Abstract

The blue light observed in sonoluminescence experiments with water is explained by Rayleigh scattered ambient UV light reflected in a blue Raman line of water. The ambient UV light incident on the spherical liquid geometry is concentrated to a high intensity and reflected in a Raman line that appears to the observer as blue light. Since Raman emission in water is highly polarized, tests to determine the polarization of the blue light are recommended. If the intensity of the blue light is significantly diminished by the use of a polarizer, then not only is the explanation of blue light given here correct, but also because the ambient UV light intensity is very low, the spherical liquid geometry may be a spherical UV lens of significant concentration. By modifying the sonoluminescence test to include an external spherical UV laser cavity driver congruent to the spherical liquid lens, the concept of a blue water laser is developed where the UV laser driver is pulsed with the acoustic field to fuse the hydrogen in water molecules in the presence of an oxygen catalyst. Potential applications of the blue water laser are industrial hydrogen and deuterium gas generators, and a low temperature, < 50 C, heavy water heater for residential heating.

Introduction

Sonoluminescence (SL) is described [1] as a non-equilibrium phenomenon in which the energy in a sound wave becomes highly concentrated so as to generate synchronous repetitive flashes of blue light in liquid water at room temperature. Measurements of each flash indicate a power of 1 mW and a duration less than 100 ps. With regard to cold fusion, SL as a significant mechanism of energy focusing in combination with a heavy D-O-D water target [2] is important because it would offer the prospect of a mechanism of fusing deuterium at room temperature.

In the standard model [3] for SL, bubble collapse energy is delivered to a number of molecules and the molecules are excited to emit blue light upon recombination. However, it is possible that the blue light observed in SL is nothing more than Rayleigh scattered light reflected in the blue Raman line of water. The Raman effect is the phenomenon of light scattering from the material medium whereby the light undergoes a frequency change in contrast to Rayleigh scattering where a frequency change does not
occur. The reflected blue Raman line from incident mercury light is observed in spectrofluorimetry [4] of water, but only at low intensity, and an even lower blue line intensity might be expected if spectrofluorimetry is made on water with ambient UV light. Hence, the geometric concentration of ambient UV light by the spherical geometry may be significant in SL. The SL explanation given here is that the low intensity ambient UV light scattered inside the spherical water geometry is concentrated at the center and after reflection in a visible blue Raman line of water is of a sufficient intensity to be visible by the observer as blue light. This SL explanation is referred hereinafter as the Light Scattering (LS) model. In contrast, the standard SL model contends the blue light is generated in the water. Since the ambient UV light is not visible, the appearance of blue light alone may have led the observers [1] to conclude that the blue light was being emitted from the water consistent with the standard SL model when, in fact, the blue light is reflected ambient UV light.

Since the visual observation [1] of blue light does not quantify the wavelength, the blue wavelength is taken to be 470 nm for the purposes of this paper. In the standard SL model, light absorption for hydrogen takes place on the order of 10 ns. However, both Rayleigh and Raman scattering do not involve light absorption and for Raman scattered blue light at 470 nm, takes place in a much smaller time, or within the period of vibration, < 1 fs. The LS model is consistent with but much faster than the < 100 ps duration reported [1], and may explain why the blue flashes cannot be resolved by the fastest photomultiplier tubes available.

SL experimental data for Rayleigh scattered UV light reflected in the Raman lines of water is not available. However, data [4] for solvents at various frequencies of exciting mercury light shows wavenumber shifts of about 0.3 / micron for all solvents containing hydrogen atoms. The Raman lines are caused by totally symmetric molecular C-H and O-H vibrations of the solvent. The data for water shows that for blue light to be emitted in a Raman line at 470 nm, the Rayleigh scattered incident UV line is required to be about 405 nm. Hence, the observed blue light at 470 nm during SL in water in the LS model is actually a Raman line corresponding to UV light at 405 nm and a wave number shift of 0.34 / micron.

In addition to reflected blue light, the ambient UV light is also reflected in UV Raman lines to produce a spectrum of reflected Raman light. Since the energy of the UV photon is greater than blue photon, the average wavelength of the reflected light is less than the 470 nm wavelength of the blue photon. Photon energy measurements [1] give a frequency of 8.0e14 Hz that corresponds to an average wavelength of 375 nm which is less than the blue wavelength of 470 nm and consistent with the LS model. This wavelength decrease may be due to a prominent Raman line at 350 nm in water [4] that is excited by a 313 nm UV line.
In the LS model of SL, the ambient UV light is focused at the center of the spherical water geometry and reflected in the Raman line of water. However, the molecular structure or how it is formed and cooperates with or scatters the UV light during SL compression or expansion is not described in the LS model. During SL expansion, the molecular order is lost because the intermolecular spacing exceeds the range of electrostatic interaction, and therefore the cooperative liquid crystal structure can only be formed in the compression phase where the order of the molecular structure is constrained to the geometry of the spherical compression field. Since the direction of the incident UV light in the spherical geometry is radial, a molecular structure comprising strings of radially disposed water molecules is indicated as the Raman scattering centers.

Currently, the reflection of color from liquids is known to most commonly occur in the liquid crystal state and specifically the chiral liquid nematic phase where the order is a twisted helical rotation. In terms of molecular order, the liquid crystal as a state of matter between the solid and the liquid state together with the molecular order in the chiral nematic state are illustrated in Figure 1. With regard to water, this means for a cooperative structure to be formed in SL, the molecules are generally, in the manner of a helix, rotated sequentially along the radially disposed strings and periodically repeat at a pitch equal to the wavelength of blue light in water. However, the hypothesized chiral liquid nematic phase, or the hypothesized blue phase for water, formed in the compression wave during SL is not known to exist at present. A brief review is presented of known chiral nematic liquid crystalline blue phases of other liquids.

Chiral or twisted helical molecular structures are known to produce blue phases in cholesteric systems [5,6] when the pitch of the helix is less than about 500 nm. The first observation of a blue phase [7] was made over 100 years ago. Upon cooling the liquid phase of cholesteryl benzoate, an appearance of a violet and blue phenomenon was observed which quickly disappeared. Currently, the molecular models [5] of the cholesteric blue phase focus on factors that affect the pitch of the helix between the nematic or liquid crystal and the isotropic liquid phase. Density or pressure and temperature changes are the common parameters affecting the helical pitch. In any event, to assess whether a liquid crystal phase change has occurred, the order parameter, \( S \), is used and is defined in terms of the average taken over all molecules in terms of the angle, \( \theta \), between the molecular pointing axis and the director.

\[
S = \langle 3\cos^2\theta - 1 \rangle / 2
\]

In the isotropic or disordered state, the order parameter is zero while in the ordered state the order parameter is unity as illustrated in Figure 1.
In cholesterogens, C-H atoms are linked to each other by chemical bonds to form a carbon based chain-like helical configuration. However, water molecules are separately distinct, and although dimer and trimer water chains of H-O-H and D-O-D clusters are well known, it is not known whether an oxygen based chain-like helical configuration of water molecules can be formed.

Water is a polar molecule with a high dipole moment and responds to incident light as an oscillating dipole. If the incident light is visualized by an electric vector, E, oscillating at a frequency, f, in water of a polarizability, \( \alpha \), the dipole moment, P, induced is,

\[ P = \alpha E \sin(2\pi ft) \]

Without SL, in an isotropic and disordered water medium without a liquid crystal phase, the water molecules function as randomly distributed scattering centers. Excitation of the molecules by UV light with a transverse electric vector, E, and frequency, f, causes the molecular dipoles to emit Rayleigh scattered light at the same frequency, f. The relation of the incident UV light to the spherical SL water geometry is illustrated in Figure 2. If the water molecules and material medium are rigid, the only scattering produced would be Rayleigh scattering. However, because of the molecular 0-H bond vibration of individual molecules at a frequency, fo, the molecular dipole is modulated and a blue Raman line at frequency (f-fo) is also scattered.

With SL and during the compression wave, the water molecules as scattering centers are ordered into radially disposed strings, but water molecules along a string are disordered in rotation. For incident UV light with a transverse polarization of frequency, f, directed in the radial direction, the electric vector, E, is orthogonal to the direction of light. However, for incident UV light with a circularly polarized content, the electric vector, E, rotates in a right or left handed manner about the direction of the light. Depending on the local constraint of adjacent molecules, the molecules rotate under the action of the dipole moment, P, tending to align the molecular dipole moment vector with the direction of the incident UV light. If the incident UV light is transversely polarized, the molecules are aligned in a nematic crystal state. If the incident UV light is circularly polarized, the molecules are aligned in a chiral nematic crystal state, or helical structure. In any event, the UV light at frequency, f, is Rayleigh scattered at the same frequency, f, and for OH vibration at frequency, fo, a Raman line at frequency (f-fo) is also scattered.

In a SL compression field, the radially disposed and rotational order of the water molecules may be increased by the alignment of the dipoles in the direction of the incident UV light electric vector, E. However, alignment can only occur if the dipole orientation response time is less than the period of UV light. In water at 20 C, the response time for dipole orientation is about...
10 ps, but is greater than the < 1 fs period of UV light. Hence, an increased order of the molecules does not occur. Instead, the molecular dipoles respond to the UV light only by small oscillations at frequency, $f$, about the angular position acquired in the compression field. There is simply not enough time for any large reorientation of the molecules to occur. At 20 C, the dielectric constant for water is large only up to about 1.e10 Hz and falls rapidly to the value for a nonpolar liquid at about 1.e11 Hz. This means any significant dipole reorientation in water can only occur for electromagnetic frequencies less than about 1.e10 Hz. Possibly the electric field of the acoustic driver at 20 kHz, itself, may be the source of increased molecular order in water during SL. Further, the rapidly fluctuating electric field of the acoustic driver may also be the source of the UV radiation, referred herein as ambient UV light. The proposed research here is to determine the optimum SL excitation carrier wave < 1.e10 Hz for the UV light, instead of the 10-20 kHz acoustic sonic carrier wave commonly used in SL.

If the water medium in SL is in a chiral nematic crystal state, most of the incident UV light will be transmitted except for the one wavelength equal to the pitch. However, whether the helical structure in the chiral nematic is right or left handed is important. If the blue light reflected is either right or left circularly polarized, the same handedness may be deduced for the pitch of the liquid crystal. This means either right or left circularly polarized UV light will penetrate to the center while the light of the other chirality is reflected back to the observer as blue light. Since the velocity of light in water is reduced by the index of refraction, the pitch in the liquid crystal is smaller than the wavelength of blue light in a vacuum. If the observer sees blue light at 470 nm and if the index of refraction of water is 1.33, then the pitch in the liquid crystalline state is about 353 nm. Hence, the UV wavelength selectively reflected from the ambient is also about 353 nm, but is less than the 405 nm UV wavelength required to produce a prominent blue Raman line at 470 nm. This means that either the chiral nematic phase does not cooperate with the LS model in the production of blue light as hypothesized, or that the index of refraction is lowered in the liquid crystal state. A study of the lowering of the index of refraction of water in a chiral nematic liquid crystal state is indicated.

With regard to cold fusion, it is an open question whether pumping UV incident light in phase with the sonic pumping and in combination with stimulated Raman scattering in water is or is not a cooperative mechanism in the production of blue light as seen by the observer. However, for UV wavelengths in the liquid crystal near the blue line, the transmission of UV energy to the center may be significant. This cooperative lasing action, collectively termed here a blue water laser, may function as a cold fusion spherical focusing device to concentrate UV energy on the water molecules at the center of the compression field and possibly fuse hydrogen and deuterium.
Molecular Water Model

Generally, the Molecular Dynamics (MD) simulation of simple monatomic liquids [9] without Coulomb charge interaction proceeds on the basis of Lennard-Jones (LJ) interatomic pair potentials to describe the internal energy. However, the MD simulation is more complex for water. The internal energy description by simple LJ pair potentials alone is not sufficient because the polarizability of water causes the long range Coulomb charge interactions to be dominant. In the liquid crystal interpretation of SL, the long range Coulomb interactions are important in developing the twisted helical structure. The first simulation of liquid water [10,11] in the early 1970's included both van der Waals and Coulombic interactions together in the manner of an effective pair potential. However, the simple point charge (SPC) developed [12] was selected here for the SL study.

The SPC model is of a tetrahedral geometry consisting of an O-H distance of 0.1 nm with point charges of -0.8476e on the oxygen position and +0.4238e on each of the hydrogen positions. The tetrahedral angle between the vector pairs connecting the oxygen and hydrogen atoms is 109.4 deg is illustrated in Figure 2. The Coulomb potential for o-o, o-h, and h-h charge separations is,

\[ V_C = q_i q_j / 4 \pi \varepsilon_0 r_{ij} \]

where, \( \varepsilon_0 = 8.854 \times 10^{-12} \text{ coul}^2 / \text{J-m} \)

The LJ potential based only on oxygen-oxygen separations is,

\[ V_LJ = 4 \varepsilon [(\sigma / r_{oo})^{12} - (\sigma / r_{oo})^6] \]

where, \( \varepsilon = 78.38 \times K_b , K_b = 1.38 \times 10^{-23} \text{ J} \), and \( \sigma = 0.316 \text{ nm} \).

MD Simulation

The MD simulation is directed to the dynamic response of bulk water at 300 K under a uniform isotropic expansion and compression. Consistent with a spherical liquid crystal structure, the isotropic geometry should be spherical with a characteristic length at least about equal to the wavelength of blue light, 470 nm. However, typical MD calculations assume a bulk fluid and are carried out in a cubic computational box with periodic boundary conditions. Although a cubic box could be assumed to be in a state of isotropic expansion and compression, the number of molecules required is significant. At 300 K the density of water [0.998 gm/cc] with a 400 nm cubic box would contain about 2 billion molecules. Hence, the attendant MD simulation would require an exorbitant amount of computation.
In order to obtain a representative MD simulation of water in a chiral nematic phase with reasonable computation times and still maintain consistency with a spherical geometry undergoing isotropic expansion and compression, a 1D chain of water molecules was selected. An exact representation would consider a spherical sector geometry with proper boundary conditions such as frictionless rigid walls that permit motion only in the radial direction. This is usually achieved by simulating the rigid walls with dummy molecules and fictitious LJ potentials. However, the rigid simulation increases the number of molecules and attendant computer time significantly. In this arrangement, a 1D chain of water molecules aligned in the radial direction with lateral constraint in the transverse directions gives a reasonable approximation to a spherical geometry with acceptable computing time. This configuration points the 1D chain in the direction of the incident UV light as shown in Figure 2.

To achieve liquid density in a 1D chain of water molecules at 300K, the initial configuration consist of about 1400 water molecules in a 0.3 x 0.3 x 400 nm computational box in the x, y, and z directions respectively. The chain is free to move in the z-direction and periodic boundary conditions are imposed at the top and bottom. In the x and y directions, periodic boundary conditions are also imposed, but lateral motion is restrained by constraining the oxygen atom to the z-axis. The hydrogen atoms are placed in a vector pair laying in the x-y plane so that their respective vector cross product was pointing parallel to the positive z-axis. The initial spacing in the model z-direction is 0.3 nm. Here, the water molecules are free to rotate about the oxygen atom. Constraining the water molecule about the center of mass is correct, but the oxygen atom was chosen as the point of rotation for analytical convenience.

The SHAKE algorithm [13] was used to maintain constant bond lengths and tetrahedral angle as well as constraining the oxygen atom of each water molecule to the z-axis. In order to include a reasonable amount of long range effect in the computation of electrostatic forces, each molecule was assumed to interact with the neat 5 molecules above and 5 below it in the 1D chain. The time step in the solution was 1 fs.

Results and Extensions

In the MD simulation, the bulk water temperature was held near 300 K. Density was changed by varying the initial spacing between the molecules in the z-direction. However, the number of molecules was adjusted to maintain the 400 nm wavelength. The crystal order parameter is computed based on the angular position of the H-O-H normal relative to the z-axis. It is found that the water molecules are ordered into a helical geometry for initial molecular spacings less than about 1 nm. The order parameter indicates a molecular rotation of about 80 degrees, but the H-O-H normal also rotates around the z-axis as shown in the simplified sketch of the blue phase of water in Figure 3.
Since the molecules are generally oriented in the manner of a twisted helical structure during SL compression, a structure that transmits ambient 400 nm UV light of a left or right chirality while reflecting the opposite chirality is predicted. The MD analysis to show that the 400 nm structure cooperates with the production of 470 nm blue light was not performed.

Because the full scope of analytical and experimental effort in the future development of the blue water laser concept is beyond the capability of the author, the following blue water laser experiments and applications are presented to the cold fusion community for review and comment.

**Confirmation of SL Model**

Polarization measurements of the reflected blue light in the SL experimental set-up [1] should be made. Since Raman emissions are highly polarized, the LS model predicts that the intensity of the blue light as viewed through the polarizer will be significantly diminished. If the blue light is found to be circularly polarized, that is, either right or left handed, it can be concluded that the water is a chiral nematic liquid crystal with the pitch equal to the wavelength of blue light in water. If the blue light is found to be linearly polarized, it can be concluded that the water is a nematic liquid crystal. In either case, the blue light in SL is caused by UV light reflected in a blue Raman line as predicted with the LS model.

**Stimulated Raman Scattering**

Stimulated Raman scattering experiments of the blue water laser directed to establishing the energy gain caused by resonance of UV ambient light with the helical structure of water in the liquid crystal state should be performed. The experimental set-up suggested is the same SL arrangement [1], except modified to include a surrounding spherical cavity coincident with the spherical compression field in the light or heavy water as shown in Figure 4. The surrounding cavity surface is lined with mercury lamps emitting UV radiation in the 300 to 400 nm range and flashed in sync with the SL acoustic frequency, or only with the SL acoustic pulsed in a steady UV radiation field. In effect, the mercury lamps function as a UV laser driver source, but other more appropriate UV exciting lines may also be used.

Of interest to cold fusion are stimulated Raman scattering experiments of the blue water laser to determine energy gain and heat produced as a function of UV wavelength. Experiments to determine the liquid crystal focusing with bulk water temperature are of importance. In carbon based molecules, hydrogen-deuterium asymmetry is known [8] to produce a twisted chiral nematic cholesterogen. However, in water molecules little is known about the effects of asymmetry in neutron mass. The effects of asymmetry of water molecules caused by neutron mass on liquid crystal structure is recommended for blue water laser research.
Blue Water Laser Applications

Conceptually, the blue water laser is a UV transparent spherical container of light or heavy water surrounded by a spherical UV laser driver cavity with the spherical acoustic driver exterior to the UV laser driver. During operation the blue water laser is a cold fusion heat source, and therefore openings are required in the spherical arrangement to permit flowing water to transfer the fusion energy to a heat sink. Openings may be made in the spherical arrangement without significantly affecting the isotropic irradiation of the water molecules. In this arrangement, the blue water laser may find application as a hydrogen or deuterium gas generator or a D-O-D water heater as illustrated in Figure 5.

At low UV energy laser driving, O-H or O-D bonds of the water molecules at center are broken and the molecules dissociate into hydrogen or deuterium and oxygen ions and, if in addition, the water includes an oxygen catalyst, recombination to hydrogen or deuterium molecules may occur. Hence, the blue water laser may find application as an industrial hydrogen or deuterium gas generator.

For high UV energy drivers and depending on the spot size, a group of water molecules may be ionized to high temperatures causing fusion of hydrogen or deuterium atoms and a fusion energy release. By providing a through flow of heavy water, the blue water laser may find application as a residential home heater by increasing ambient temperature water to about 50 C without a loss of the spherical liquid crystal focusing structure. However, oxygen catalysts may be precluded here because of potential quenching of the hydrogen or deuterium fusion plasma. Further, the fusion plasma may also be quenched by the oxygen in the water molecule. Conversely, the quench in fusing of water molecules in the presence of oxygen catalysts may serve as a natural safety mechanism to prevent a runaway fusion process. The fusion of water molecules in the presence of oxygen and oxygen catalysts is recommended for future blue water laser research.

In both low and high UV energy driver applications, the UV radiation from the surrounding spherical cavity is concentrated at its center by the geometric focusing. Hence, contamination of the hydrogen and deuterium plasma by oxygen and oxygen catalysts may not be a problem because the very large concentration of UV energy may accommodate the contamination and still achieve fusion temperatures. Because of the significant concentration of UV driver energy, it is possible that ambient UV light alone is sufficient to cause hydrogen or deuterium fusion in water molecules, and therefore it is not whether cold fusion can occur during SL, but rather why has cold fusion not been detected to date. The answer given here is that for a small number of fusing water molecules, the low level energy release and helium nuclear products would be difficult to detect. However, with higher UV energy lasers, nuclear products may be detectable.
Discussion and Summary

The blue water laser is similar to the Inertially Confined Fusion Reactor (ICFR) hot fusion concept [14] where fabricated D-T fuel pellets are ignited at fusion temperatures by imploding the fuel pellets through laser ablation of the exterior pellet surface. However, the blue water laser is a far simpler concept than the ICFR because fuel pellets do not need to be fabricated as the water molecules at the focal point of the liquid crystal structure function as the fuel pellet. Further, the mercury lamp arrangement is a simple laser driver. Since the spherical liquid crystal structure is perfectly reformed after each SL pulse, a continual and reliable flow of fuel is provided for repetitive ignition and a likewise channel is provided for the UV light to irradiate the water molecules at the center of the spherical liquid crystal structure.

The advantage of the blue water laser over conventional ICFR concepts is that a very small quantity of D-O-D fuel is repetitively ignited. This means that the UV energy required for D-D ignition is small and the external UV laser energy may also be small because of the geometric concentration by the spherical lens. Further, since the D-D energy release is small, only a small temperature rise and shock pulse in the bulk water occurs during each ignition. Still further, the blue water laser would make possible the neutron free D-D reaction at reasonable UV power instead of opting for the lower ignition energy D-T reaction with attendant neutron radioactivity problems common in ICFR concepts. Still further, miniature blue water lasers may be envisioned instead of the large size of ICFR laser drivers.

In contrast to ICFR concepts that fuse D-T fuel, the blue water laser concept attempts to fuse deuterium in heavy water by UV irradiation of D-O-D molecules. It should be noted that the blue water laser is a cold fusion device because the liquid crystalline structure required in the transmission of UV radiation to the fusing water molecules would only operate, say below 50 C, even though the local hot fusion D-D reaction is actually producing the heat. However, the quenching of the D-D plasma temperatures by the oxygen catalysts or the oxygen in the D-O-D water molecules or the helium reaction product itself may be a difficult obstacle for the blue water laser concept to overcome. If not, miniature blue water lasers can serve as a limitless energy source in providing residential home heating. Otherwise, the blue water laser is likely to find commercial application as a hydrogen or deuterium gas generator.
Figure 1  Liquid Crystal Notation

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Figure 2  Spherical Water Liquid Crystal Geometry, Radially Disposed Strings of Molecules, and Water Molecule Model Geometry
Figure 3 Simplified Sketch of the Blue Phase of Water

Figure 4 Blue Water Laser Concept
Figure 5  Blue Water Laser Applications