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Experimental Analysis of Water-1MHz-gasified with O_2, and Simulation Analysis of Physicals Parameters Effect of Solvents in Megasonic Cleaning

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***Abstract*—Aqueous chemicals and solvents are used heavily in semiconductor manufacturing, and device manufacturers are focused on advancing these cleaning liquids to the next technology node. The scientific results confirm that ultrasonic agitation can improve the removal of particles. Megasonic energy has been proven to improve particle elimination in semiconductor devices in cleaning procedures. On the other hand, applied ultrasonic energy may damage the sensible devices in the cleaning process. In order to better comprehend, we explore in this paper the impact of different liquid properties by showing the transient cavitation threshold by performing some simulations with the analytical Blake model and the numerical Gilmore model. The experimental setup firstly to understand the temporal and spectral response of the increasing of the electrical power, and secondly to investigate that increasing the gas level in the cleaning bath in Water-1MHz-gasified with O_2 modifies the acoustical pressure in the medium. We can conclude that the experimental measurements and simulation studies of the applicable sound wave field and cavitation level provide an important indication of the medium's properties. By proceeding in this manner, we can find the impact parameters on the onset of transient cavitation and the safe area to treat client wafers. At this point, we can figure out the cavitation threshold that works for us and safely translate it from one chemical process to another.**

***Keywords*— Threshold cavitation; megasonic; signal processing; solvents; bubbles dynamics.**

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I. INTRODUCTION

The semiconductor industry and devices manufacturers used the chemical solvent in their cleaning process [1]. However, they are more inconvenient with this cleaning method, such as corrosion, pattern collapse, surface damage of sensitive materials, and wetting trenches in hydrophobic materials. It was found that megasonic energy can improve the removal of particles from semiconductor devices during cleaning processes [2]–[9], provide megasonic energy that significantly improves particle removal [2]–[4], [10], [11], and develop a deeper comprehension of the transducer response in cavitation environmental and megasonic conditions [8], [12]. Thus, megasonic cleaning is increasingly popular among semiconductor manufacturers, with decreasing process times using megasonic [13]. Nevertheless, the applied ultrasonic energy could cause damage to sensitive nanotechnologies components [14]. The mechanical system could introduce the power needed to remove sufficient particles without damaging them by conceiving a dispersion wave to control cavitation in different solvents [15].

To comprehend the megasonic energy impacts on a different range of solvents [16], the research has been conducted with a small sonic shaker to learn more about chemical reactions to sound and to determine the cavitation threshold for various types of liquids. These findings and data are expected to guide the experiments and provide insight into the basic chemicals and liquid preparations ready to use when applied with sonochemistry. Furthermore, we might be able to clarify why certain cleaning approaches have a significant advantage in using ultrasonic cleaning for nano-structures, whereas other cleaning approaches adversely affect the nanostructures.

This research suggests numerical and analytical modeling studies that show that the threshold for transient cavitation is decreased via density decrease, surface tension decrease [17] and vapor pressure increase. The decreasing transient

cavitation threshold causes a more effective removal performance due to the enhanced bubble interaction by a drag force, wave shocks, and jetting. In this paper, we show that increasing the temperature in water affects the transition from stable to transient cavitation and the erosion efficiency, and in solvents, with efficiency in eliminating the weak film. Finally, we perform an experiment that shows that increasing the electrical power transferred to the piezoelectric transducer and increasing the gas content strongly influences the acoustic pressure.

We organize the remainder of this paper as follows. After a brief introduction, Part 2 explains that the intensity of the sound I is proportional to the square of the maximum pressure amplitude P_A in chemical cleaners and the concept of cleaning employed in this investigation. In the third section, we first report all the results found from voltage analysis, FFT, gasified water effect experiments, and then the simulation of the pressure variation as a function of the medium characteristics. In the fourth section, we present the conclusion on constructing our dataset from experimental and hydrophone measurement simulations to quantify a hybrid megasonic/chemical solvent technique to monitor the cavitation threshold to achieve safety and damage-free cleaning.

II. Materials and Methods

To study the impact of the different liquid properties on ultrasound cleaning mechanisms and the impact of physical parameters on bubble dynamics. We do an experimental study to investigate the electrical energy optimization sent to the piezoelectric transducer [1], and the acquisition of the signal measured by the microphone (Fig.1) in order to calculate the response of the peak-to-peak voltage (Fig. 5) and present a spectral analysis of the two liquids (water and IPA) by calculating their Fast Fourier transforms (Fig.6).

The sound energy transmitted by the piezoelectric transducer with an equal frequency 1.08 MHz, generates a cavitation phenomenon, hence the usefulness of studying the impact of external parameters such as frequency, voltage on cavitation production, and also explore the impact of the solvent's physical properties on the transition from stable to transient cavitation, that is why we realize a simulation of the temperature (Fig. 13), the surface tension (Fig. 9), the vapor pressure (Fig. 12) impacts. Finally, we study the response comparison between the Blake threshold and Glimore Model (Fig. 14).

A. Cleaning Concept and Experimental Setup

We work to develop cleaning technologies for advanced IC fabrication processes. Traditional cleaning techniques rely on aqueous chemistry to remove particle contamination from surfaces. However, this is no longer possible for modern technologies and physical forces enhance chemical action. We research the application of ultrasonic energy. A power source is connected to a piezo-electric transducer at different input voltages from 5 V to 80 V, which is immersed in the cleaning bath. Typical resonance frequencies of the transducer are of the order of 1MHz. A hydrophone with broadband between 0.2 and 10 MHz, used to capture the signal of the transition from stable to transient cavitation for all liquids (IPA, Water, NMP, DMSO) [3], [18], [19]. The intensity of the sound I is proportional to the square of the maximum pressure amplitude P_A in the cleaning chemicals and calculated by this equation (1):

$$I = \frac{1}{Q} * \frac{{P_A}^2}{2Z_m} \quad \left(\frac{W}{cm^2}\right) \tag{1}$$

It is the electrical power I from a pressure field MHz generated in a liquid. The experiments have shown that the power I which arrives at the substrate surface can vary. Important parameters are the occurrence of standing waves, the position of the substrate, and possibly many others. Such parameters may be visible as a change in the complex impedance of the transducer.

This assignment consists of different tasks that should help us improve the system's power transfer.

The power applied of sound I is proportional to the square of the maximum pressure amplitude P_A, are dependent on the transducer-liquid coupling (e.g., quartz wall): Q and the acoustic liquid impedance [20] shown in Eq. (2):

$$Z_m = \rho * c \ (kg * m^{-2} * s^{-1}) \tag{2}$$

With ρ being the density of the liquids and c being the velocity of the sound waves moving through the fluid. The experimental maniple is realized with the power supply of the transducer operated by a Hewlett Packard HP generator, and the voltage source is amplified by 100 using HAS 4101 device to aliment a 1.08 MHz transducer.

A hydrophone with the following characteristics with a diameter of 2.5 mm PZT is used to detect the transition signal between stable and transient cavitation. The bandwidth of the microphone varies between 0.2 and 10 MHz, connected directly to a digital oscilloscope that is connected to a PC that controls the voltage source and analyses the data collected from the oscilloscope with LabVIEW code.

In this way, we are looking for the time and frequency presentation of the bubble collapse signal. Figure 1 shows the experimental design used to detect the cavitation signal and process the signal with the Fast Fourier transform.

Fig. 1 Schematic of a liquid cell.

B. Simulation Concept

To understand how different liquids respond to a sound field and can bubble dynamics be predicted [21], they are two approaches for modeling bubble dynamics: analytical [17] and numerical [22], [23]. We calculate the transient cavitation threshold with the Rayleight-Plesset model for incompressible fluid to obtain the analytical result (Blake threshold).

1) Pressure and Bubble dynamics: This variation of pressure response is caused by the acoustic impedance (see

Equation 2), which is defined as the product of density and the speed of sound in that medium. The ultrasonic energy sent into the liquid at a certain electrical power I will generate a pressure in the medium presented by P_a. Cavitation: bubble seeds grow in the tensile pressure cycle and collapse in the compressive cycle [24].

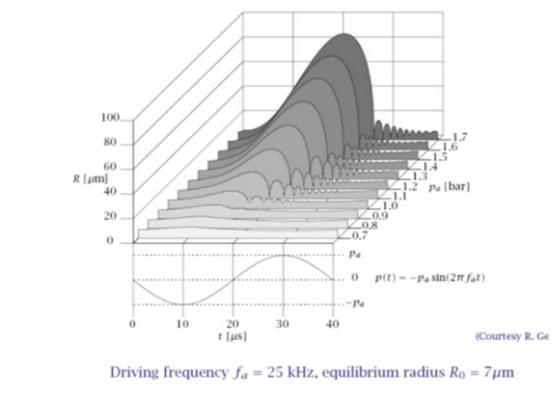

Fig. 2 From pressure to bubble dynamics [24].

Bubble seed with radius R_0 in a MHZ field with amplitude pressure P_a. The figure 2 show that with increasing driving radial pressure Pa motion R(t) increases and the Cavitation becomes transient if $R_{max}>2R_0$ [24].

2) Bubble dynamic or equations single bubble: We search how do different liquids respond to a sound field with simulated bubble dynamic [25], [26] and calculated the threshold: transient cavitation by two models Rayleigh-Plesset for non-compressible fluid (Blake threshold), and Gilmore for compressible fluid.

- *Non-compressible fluid (Analytical Model)*

We start with the first model: in Figure 3, we showed the liquid's pressure at the bubble's wall.

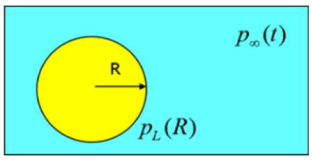

Fig. 3 Bubble Simulation.

The liquid pressure at the wall of the bubble is [17]:

$$P_L(R) = \left(P_0 + \frac{2\sigma}{R_0} - P_v\right)\left(\frac{R}{R_0}\right) + P_v - \frac{2\sigma}{R_0} P_L(R) = \left(P_0 + \frac{2\sigma}{R_0} - P_v\right)\left(\frac{R}{R_0}\right) + P_v - \frac{2\sigma}{R_0} \quad (3)$$

The radius of the bubble and the initial radius of the bubble are R and R_0, and σ is the usual surface tension coefficient given in N/m or J/m2. And the driving pressure is:

$$P_\infty(t) = P_0 - P_A \sin(wt) \quad (4)$$

- *The equation of Incompressible liquid with Rayleigh-Plesset model*

Where Ṙand R̈ are the first and the second order derivatives of the bubble radius concerning time, and ρ is the volumetric mass density of the medium. The final equation that describes the explosive growth bubble is:

$$P_B = P_0 - P_v + \frac{4\sigma}{3}\left(\frac{3\gamma}{2\sigma}\left(P_0 + \frac{2\sigma}{R_0} - P_v\right) {R_0}^{3\gamma}\right)^{-\frac{1}{3\gamma-1}} \quad (6)$$

Where γ is the heat capacity ratio of the enclosed gas.

- *Compressible fluid (Numerical Model)*

For Compressible liquid, the Gilmore model is necessary at high wall speeds. The equation of compressible liquid: with Glimoe model [22], [23], [27], [28] is given as:

$$\left(1 - \frac{\dot{R}}{C}\right) \times \ddot{R} + \frac{3}{2} \times \left(1 - \frac{\dot{R}}{3C}\right) \times \frac{\dot{R}^2}{R} = \left(1 + \frac{\dot{R}}{C}\right) \times H + \left(1 - \frac{\dot{R}}{C}\right) \times R \times \frac{\dot{H}}{C} \quad (7)$$

C is the sound velocity of the liquid at the wall of the bubble and H is the enthalpy difference of the liquid at the wall of the bubble and at infinity.

Enthalpy H is given as:

$$H = \frac{1}{\rho_0}\left(\frac{n}{n-1}\right)\left(\frac{1}{P_0+B}\right)^{\frac{-1}{n}}\left[(P_L(R)+B)^{\frac{n-1}{n}} - (P_\infty + B)^{\frac{n-1}{n}}\right] \quad (8)$$

The speed of sound of the liquid is given as:

$$C = \sqrt{{c_0}^2 + (n-1)^2} \quad (9)$$

The equation of the state liquid is given as:

$$\frac{p+B}{p_0+B} = \left(\frac{\rho}{\rho_0}\right)^n \quad (10)$$

Here B and n are constant in the Tait equation of state for the liquid.

III. Results and Discussion

This research is devoted to combining chemistry through solvents and physics through ultrasound to prove that using megasonic in a cleaning process can reduce the amount of chemical solution and ultrapure water used by simplifying the cleaning process. This research seeks to optimize sound energy with an extremely powerful cleaning effect without damaging the semiconductor substrate. This study is devoted to the study of the effect of the combination in a cleaning process which includes a first part talking about the application of megasonic frequencies to chemical solutions in a cleaning bath to remove metals and fine particles adhering to the substrate, a second part of the work on the realization of a signal processing on the information detected by the microphone in order to map in frequency any chemical solvent used in this study. The third part of the study is dedicated to the effect of applying megasonic frequencies to the degassed water in the cleaning bath to clean the substrate, a fourth part dedicated to program and perform simulation on Bubble Dynamics Models such as the Rayleight model and the Glimore model, and a final part that concludes our research goal which is to find a correlation between erosion and the change of physical parameters in the water and solvents used for the cleaning process.

We build a setup to comprehend the physical and chemical forces in combination. Figure 1 shows the configuration we used to study the liquids. Data is sent to a digital oscilloscope,

and pressures are registered for specific chemicals. We can conclude that the cavitation threshold oscillation varies with the pressure produced in the solvent [29]. Figures 4 and 5 show when the signal deforms to check the cavitation signal using the peak-to-peak voltage of the signal and processing with FFT in figure 6.

A. Hydrophone Measurement

Figure 4 and Figure 5 show the impact of the augmentation of the electrical power; we can see the transition from stable to transient cavitation [30] when the average results of the hydrophone become nonlinear.

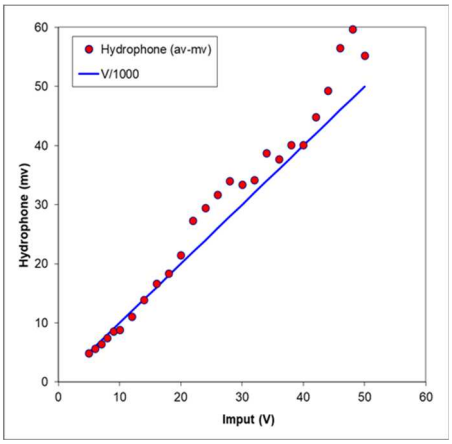

Fig. 4 Hydrophone Measurement in water for different inputs.

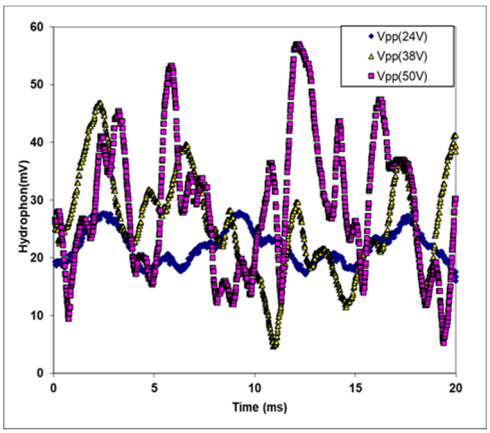

Fig. 5 Voltage Peak to Peak analysis in water.

The cavitation intensity strongly correlates with the electrical energy sent to the piezoelectric transducer. Hence, our study's interest is to optimize the electrical energy transferred to the piezoelectric transducer [30]. It is expected to link the optimization of the electrical energy transferred from the source power to the transducer and to realize a characterization voltage and frequency from the transition between stable and transient cavitation for different solvents.

We measure cavitation by extrapolating the spectral broadband components from 10 kHz to 5 MHz. As illustrated schematically in Figure 6, the sound pressure spectrum is classified into three types of frequency components. The first is the largest peak in the vicinity of f_0, assigned to the direct field. The second is the smaller peaks assigned to stable cavitation. The third is the broadband noise between the peak, assigned to transient cavitation [31]. In Figure 6, we see the energy transferred from the fundamental to the subharmonics due to the cavitation. For this waveform, we can obtain a frequency analysis as shown in Figure 6. which shows the difference of fundamental harmonic, sub-harmonic, and ultra-harmonic between water and IPA [32].

From Figure 6, we conclude by FFT calculation this difference between solvent used in our cleaning concept for optimizing cavitation energy from the transition from stable to transient cavitation via the energy transferred from the fundamental harmonic to the subharmonic and ultra harmonic which is presented by the changes in the amplitudes of the harmonics. The FFT calculation allows a spectrum variation for each solvent used in the cleaning process.

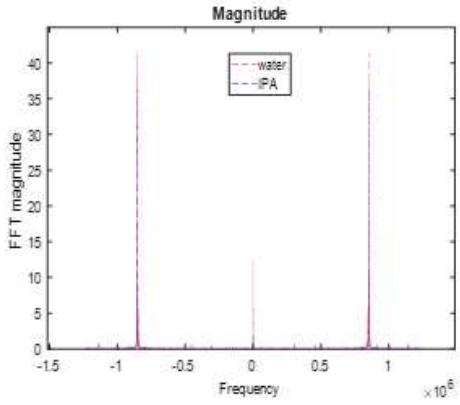

Fig. 6 Frequency spectrum of water and Isopropyl alcohol (IPA).

B. Experimental Analysis: Impact of gasification level

Figure 7 illustrates a resemblance of the simulation equation (1) to the experimental data, and the increase in gas content strongly influences the acoustic pressure. Increasing amounts of bubbles impact the Sound absorption by bubbles and change the speed of sound, influencing the value of acoustic impedance represented by Equation (2).

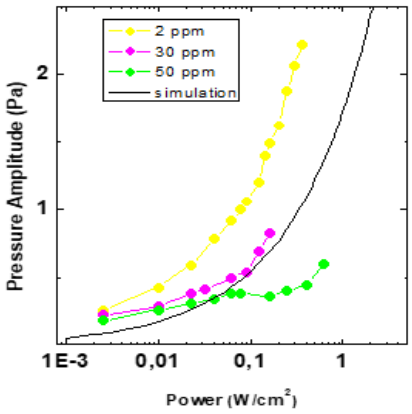

Fig. 7 Water-1MHz-gasified with O_2

In gasified aqueous liquids, the gas levels in an aqueous liquid can change the acoustical characteristics of the medium. In particular, this is interesting as literature [33]–[35] usually focuses on the power being applied while cleaning and causing damage, whereby the results can be confounded as there are some changes in the pressure that is applied which a particle or setup is getting that are not considered. On our chemical bath, we see a decrease in the cavitation threshold due to the increase in the dissolving O_2 in

the water, with this increasing gas level we decrease the acoustic pressure in the water. The current discovery suggests that using water supersaturated with dissolved gas O_2 is also beneficial for high frequency ultrasound like cleaning of silicon wafers by megasonics [36]–[38]. Experimental data shows that more factors than acoustic impedance and the gasification level should be considered, like surface tension, vapor pressure, density, and temperature, hence the interest in building a simulation model to calculate these parameters and show his important trends.

C. Simulation Analysis

We perform a simulation with Blake's model [39] at a frequency of 1 Mhz. Figure 8 and Table 1 illustrate the decrease of the transient cavitation threshold with the decrease of the surface tension, the decrease of the density, and the increase of the vapor pressure [20].

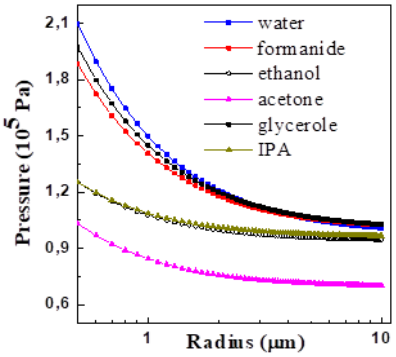

Fig. 8 Influence of the bubble radius on the acoustic cavitation.

TABLE I
VAPOR PRESSURE AND SURFACE TENSION.

Liquid	Threshold (10^5Pa) R_0=500 nm	P_V(kPa)	$\sigma(\times 10^{-3}\ N.m^{-1})$
Water	2.1	2.33	72.75
glycerole	1.97	0.0001	63.4
Formanide	1.88	0.002	58.2
IPA	1.25	4.1	21.8
Ethanol	1.25	5.94	22.75
Acetone	1.03	30.8	23.7

Figure 8 and Table 1 show the influence of P_A on acoustic cavitation at $R_0 = 500\ nm$ et $f = 1\ MHz$

D. Surface tension Effect

The simulation of the pressure using the analytical model [28] (1MHz, 2bar) shows in Figure 9 that the largest influence for small bubbles and small shift resonant size to small Radius [40]–[42].

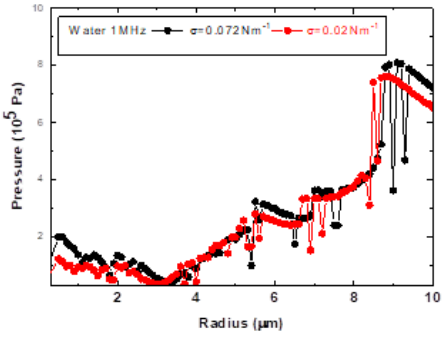

Fig. 9 Surface Tension Effect.

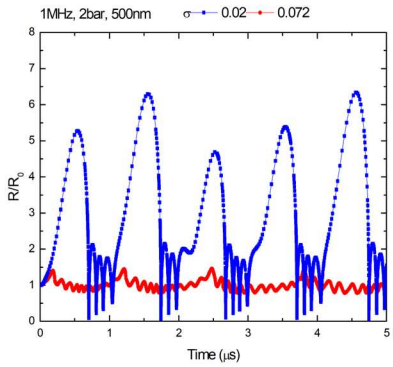

Fig. 10 Bubble radius variation for different surface tension in water: R_0=0.5 µm.

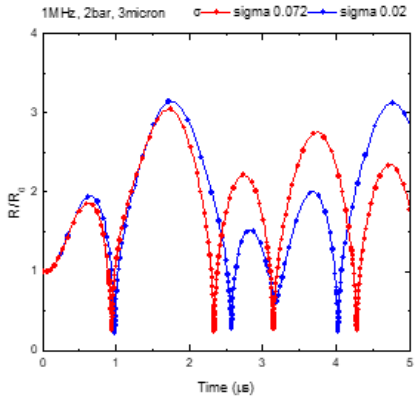

Fig. 11 Bubble radius variation for different surface tension in water: R_0=3 µm.

Figures 10 and 11 demonstrate that our simulation results on the effect of the change in surface tension agree well with the conclusions obtained by the study [43], which shows that for isolated bubbles in front of a wall, the stability of the bubbles in the liquid medium is reduced by low surface tension, and by a decrease of the cavitation threshold with the decrease of the surface tension.

E. Vapor Pressure Effect

The result of our analytical simulation of the pressure is presented in Figure 12. This approach shows the influence of the increasing vapor pressure in 20 °C which Pv=2338 Pa.

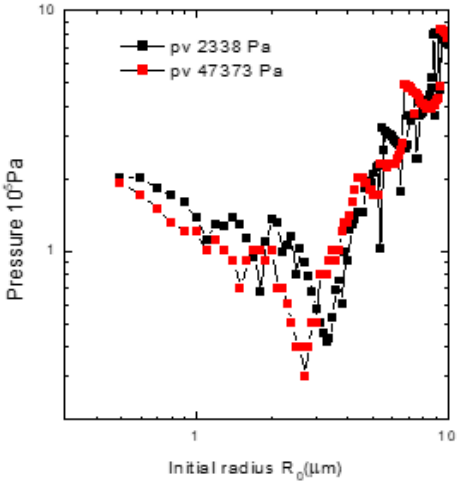

Fig. 12 Vapor Pressure Effect.

It is obvious that vapor pressure does not remain constant with increasing temperature but increases rapidly. Consequently, there is a rapid increase in vapor pressure with increasing temperature, and the cavitation threshold decreases accordingly. The corollary is that liquids with high vapor pressure or low surface tension cavitate at a lower intensity. We conclude that the higher vapor pressure influence directly the threshold cavitation (Lower threshold) [44].

F. Temperature Effect

The numerical simulation [24], [45] shows that the Bubble action increases in hot temperature at a fixed pressure. Figure 13 and Table 2 show the increased bubble action at higher temperatures [46].

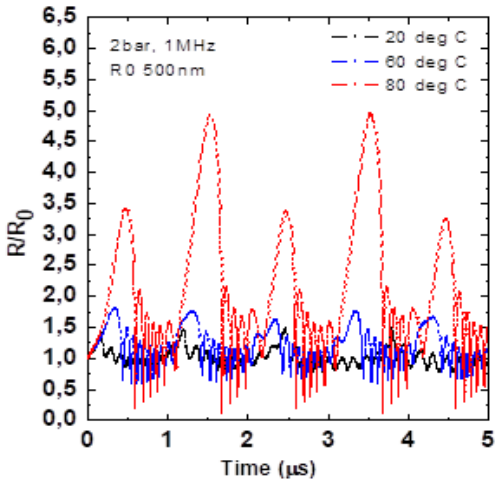

Fig. 13 Bubble growth of hot and cold water.

TABLE II
TEMPERATURE VARIATION EFFECT

Temperature (°C)	P_V (kPa)	$\sigma(\times 10^{-3}\ N.m^{-1})$
20	2.33	72.75
60	19.932	66.0
80	47.343	62.0

The last factor to consider here, known to affect the cavitation threshold, is temperature. It has been established that the threshold limit increases with decreasing temperature. This may be due in part to the increase in surface tension (σ) or viscosity (μ) of the liquid as the temperature decreases or to the decrease in vapor pressure (P_V) of the liquid. To better understand how these parameters (σ,μ,P_V) affect the cavitation threshold, we are programming a code to simulate an isolated bubble, of radius R_0, in water at a hydrostatic pressure (P_h) of 1 atm.

The results obtained from this model approach provide promising measures. We show that increasing the temperature in the water impacts the threshold of transient cavitation and the particle-removing performance. We can help build up a set up to optimize the power transferred from the piezoelectric transducer to the liquids to control megasonic agitation on Nano-structures [47].

G. Simulation of the Transient cavitation threshold of water

The analytical result correlates well with Glimore, the numerical model for small R_0 in water [48]–[50] for a frequency equal to 1 MHz in frequency and a temperature equal to 20 degrees.

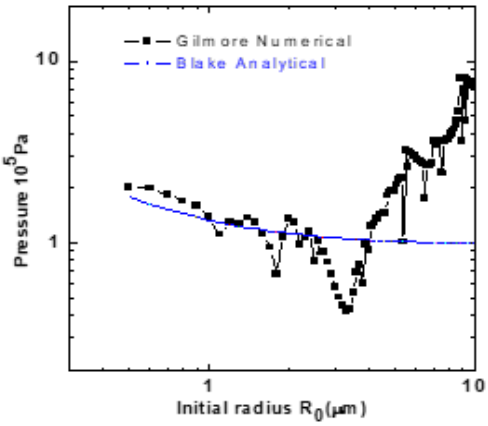

Fig. 14 Comparison between Blake and Glimore Model.

Figure 14 shows the resonant size, which indicates the transition from the stable (small oscillations around equilibrium radius) to the transient cavitation (Large oscillations and bubble collapse), and this increase of the pressure began for an initial radius equal to 3 µm. The Blake model gives us more information for small Bubbles [51], in case exploring the Glimore model for large Bubbles is interesting.

IV. CONCLUSION

The main objective of this study is the experimental determination of some parameters like the increasing of the electrical power and the control of gasification level with increasing O_2 gas content that strongly influences the acoustic pressure. The modeling result for water confirms that surface tension is an important influencing parameter on the transient cavitation threshold on small bubbles and varies with temperature, showing a decrease in surface tension with increasing temperature. If we can assume that P_V remains constant with increasing temperature, then there will be a small increase in P_V and a decrease in the pressure P_a required to cause cavitation.

Finally, we can build our dataset by quantifying experimental and simulation results using a megasonic and chemical solvent combination technique to monitor the cavitation limit and realize safe and non-damaging cleaning. Experimental measurements and simulation studies of the applied acoustic sound and cavitation limit reveal significant knowledge of the liquid's properties. As a result, we can work faster to achieve a positive result that assists in designing ultrasonic cleaning to clean sensitive Structures and in creating adequate directives for vendors and chemical customers.

In future work, we would like to model induced shock waves, jets, and resulting drag force FD and consider that more factors than acoustic impedance influence the conversion from power I to pressure field Pa.

NOMENCLATURE

P_∞	Driving pressure	Pa
$P_L(R)$	Liquid pressure at bubble wall	
ρ	Density	$Kg.m^{-3}$
σ	Tension Surface	$N.m^{-1}$
C and c	The speed of sound of the liquid	$m.s^{-1}$
$\ddot{R}$	The second order derivatives of the bubble radius	$m.s^{-2}$
P_v	Vapour pressure	Pa
P_h	Hydrostatic Pressure	atm
R	Bubble Radius	m
R_0	Initial Bubble Radius	m
H	Enthalpy	J
γ	The heat capacity ratio	Constant
$\dot{R}$	The first order derivative of the bubble radius	$m.s^{-1}$
I	Power	$W.cm^{-2}$
P_A	Amplitude Pressure	Pa
P_a	Amplitude Pressure	Pa

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