Besides the longitudinal excitations, small extra excitations can be observed as shoulders between the quasielastic peak and longitudinal acoustic excitation peaks at about 7 meV for liquid Ga, 13 meV for liquid Cu, and 17 meV for liquid Fe. With decreasing Q, such small extra modes become invisible below $Q \sim 8$ nm^{-1}.

In order to clarify the contribution of the extra excitations, the $S(Q,\omega)$ data were analyzed by using a damped harmonic oscillator (DHO) model [16] expressed as,

$$\left[\frac{1}{1 - e^{-\hbar\omega/k_B T}} \right] \frac{A_Q}{\pi} \frac{4\omega\omega_Q\Gamma_Q}{(\omega^2 - \omega_Q^2)^2 + 4\Gamma_Q^2\omega^2}, \quad (1)$$

for 'two' excitation modes each and a Lorentzian for the quasielastic line. Here, A_Q and ω_Q are the amplitude and

energy of the inelastic excitation modes, respectively, and Γ_Q is the width close to half-width at half-maximum.

Solid curves on the data in Fig. 4 indicate the best fits of the double DHO model, convoluted with the resolution function, to the experimental data. This double DHO model reproduces well each of the experimental $S(Q,\omega)$ function. The thin dotted curves are Lorentzians for the quasielastic peak, and the thick dashed and thin chain curves are the DHO functions for the transverse and longitudinal inelastic modes, respectively. As Shown in Fig. 4, the transverse modes are similar to the longitudinal modes in intensity or height in each liquid metal at $Q = 10 \sim 12$ nm^{-1}. However, the intensity of the transverse mode largely decreases with decreasing Q in each liquid metal (not shown), and below $Q \sim 8$ nm^{-1}, fits using single DHO function were sufficient with the fit routines giving the transverse mode intensity nearly zero. Thus, the transverse excitation modes may either merge into the quasi elastic peak or rapidly decrease in intensity with decreasing Q.

DISCUSSION

Figure 5(a) shows the dispersion relation of the transverse (open circles) and longitudinal (solid triangles)

acoustic phonon excitation modes in liquid Ga [10, 11] obtained from the fit. The small solid circles indicate the previous longitudinal results [8]. The present longitudinal results agree well with previous ones [8, 17, 18]. The dashed line is the dispersion of hydrodynamic sound at the low Q limit determined by the adiabatic sound velocity [19]. The dynamical sound velocity, ω_Q/Q, of the transverse mode would be slightly larger than 1050 m/s, much less than a half (36%) of the longitudinal sound velocity. The microscopic shear modulus of liquid Ga can be estimated to be about 6.5 GPa, which is about 1/6 of the crystal value of 40 GPa [21].

González and González carried out an orbital-free *ab initio* MD simulation on liquid Ga at 100°C, and discussed the transverse current correlation functions [20]. This simulation has repeated at 40°C, and the dotted curve in Fig. 5(a) represents the obtained transverse phonon excitation energies [10]. These theoretical values are slightly smaller than the present experimental values, and continue to the lower Q values.

Since the transverse phonons do not create the density fluctuations towards the direction of scattering vector, $\vec{Q}$, the transverse phonons were believed not to be detected from scattering experiments. This problem may be solved by taking the mixing of the longitudinal and transverse modes into account as discussed in [10, 11]. Due to the lack of the translational invariance, the pure symmetry character of the two modes is lost, and both the modes contribute to some extent to both the current spectra. Thus, the transverse modes can be detected through the quasi-transverse sound branches in the *longitudinal* current correlation spectrum.

In liquid Ga, the above-mentioned MD simulation also revealed the quasi-transverse branch in the longitudinal current spectra as small peaks or shoulders. These energies are shown by the solid curve in Fig. 5(a), and almost coincide with the peak positions in the transverse current spectra (dotted curve), and the experimental values. This is clear evidence of the existence of the transverse phonon modes in liquid Ga measurable by IXS.

Figure 5(b) shows the dispersion relation of the transverse (open circles) and longitudinal (solid triangles) acoustic phonon excitation modes in liquid Cu obtained from the fit. The small solid circles indicate the previous longitudinal results [22], and the present longitudinal results agree well with previous ones. The dashed line is the dispersion of hydrodynamic sound at the low Q limit determined by the adiabatic sound velocity [23]. The dynamical sound velocity, ω_Q/Q, of the transverse mode is about 2650 m/s, much larger than a half (about 77%) of the longitudinal sound velocity. The microscopic shear modulus of liquid Cu can be estimated to be about 56 GPa, which is slightly smaller than the *fcc* single crystal value of 75 GPa [24], but surprisingly much larger than

TABLE 1. The ω_Q, Γ_Q, $\tau(Q)$, and $L(Q)$ values for liquid Ga, Cu, and Fe at $Q = 10.6$, 10.7, and 12.0 nm^{-1}, respectively.

		ω_Q [meV]	Γ_Q [meV]	$\tau(Q)$ [ps]	$L(Q)$ [nm]
Ga*	transverse	*7.0	*5.2	*0.40	*0.40
	longitudinal	*17.9	*4.1	*0.50	*1.28
Cu	transverse	18.7	9.1	0.23	0.60
	longitudinal	24.3	4.1	0.51	1.75
Fe	transverse	23.1	17.1	0.12	0.35
	longitudinal	29.3	5.5	0.38	1.41

* Ref. [10, 11]

the polycrystal value of 47 GPa [24].

Figure 5(c) shows the dispersion relation of the transverse (open circles) and longitudinal (solid triangles) acoustic phonon excitation modes in liquid Fe obtained from the fit. The small solid circles indicate the previous longitudinal results [25], and the present longitudinal results agree well with previous ones. The dashed line is the dispersion of hydrodynamic sound at the low Q limit determined by the adiabatic sound velocity [26]. The dynamical sound velocity, ω_Q/Q, of the transverse mode is about 2900 m/s, much larger than a half (about 76%) of the longitudinal sound velocity. The microscopic shear modulus of liquid Fe can be estimated to be about 59 GPa, which is almost a half of the *bcc* single crystal value of 116 GPa [24], and about 70% of the polycrystal value of 82 GPa [24].

From the DHO fits, the mode widths, Γ_Q, of the transverse and longitudinal excitations can be obtained. Using the Γ_Q values, the lifetimes, $\tau(Q)$, of these phonon excitations can also be estimated by taking the Heisenberg's uncertainty principle into account to be proportional to the inverse of Γ_Q, i.e., $\tau(Q) = h/(2(h/2\pi)\Gamma_Q) = \pi/\Gamma_Q$, where h is the Planck constant. Furthermore, the propagating lengths, $L(Q)$, of the phonons can be approximated by multiplying $\tau(Q)$ with the dynamical velocity of sound, ω_Q/Q, expresses as $L(Q) = \pi/\Gamma_Q \times \omega_Q/Q = \pi\omega_Q/Q\Gamma_Q$. Table 1 shows the summary of these values for liquid Ga, Cu, and Fe at $Q = 10.6$, 10.7, and 12.0 nm^{-1}, respectively, together with ω_Q. The Γ_Q, $\tau(Q)$, and $L(Q)$ values slowly change with Q as shown in Fig. 3 of Ref. [10] for liquid Ga.

In liquid Ga, Γ_Q of the transverse excitations is 5.2 meV comparable to its ω_Q of 7.0 meV, indicating a highly damped feature. It is slightly larger than the longitudinal one, although ω_Q of the transverse mode is much less than a half of the longitudinal mode at the same Q value.

The $\tau(Q)$ value of the transverse phonons is 0.40 ps, which is almost the same as that of the longitudinal ones. Interestingly, this timescale matches well the lifetime
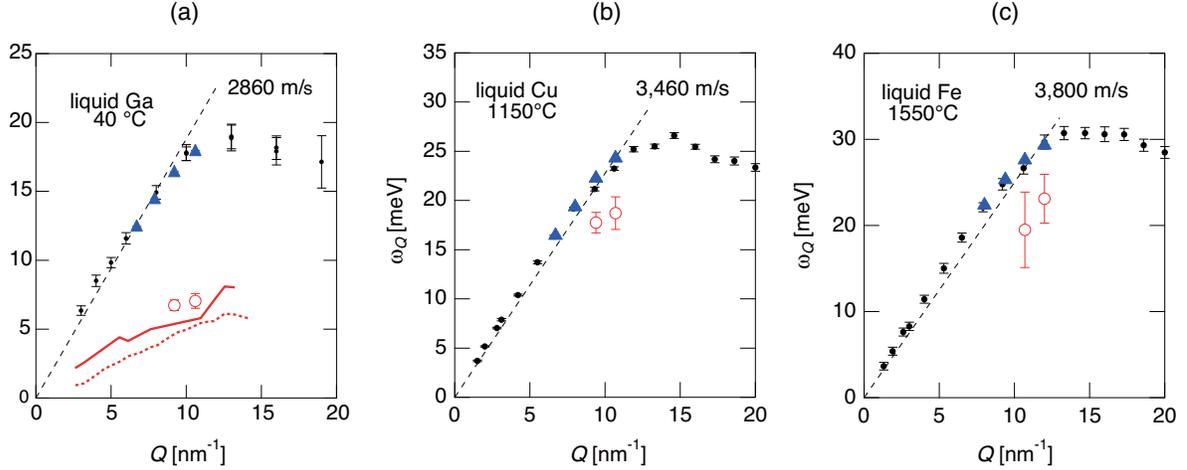
FIGURE 5. (Color online.) The dispersion relation of the transverse (open circles) and longitudinal acoustic phonon modes in liquid (a) Ga [10, 11], (b) Cu, and (c) Fe obtained from the fit. The small solid circles indicate the previous longitudinal results, and the dashed line the dispersion of hydrodynamic sound at the low Q limit determined by the adiabatic sound velocity. The solid and dotted curves indicate the results of *ab initio* MD simulations. (a) is after Ref. [10].

of short-living covalent bonds (0.39 ps at 100°C) [9] obtained from the Gaussian line width of the quasielastic peak near the $S(Q)$ maximum. Such short-living bonds may also indicate the lifetime of cages formed in liquid Ga instantaneously. Another timescale obtained from the macroscopic experiments is the Maxwell relaxation time, τ_M, which can be evaluated from the elastic modulus and shear viscosity. The estimated τ_M value is about 0.30 ps, which is again in the same time range as the above microscopic value.

The $L(Q)$ value of the transverse phonons is 0.40 nm, which is much shorter than that of the longitudinal ones of 1.28 nm. Since the transverse phonons can be generated only in the solid-like cages while the longitudinal ones can survive even in liquids, this $L(Q)$ value of 0.40 nm can be considered as the size of the cages formed in liquid Ga, where the transverse phonon packets are localized. Ioffe and Regel [27] proposed a criterion ($L_{IR} = 2\pi^2/Q$), which is considered as a boundary between the propagating and localized wave modes, corresponding to $L_{IR} = 1.86$ nm at $Q = 10.6$ nm^{-1}. With this criterion, both the transverse and longitudinal phonons in liquid Ga are localized at this Q value.

In liquid Cu, Γ_Q of the transverse excitations is 9.1 meV, which is much broader than that in liquid Ga, but almost a half of its ω_Q of 18.7 meV, indicating a less damped feature compared to liquid Ga. It is more than twice as large as that of the longitudinal phonons, 4.1 meV, different from that in liquid Ga. The $\tau(Q)$ value of the transverse phonons is 0.23 ps, which is less than a half of that of the longitudinal ones. The $L(Q)$ value of the transverse phonons is 0.60 nm, which is much shorter

than that of the longitudinal ones of 1.75 nm as expected, and by 50% longer than that in liquid Ga. Compared to $L_{IR} = 1.84$ nm, the transverse and longitudinal phonons in liquid Cu are highly and slightly localized at $Q = 10.7$ nm^{-1}, respectively. Analogous to liquid Ga, the transverse phonons in liquid Cu are located in clusters with the lifetime of 0.23 ps and the size of 0.60 nm.

In liquid Fe, Γ_Q of the transverse excitations is 17.1 meV, which is extremely broader than those in liquid Ga and Cu, and comparable to its ω_Q of 23.1 meV in liquid Fe as in liquid Ga. It is about three times larger than that of the longitudinal phonons of 5.5 meV. The $\tau(Q)$ value of the transverse phonons is 0.12 ps, which is extremely smaller than those in the other liquid metals, and less than a half of the longitudinal value in liquid Fe. The $L(Q)$ value of the transverse phonons is 0.35 nm, which is much shorter than that in liquid Cu but comparable to that in liquid Ga. Compared to $L_{IR} = 1.64$ nm, the transverse and longitudinal phonons in liquid Cu are again highly and slightly localized at $Q = 12.0$ nm^{-1}, respectively. Analogous to liquid Ga, the transverse phonons in liquid Fe are located in clusters with the lifetime of 0.12 ps and the size of 0.35 nm.

The Poisson's ratio, σ, is obtained from the longitudinal and transverse velocities of sound, c_l and c_t, respectively, as

$$\sigma = \frac{1}{2} \frac{c_l^2 - 2c_t^2}{c_l^2 - c_t^2} \qquad (2)$$

When a material is compressed in one direction, it usually tends to expand in other two directions perpendicular to the compressing direction. The σ value is the ratio of deformations, indicating the stiffness of bond angles

in a material, and can range from 0.5 to –1.0. The former value is the case of a perfectly incompressible material deformed elastically at small strains like an ideal liquid. On the other hand, the latter value represents another ideal material that shrinks in all the directions when compressed (or expands when stretched), indicating perfectly rigid bond angles.

The macroscopic σ values of typical metal crystals are about 0.3, and that of polycrystalline Ga is a slightly smaller value of 0.22 [21]. However, the microscopic value of liquid Ga obtained from the IXS experiment is about 0.42 [11], which is very large as a usual metal value, and similar to a value of rubber, 0.46–0.49. Thus, such a large σ value suggests that the cages formed by instantaneous covalent bonds in liquid Ga are easily deformable like a rubber made of polymer chains.

The microscopic σ value of liquid Cu can be roughly estimated to be –0.2, which is surprisingly a large negative value, and an extremely unusual value in comparison to the macroscopic crystal value of 0.343 [24]. This means that when liquid Cu is compressed in one direction, liquid also tends to shrink in the perpendicular directions, having a strong tendency to keep the shape of clusters remaining unchanged. It is ideally possible for the σ value to be negative. With reality, however, only a few materials show negative σ, such as $\alpha-$crystbalite [28].

The microscopic σ value of liquid Fe can be roughly estimated to be –0.2, which is again an extremely unusual value in comparison to the macroscopic crystal value of 0.293 [24]. This shows again a microscopic behavior in the elastic properties in liquid Fe similar to those in liquid Cu. Thus, it is concluded that the clusters in liquid Cu and Fe have very large shear modulus in the microscopic sense, and their bond angles are extremely rigid.

The most plausible candidate for such a microscopic cluster in liquid Cu and Fe is an icosahedron that Frank proposed in supercooled liquids in 1952 [29]. As shown in Fig. 6, this is a compact cluster composed of 13 atoms. The space cannot be filled out with only this cluster, and thus, it cannot be a unit cell for a crystal. However, it is very dense locally, and very stable energetically. For example, provided that the atoms are bound using a potential of Lennard-Jones type, the total energy of this cluster is lower by 8.4% than that of a dense-packed fcc or hcp structure.

Later, the existence of icosahedral clusters was confirmed experimentally and theoretically even in normal liquids. For example, that in liquid Cu was suggested by detailed XAFS measurements and reverse Monte Carlo calculations using these data, and it was reported that about 10% of Cu atoms belong to icosahedral clusters [30]. An *ab initio* MD simulation revealed that the above ratio is also ten-odd % [31].
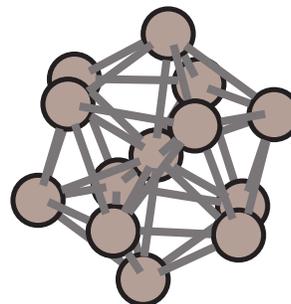
FIGURE 6. (Color online.) Schematic view of an icosahedral cluster proposed by Frank [29].

The existence of icosahedral clusters was also confirmed in liquid Fe. They were found by a neutron scattering experiment using a levitated liquid Fe sample [32]. An *ab initio* MD simulation also confirmed it [33]. From the MD results, distributions of bond orientational direction order parameters were obtained, and indicate that more than 15% of Fe atoms belong to slightly accommodating or deformed icosahedra although the perfectly ideal icosahedra are rarely seen.

The previous IXS experiment on liquid Fe [25] showed that the slow viscoelastic decay rapidly increases at $Q < 4$ nm^{-1}. Since this Q value corresponds to the length scale larger than 1.6 nm, a half of $L(Q)$ for the transverse excitations, the above IXS result may indicate a feature that the Fe atoms are strongly captured by small icosahedral clusters on the ps time scale.

The σ values in liquid Cu and Fe can be understood by considering the microscopic properties of icosahedral clusters. The length scales of the transverse and longitudinal excitations are different from each other, i.e., the $L(Q)$ values indicate that the transverse mode is surely reflected by the elastic properties within the icosahedral clusters, while the longitudinal mode may include those outside the clusters to some extent. Thus, the negative σ values in liquid Cu and Fe do not indicate extremely rigid elastic properties of the icosahedral clusters directly. Nevertheless, these σ values qualitatively reveal *instantaneously* rigid behaviors, in particular rigid bond angles, of the icosahedron since it is the highest close-packed structure with the packing fraction $\eta = 0.755$ for the central atom, rather than crystal Cu with a fcc structure ($\eta = 0.680$) and crystal Fe with a bcc structure ($\eta = 0.740$). They are in contrast to liquid Ga, where the clusters formed by instantaneous covalent bonds are easily deformable like a rubber.

From the *ab initio* MD simulations on liquid Cu [31] and Fe [33] by Ganesh and Widom, it was reported that the portion of the Cu atoms in the icosahedra is smaller than that of the Fe atoms. The author discussed the ori-

gin of this difference based on the corresponding crystal structures. The *bcc* structure stable in Fe can transform into an icosahedral cluster by producing bonds between the second-neighboring atoms. Thus, *bcc*-like liquid Fe can easily transform into icosahedral clusters. On the other hand, the *fcc* structure stable in Cu cannot change easily into an icosahedral cluster, and complicated processes may be needed for the transformation from *fcc*-like liquid to icosahedral clusters in liquid Cu. Thus, it is speculated that the height of energy barrier between *bcc*-like liquid and icosahedral cluster in liquid Fe must be lower than that between *fcc*-like liquid and icosahedral cluster in liquid Cu.

This idea can adopt the difference in the lifetime of the transverse modes obtained the present IXS experiment, i.e., $\tau(Q)$ in liquid Cu is about twice as long as $\tau(Q)$ in liquid Fe. An icosahedral cluster formed in liquid Fe can easily change back into *bcc*-like liquid with a short lifetime. On the other hand, once an icosahedral cluster is produced in liquid Cu, a longer lifetime is needed until the cluster returns to the *fcc*-like liquid.

CONCLUSION

The IXS experiments performed recently showed the existence of transverse phonon excitation modes in liquid Ga [10, 11] and liquid transition metals, Cu and Fe. At a glance, this findings contradict the description in high-school physics textbooks, 'There are no transverse waves in liquids.' This discrepancy arises from the differences in time- and length-scales as mentioned the introductory section.

From the detailed analyses, it is concluded that solid-like cages are the origin of the existence of transverse modes in liquid metals. In liquid Ga, clusters with short-living covalent bonds are formed with a lifetime of 0.40 ps [10, 11]. In liquid Cu and Fe, icosahedral atomic configurations produce such clusters with shorter lifetimes of 0.23 and 0.12 ps, respectively.

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