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The importance of laser-generated bubble expansion and cavitation erosion mechanisms for pulsed laser interactions and nanoparticle formation in liquid

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GE Research



Cavitation bubble effect in localized power deposition processes in liquids

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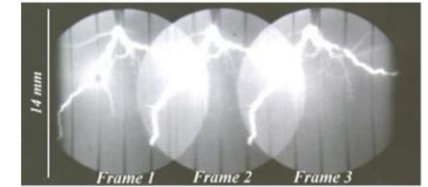


Bubble examples/scale



Localized energy deposition in liquids where bubbles play roles:

-underwater arc/spark discharges
/oil & gas application, rock breaking well restimulation/



-micro-EDM
/hole making in metals and metal alloys/

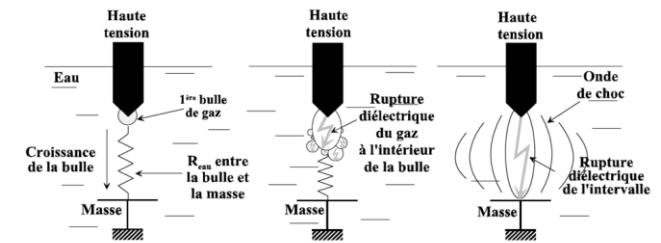
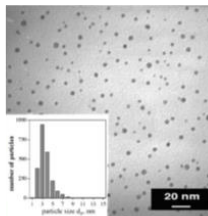
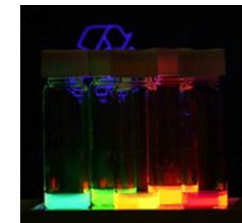
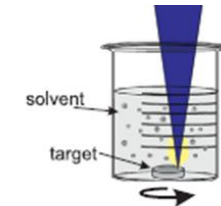
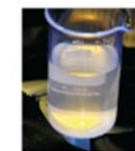
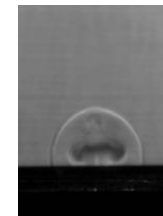
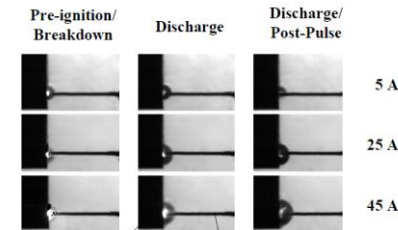


Figure 1-5 : Schématisation de la propagation sous polarité positive d'une décharge électrique subsonique dans de l'eau (200µs/cm) [7]

-laser -material interaction in liquids
/pinning, eye surgery, ablation/

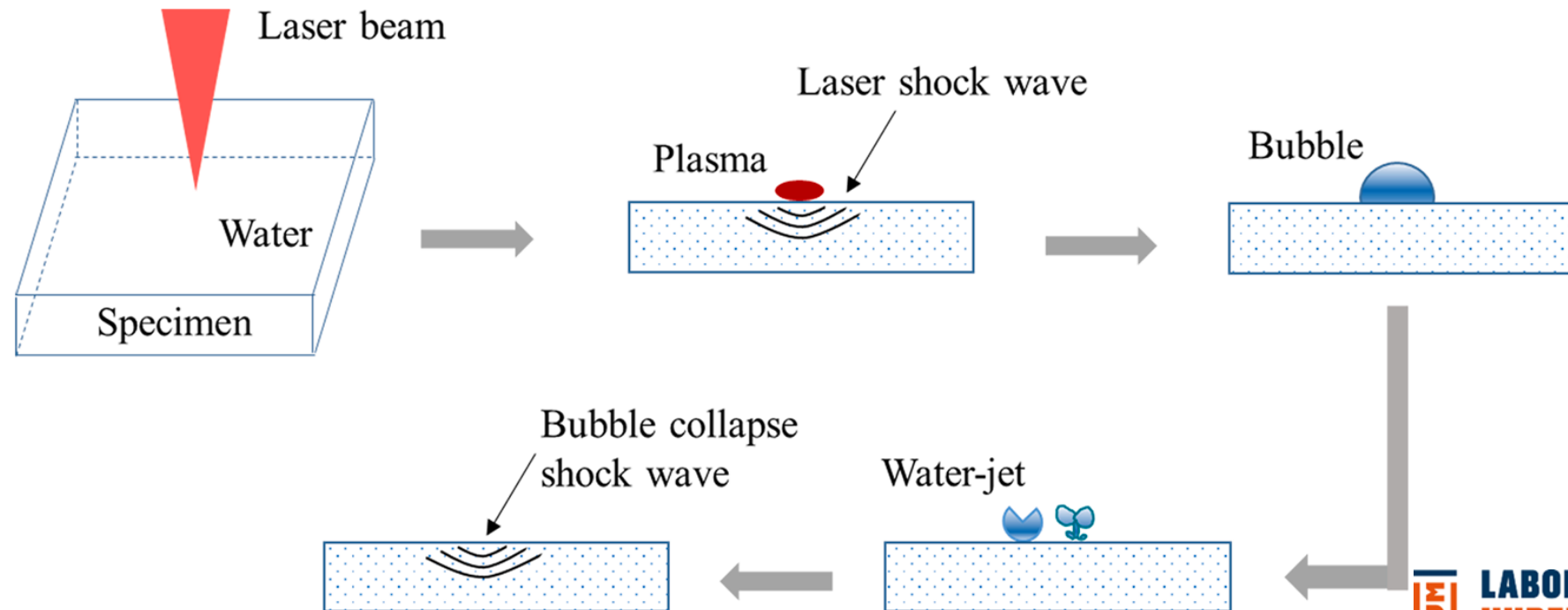


Pressure wave generated by underwater electrical discharge: Application to electrical fracturing PhD thesis, Justin Martin Université de Pau, France
https://www.researchgate.net/publication/253954969_Origin_of_Gas_Bubbles_in_a_Small_Work_Gap_During_the_Micro-EDM?enrichId=rgreq-8a7afbbbfe180b802dacc1f8945718e-XXX&enrichSource=Y292ZXJQYWdlOzI1Mzk1NDk2OTtBUzo%3D%3D&el=1_x_2&_esc=publicationCoverPdf
 On nanoparticle formation by laser ablation in liquids
 TE Itina - The Journal of Physical Chemistry C, 2011

Why bubbles are important?



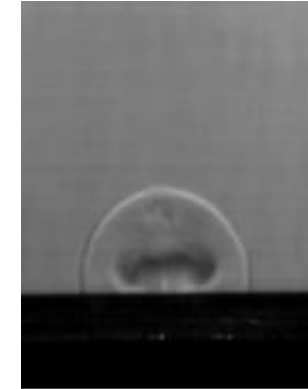
- Bubble collapse results in large pressure increase
- Shock waves
- Surface material splashing
- Jets



Bubble formation theory

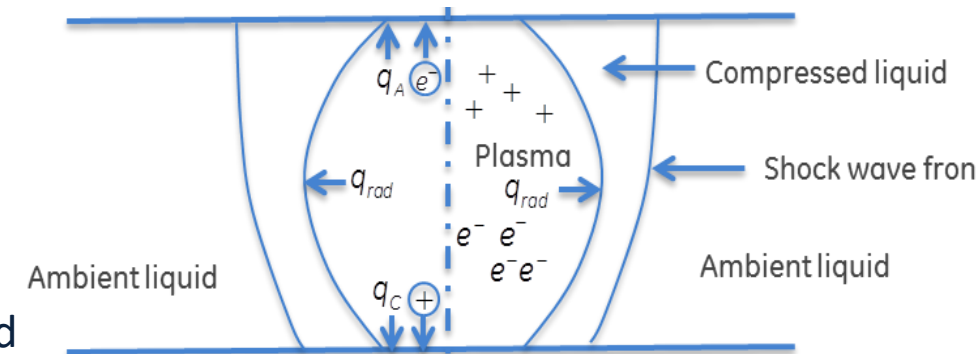


- Still not widely used
- Radiation absorption often wrongly neglected



Underwater localized energy deposition (OD) implemented in MATLAB GRC Model Highlights

- Bubble is treated as a thermodynamic system whose state is set by P , T and R
- Spherical bubble dynamics in a compressible liquid (Keller-Kolodner* model)
- Heat loss mechanisms include radiation and vapor condensation/evaporation
- Pressure computed using ideal gas law with dissociation
- Acoustic pressure rise in surrounding liquid is calculated
- Radiative heat flux computed for specified pressure, temperature and bubble size – lookup tables generated for given ranges of above parameters



Bubble formation theory



Bubble dynamics

$$\left(1 - \frac{\dot{R}}{c_\infty}\right) R \ddot{R} + \frac{3}{2} \left(1 - \frac{\dot{R}}{3c_\infty}\right) \dot{R}^2 = \left(1 + \frac{\dot{R}}{c_\infty} + \frac{R}{c_\infty} \frac{d}{dt}\right) h_B$$

$$h_B = \int_{\rho_\infty}^{\rho} \frac{dp}{\rho} \quad \frac{\rho + B}{\rho_\infty + B} = \left(\frac{\rho}{\rho_\infty}\right)^n \quad c_\infty^2 = \frac{n(\rho_\infty + B)}{\rho_\infty} \quad h_B = \frac{c_\infty^2}{n-1} \left(\left(\frac{\rho + B}{\rho_\infty + B}\right)^{(n-1)/n} - 1 \right) \quad \dot{h}_B = \frac{\dot{\rho}_B}{\rho_B + B} \left(\frac{n-1}{n} h_B + \frac{c_\infty^2}{n} \right)$$

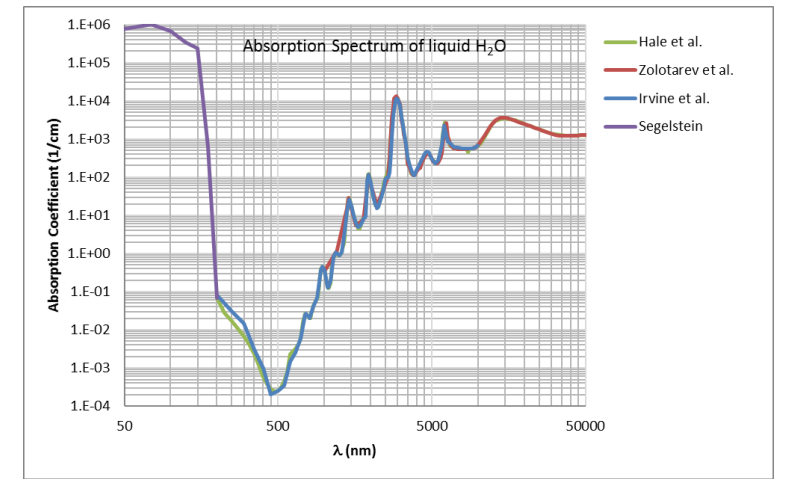
$$p_B = P - \frac{1}{R} (2\sigma + 4\mu\dot{R}) \quad \dot{\rho}_B = \dot{P} - \frac{4\mu}{R} \ddot{R} + \frac{\dot{R}}{R^2} (2\sigma + 4\mu\dot{R})$$

$$\frac{d}{dt}(\rho V) = -\dot{m}_{out} \quad \frac{\rho V}{n(\rho_\infty + B)} \frac{dp_\infty}{dt} = \rho 4\pi R^2 \frac{dR}{dt} - k(p_\infty - p_0) \quad \dot{P} = \eta P \left[\left(\frac{\partial g}{\partial \alpha} \frac{1}{g} \left(\frac{\partial \alpha}{\partial T} \right)_P + \frac{1}{T} \right) \dot{T} + \frac{3gRT}{PR} \dot{m}_T - \frac{3\dot{R}}{R} \right]$$

$$PV = Mg(\alpha)RT \quad U = MR_g \left(3T \left(1 + \frac{\alpha}{2} \right) + \alpha \frac{L_{dis}}{R_g} \right)$$

$$Q = 4\pi R^2 q = 4\pi R^2 (q_{in} - q_{BB} - q_M)$$

$$q_{in}(t) = P_0 \left(1 - k(t/t_d)^2 \right) \sin(\pi t/t_d) / 4\pi R^2 \quad q_{BB} = (1 - \phi(x, T)) \varepsilon \sigma (T^4 - T_\infty^4) \quad q_M = [\dot{m}_T + \dot{m}_E \Theta(\dot{m}_E)] \int_{T_E}^T c_p(T) dT$$



A. Lezzi and A. Prosperetti, "Bubble Dynamics in a Compressible Liquid. Part 2: Second Order Theory", J. Fluid. Mech. 185, 289 (1987).

R.H. Cole, "Underwater Explosions", Princeton Univ. Press, Princeton NJ (1948)

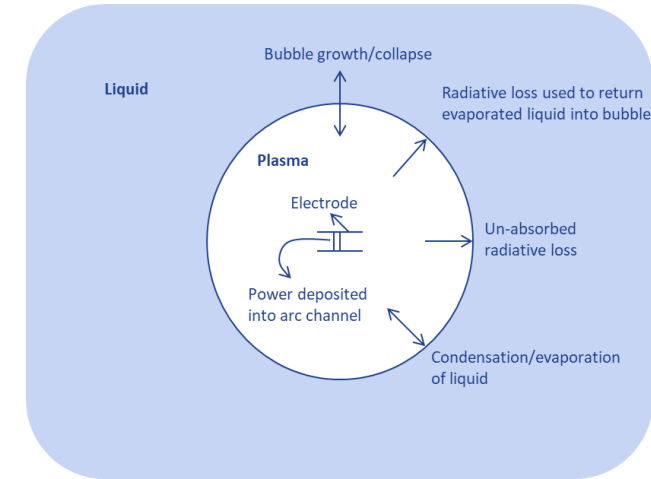
J.A. Cook et al., "A Spark-generated Bubble Model with Semi-empirical Mass Transport", J. Acoust. Soc. Am. 101, 1908 (1997).

Bubble formation model

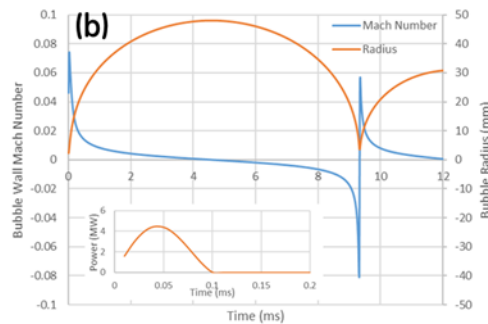
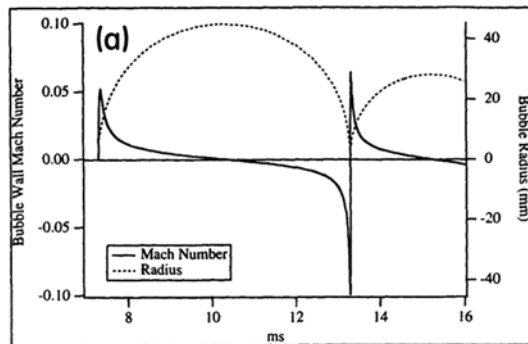


Model assumptions

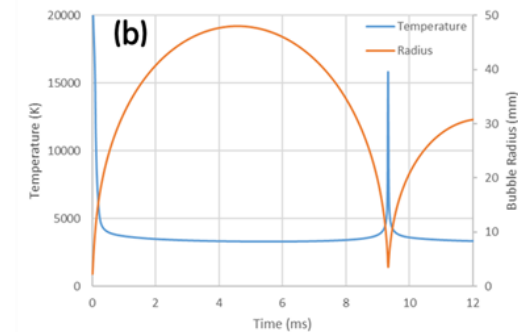
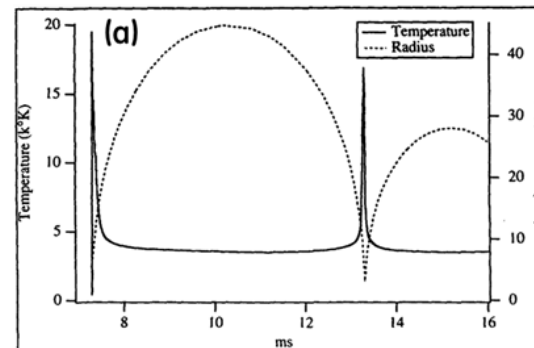
- 1) The contents of the **bubble are homogeneous and in thermodynamic equilibrium.**
- 2) The gas in the bubble obeys the **ideal gas law**, with modifications to account for the fact that water vapor in the bubble is dissociated. Ionization is neglected.
- 3) The bubble is **optically thick**, wherein emissivity of the bubble was calculated using the Rosseland weighting approach, which calculates a frequency averaged photon mean free path.
- 4) **A dissipation length was assumed** to calculate the fraction of emitted radiation absorbed by the surrounding water.
- 5) Mass flow from evaporation and condensation - model by Schrage.
- 6) Thermal loss from the bubble due to conduction into liquid was ignored



Model validation



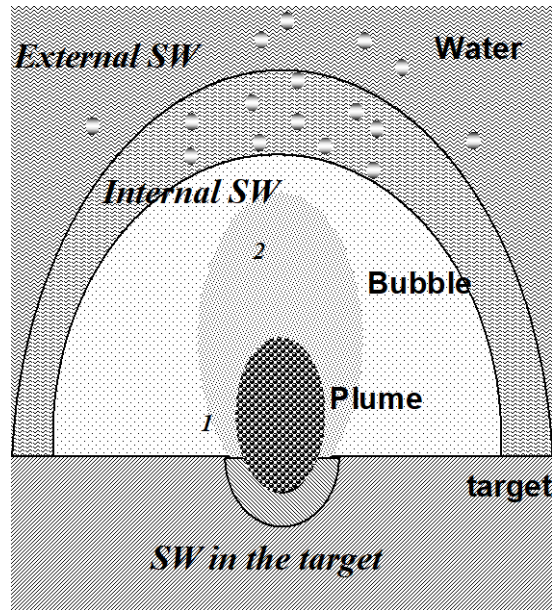
Comparison between calculated bubble radius and wall Mach number for a discharge energy of 270 J from a) Cook technical report, and b) this work.



Comparison between calculated bubble radius and temperature for a discharge energy of 270 J from a) Cook technical report, and b) this work.

J.A. Cook et al., "A Spark-generated Bubble Model with Semi-empirical Mass Transport", J. Acoust. Soc. Am. 101, 1908 (1997).
 R.W. Schrage, "A Theoretical Study of Interphase Mass Transfer", Columbia U.P., New York (1953).
 M.S. Plesset and A. Prosperetti, "Bubble Dynamics and Cavitation", Annu. Rev. Fluid Mech. 9, 145 (1977).
 B. Ramamurthi, T. Sommerer Analysis of an in-liquid Arc System for Oil & Gas Well Re-stimulation GE GRC Report, 2016

Laser ablation in liquids



1. Early stage – laser energy absorption, material ejection, plume formation

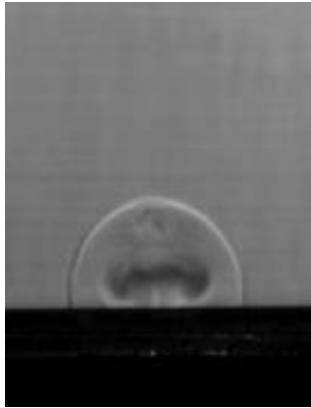
2. Intermediate stage – plume expansion, SWs propagation, cavitation bubble development, oscillations

3. Late stage – Bubble collapse, plume mixing with the liquid, NP coalescence/aggregation processes.

Pressure on the target:

- from laser heating : SW propagation in the target and rarefaction wave (tensile pressure) is formed behind
- from the backscattering plasma plume: additional heating and pressure
- from the collapsing cavitation bubble and water micro-jet

Laser ablation in liquids



-bubble formation (liquid)

-confinement=> different ablation threshold and yield

-shock wave formation

What are the roles of laser, plasma and of cavitation bubble?

Confinement by liquid

$$R_n(t) = \left\{ R_{na}^3 + \frac{R_{nb}^3 - R_{na}^3}{2\tau} \left[t - \frac{\tau}{\pi} \sin\left(\frac{\pi}{\tau} t\right) \right] \right\}^{1/3}$$

Vogel et al., J. Acoust. Soc. Am. 100(1), 1996

=>Hydrodynamic modeling

- **Gold target in water**
- *2T semi-empirical equations of state (for metal, gold here)*
- *EOS for water*

$$I(t) = I_0 \exp(-4 \ln 2 t^2 / \tau^2), \quad \tau = 200 \text{ fs}, \quad 800 \text{ nm}, \quad I_0 = 2, 3, 4, 5 \times 10^{13} \text{ W/cm}^2$$

Laser ablation in water



Bubble radius/ pressure vs time: examples of bubble behavior

Experiment

Model

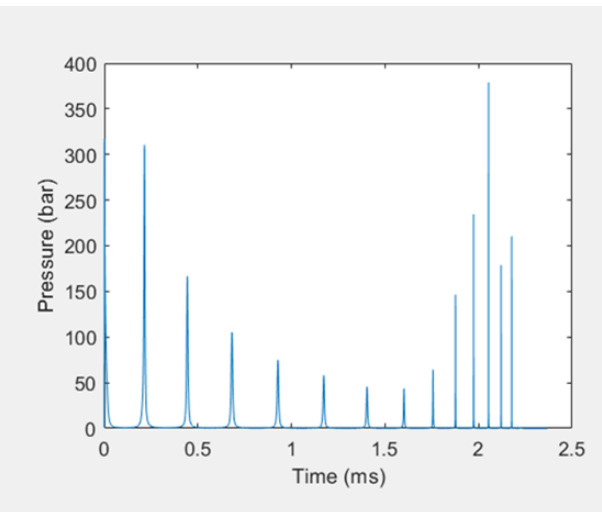
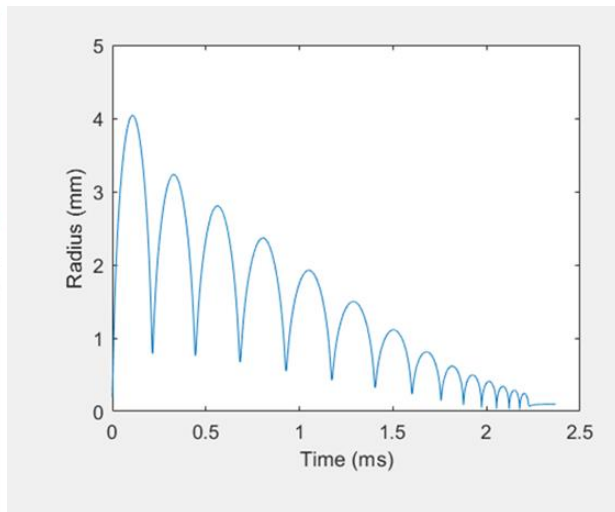
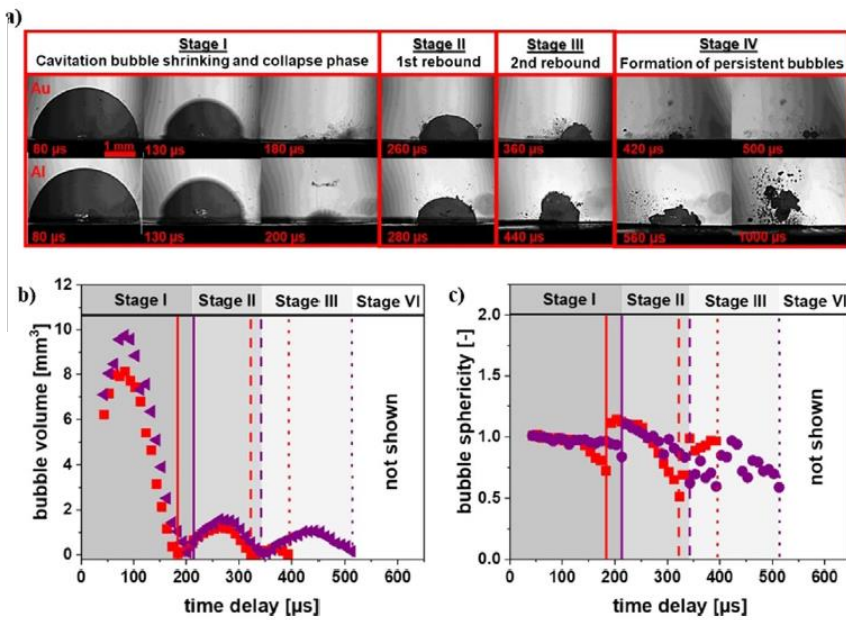
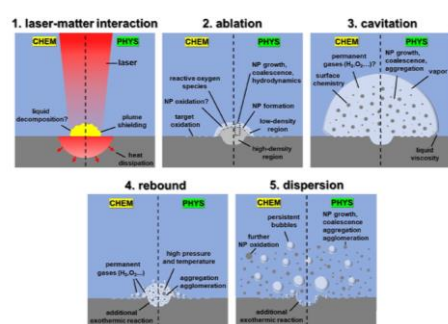
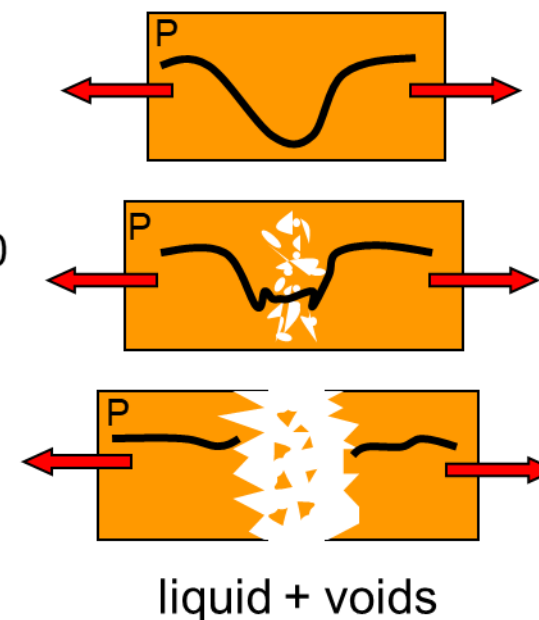
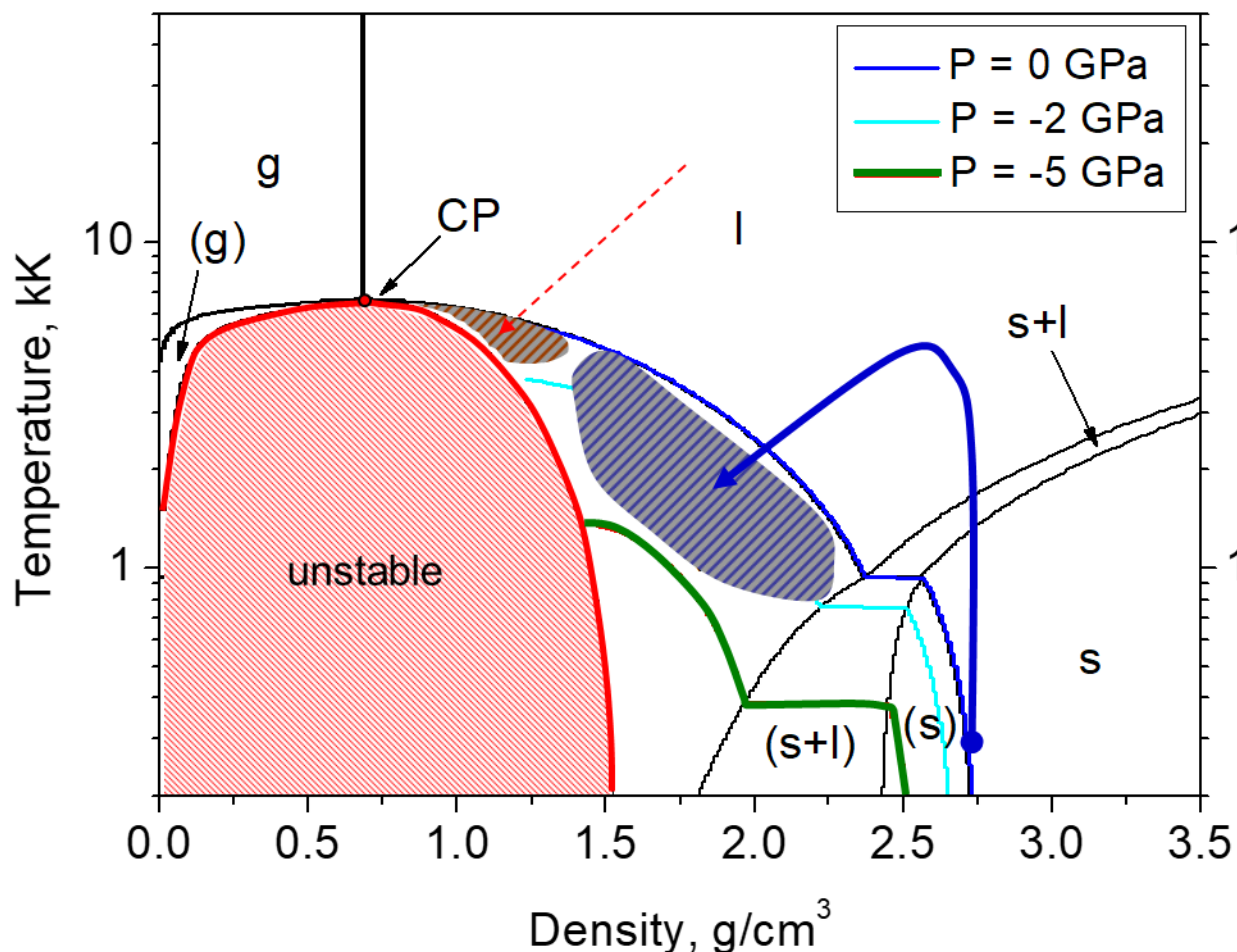


Figure 7. (a) Temporal evolution of the cavitation bubble on gold (upper picture series) and aluminum target (lower picture series) immersed in water at a theoretical, incident laser fluence of 313 J cm^{-2} . (b) Temporal evolution of the cavitation bubble volume and (c) calculation of the bubble sphericity (hemispherical = 1.0) as a function of time. Au = red squares, Al = purple circles.

Mark-Robert Kalus, Stephan Barcikowski, and Bilal Gökçe How the Physicochemical Properties of the Bulk Material Affect the Ablation Crater Profile, Mass Balance, and Bubble Dynamics During Single-Pulse, Nanosecond Laser Ablation in Water
 Chemistry – A European Journal | Full Paper | doi.org/10.1002/chem.202005087

Spallation (material fragmentation due to expansion)



Pore coalescence affects time to fracture

Fragmentation criterium

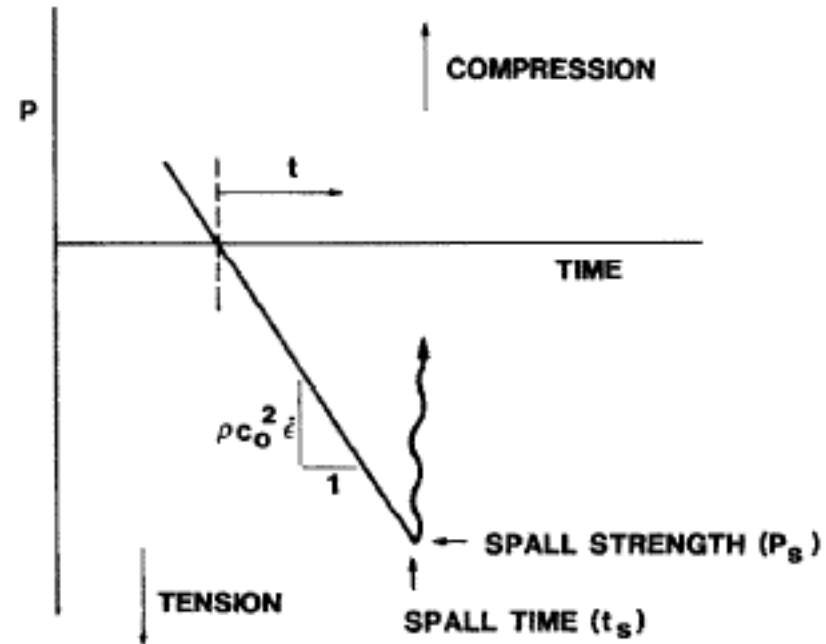


Energy minimization

$$P_s = (6\rho^2 c^3 \sigma \dot{\epsilon})^{1/3}$$

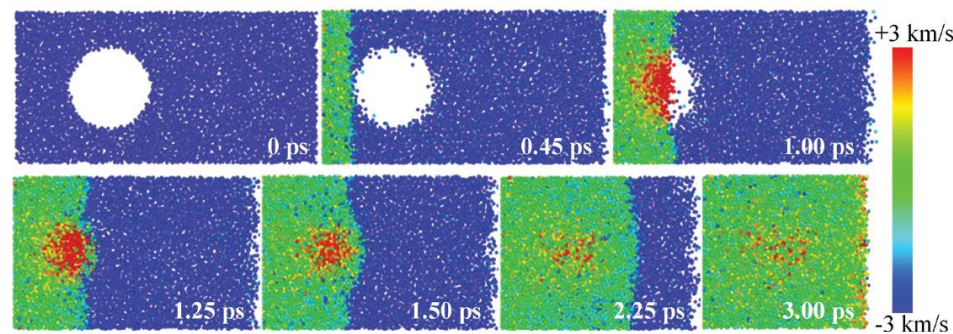
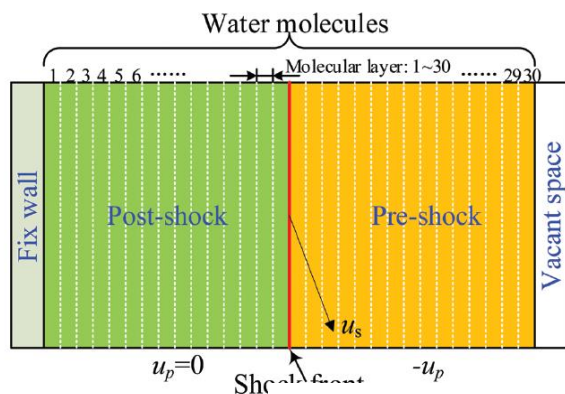
$$t_s = (6\sigma / \rho \dot{\epsilon}^2 c^3)^{1/3}$$

$$\sigma = \sigma_0 (1 - T/T_c)^{1.25}$$



D. Grady, J. Mech. Phys. Solids **36**, 353 (1988).

Bubble MD simulations



Sequence of snapshots of the shock wave propagation through the water for $D = 5.0$ nm at $u_p = 3.0$ km s⁻¹.

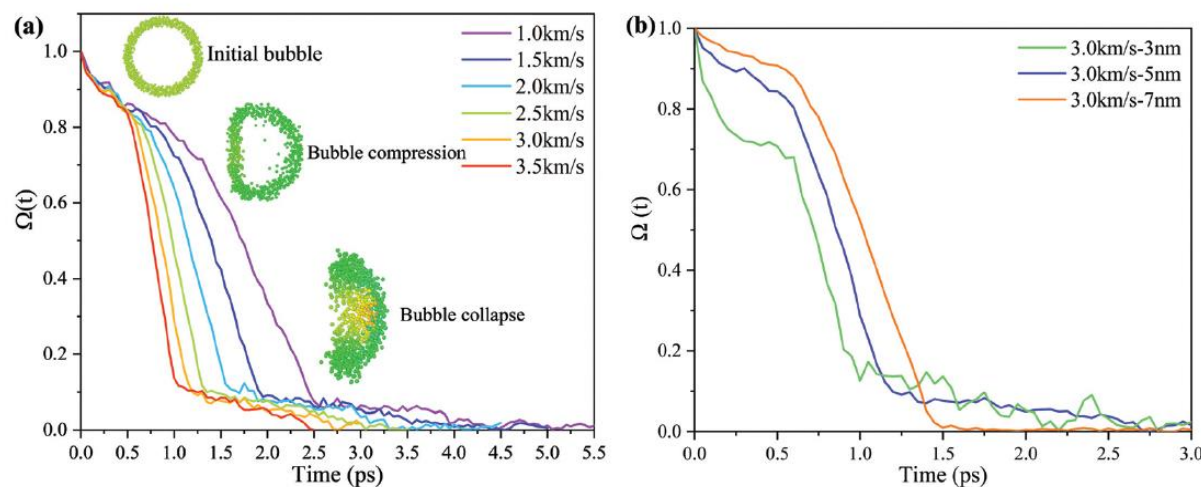


Fig. 9 Normalized bubble volumes $\Omega(t)$ versus time for the different particle velocities u_p and bubble diameters D : (a) $D = 5$ nm, $u_p = 1.0, 1.5, 2.0, 2.5, 3.0$ and 3.5 km s⁻¹; (b) $D = 3, 5$ and 7 nm, $u_p = 3.0$ km s⁻¹.

Summary and future work



- Cavitation bubbles are important phenomena to account when there is a localized large energy deposition in liquids
- Bubble formation theory exists and provides good insight into bubble dynamics
- Large pressure at the bubble collapse stage results in surface material splashing, shock waves both in liquids and surface materials
- MD simulations of bubble formation have recently been successful
- Future work can focus on a creation of a comprehensive model for laser ablation in fluids accounting for a cavitation bubble effect

Questions?



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Contact: seleznev@ge.com