



Shock-induced collapse of a vapor nanobubble near solid boundaries



Francesco Magaletti, Mirko Gallo, Luca Marino, Carlo Massimo Casciola*

Dipartimento di Ingegneria Meccanica e Aerospaziale, Università di Roma "La Sapienza", via Eudossiana 18, 00184 Roma, Italy

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ABSTRACT

The collapse of a nano-bubble near a solid wall is addressed here exploiting a phase field model recently used to describe the process in free space. Bubble collapse is triggered by a normal shock wave in the liquid. The dynamics is explored for different bubble wall normal distances and triggering shock intensities. Overall the dynamics is characterized by a sequence of collapses and rebounds of the pure vapor bubble accompanied by the emission of shock waves in the liquid. The shocks are reflected by the wall to impinge back on the re-expanding bubble. The presence of the wall and the impinging shock wave break the symmetry of the system, leading, for sufficiently strong intensity of the incoming shock wave, to the poration of the bubble and the formation of an annular structure and a liquid jet. Intense peaks of pressure and temperatures are found also at the wall, confirming that the strong localized loading combined with the jet impinging the wall is a potential source of substrate damage induced by the cavitation.

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1. Introduction

The collapse of vapor bubbles near solid boundaries has been deeply investigated in the last century. The triggering episode goes back to the finding of the destructive effects of cavitation phenomena on the propellers of the great ocean liners at the beginning of the 20th century. Similar effects have been observed successively on the blade of big hydraulic machines like turbines and pumps (Silberrad, 1912; Leighton, 2012). Only recently, due to the increasing impact of the micro and nano-technologies, the attention from millimeter-size bubbles has shifted downwards, toward micro or sub-micro bubbles. Indeed in microfluidic devices, the so called *lab on a chip*, cavitation phenomena can be employed for microfluidic pumping (Dijkink and Ohl, 2008), to enhance mixing by means of vorticity generation during the final stage of bubble collapse and for surface cleaning purposes (Ohl et al., 2006). Cavitation bubbles are also used in advanced medical procedures like high intensity focused ultrasound (HIFU) and extracorporeal shock wave lithotripsy (ESWL) (Coussios and Roy, 2008) to enhance drug delivery or increase local heat deposition deep within the body, to control localized cell membrane poration (Sankin et al., 2010), and to comminute kidney stones (Zhu et al., 2002). Moreover, the use of femtosecond lasers, generating nanometric bubbles, has recently

found important applications in nanosurgery of cells and tissues (Vogel et al., 2005; 2008).

The experimental investigation has played the most important part in the understanding of bubble–wall interactions, so far. The improvements in the bubble generation techniques led to cleaner and better reproducible data, starting from the kinetic impulse technique (Benjamin and Ellis, 1966). This approach suffers from the disadvantage that the bubble must be located before the application of the impulse. Successively the problem of localization has been overcome by means of the generation of the bubble by using an electric spark (Naudé and Ellis, 1961; Tomita and Shima, 1986). As a drawback, the electrodes perturb the bubble motion in the last stage of the collapse. At the moment, the best bubble generation technique is, probably, the non-intrusive pulsed-laser discharge (Vogel et al., 1989) that can focus an intense local heating and vaporization of the liquid through application of a thermal impulse. The visualization of the bubble dynamics can be performed by illuminating the scene with diffuse backlighting (Blake and Gibson, 1981) and by means of high-speed cameras, up to 20 million frames per second (Ohl et al., 1995). More recently, the μ -PIV technique has been used to measure the flow field during the bubble collapse (Sankin et al., 2010). The experiments allowed the visualization of the jet formation during the bubble collapse near solid surfaces and the assessment of the role of shock-wave emission, jet-wall interaction and chemical effects on cavitation damage (Benjamin and Ellis, 1966; Plesset and Ellis, 1955). Notwithstanding the extreme frame-rate of modern cameras, the complete and detailed description of thermo-acoustic and

* Corresponding author.

E-mail address: carlomassimo.casciola@uniroma1.it (C.M. Casciola).

URL: https://sites.google.com/a/uniroma1.it/prova_fumacs2/ (C.M. Casciola)

flow fields, is still lacking. The temperature and pressure inside the bubble at the collapse instant is not easily accessible with non-intrusive measurements. The pressure indeed can be only extrapolated by measuring it with a hydrophone at some distance from the bubble and by assuming a classical $1/r$ decay (Lauterborn and Vogel, 2013). The temperature instead can be estimated by matching a blackbody radiation with the measured spectrum of the emitted light upon collapse (Flannigan and Suslick, 2005).

On the other hand, the mathematical modeling of cavitation is still a great challenge. The cornerstone in the theory of bubble dynamics was the pioneering work of Rayleigh (1917) who described the collapse of a bubble immersed in a unbounded incompressible liquid. Despite the significant simplifying assumptions, the correspondence with experimental results is still impressive. The model has been successively refined by taking into account compressibility effects in the liquid (Keller and Kolodner, 1956; Hickling and Plesset, 1964) and the presence of a dilute gas in the bubble. These refined models provided an estimate of the pressure peaks reached inside the bubble on the order of hundred times the pressure of the liquid environment. Numerical simulations and more complex analysis followed (Plesset and Chapman, 1971; Plesset and Prosperetti, 1977; Shima and Sato, 1981) in order to describe the effect of a nearby boundary. Different numerical techniques have been used in order to capture the interfacial dynamics, ranging from the Boundary Element Method (BEM) for irrotational conditions (Blake and Gibson, 1981) to the Arbitrary Lagrangian Eulerian (ALE) schemes (Tipton et al., 1992; Ding and Gracewski, 1996). Recently more sophisticated models have been proposed to gain new insights on the effects of dissolved gas and phase change (Akhatov et al., 2001) and to obtain a deeper knowledge in fascinating phenomena like sonoluminescence (Brenner et al., 2002). Of particular interest is the diffuse interface approach which enables a natural description of interfacial flows, changes of topology, vapor/liquid and vapor/supercritical fluid phase changes which have been shown to be crucial for the correct description of the final stages of the bubble collapse (Magaletti et al., 2015).

In this work we will exploit the diffuse interface model to numerically investigate the collapse of a sub-micron vapor bubble near solid boundaries. The effect of the initial bubble–wall distance will be analyzed and the visualization of the entire flow and thermo-acoustic fields will be provided. Particular attention will be paid to the stress distribution on the solid wall and we will address the role of the different pressure waves on cavitation damage.

The paper is organized as follows: in Section 2 the diffuse interface model and the relevant conservation equations is derived; Section 3 provides details on the numerical scheme and describes the numerical setting of the simulations; finally, the results of the numerical experiments will be discussed in Section 4 to finally draw conclusions and provide final comments in the last Section 5.

2. Mathematical model

Thermodynamics of non-homogeneous systems

We exploit an unsteady diffuse interface description (Anderson et al., 1998) of the multiphase flow in a domain \mathcal{D} based on the van der Waals gradient approximation of the free energy functional $F[\rho, \theta]$ (Dell'Isola et al., 1995; Jamet et al., 2001):

$$F[\rho, \theta] = \int_{\mathcal{D}} \hat{f} dV = \int_{\mathcal{D}} \left(\hat{f}_0(\rho, \theta) + \frac{\lambda}{2} |\nabla \rho|^2 \right) dV, \quad (1)$$

where $\hat{f} = \hat{f}_0 + \lambda/2 |\nabla \rho|^2$ with $\hat{f}_0(\rho, \theta)$ the classical Helmholtz free energy density per unit volume of the homogeneous fluid at temperature θ and mass density ρ . The coefficient $\lambda(\rho, \theta)$, in general function of the thermodynamic state, embodies all the information on the interfacial properties of the liquid–vapor system (i.e.

surface tension and interface thickness). In particular, for a van der Waals fluid, the free energy reads

$$\hat{f}_0(\rho, \theta) = \bar{R} \rho \theta \left[-1 + \log \left(\frac{\rho K \theta^{1/\delta}}{1 - b\rho} \right) \right] - a\rho^2, \quad (2)$$

with $\delta = \bar{R}/c_v$, \bar{R} the gas constant, c_v the constant volume specific heat, a and b the van der Waals coefficients and K a constant related to the de Broglie length (Zhao et al., 2011).

Equilibrium conditions

The present paragraph summarizes, for the reader convenience, results concerning thermodynamic equilibrium for systems described by the free energy functional (1). Although well known to specialists, we deemed useful to present a short summary to rationalize this classical material which is hardly described comprehensively in literature, Jamet (1998).

At given temperature, equilibrium is characterized by the minimum of the free energy functional in Eq. (1), where variations are performed with respect to the density distribution ρ . The evaluation of the functional derivative leads to the following equilibrium condition:

$$\mu_c^0 - \nabla \cdot (\lambda \nabla \rho) = \text{const}, \quad (3)$$

where the temperature is constrained to be constant, $\theta = \text{const}$, and $\mu_c^0 = \partial \hat{f}_0 / \partial \rho|_{\theta}$ is the classical chemical potential. The equation defines a generalized chemical potential $\mu_c = \mu_c^0 - \nabla \cdot (\lambda \nabla \rho)$ that must be constant at equilibrium.

The consequence of the above equilibrium conditions is better illustrated in the simple case of a planar interface, where the only direction of inhomogeneity is x , under the assumption of constant λ . The constant temperature appears in the equilibrium problem as a parameter and will not be further mentioned throughout the present section. Hence, determining the equilibrium density distribution amounts to finding a solution of

$$\mu_c = \mu_c^0(\rho) - \lambda d^2 \rho / dx^2 = \mu_{eq}, \quad (4)$$

where the chemical potential in the bulk fluid (the vapor phase, say), far from the interface where $d\rho/dx = 0$, determines the constant $\mu_{eq} = \mu_c^0(\rho_V) = \mu_c^0(\rho_L)$. By multiplying Eq. (4) by $d\rho/dx$ and integrating between $\rho_{\infty} = \rho_V$ and ρ , leads to

$$\hat{w}_0(\rho) - \hat{w}_0(\rho_V) = \frac{\lambda}{2} \left(\frac{d\rho}{dx} \right)^2, \quad (5)$$

where $\hat{w}_0(\rho) = \hat{f}_0(\rho) - \mu_{eq}\rho$. Eq. (5) shows that \hat{w}_0 has the same value in both the bulk phases, where the spatial derivative of mass density vanishes: $\hat{w}_0(\rho_L) = \hat{w}_0(\rho_V)$.

The grand potential, defined as the Legendre transform of the free energy,

$$\Omega = F - \int_{\mathcal{D}} \rho \frac{\delta F}{\delta \rho} dV = \int_{\mathcal{D}} \hat{w} dV, \quad (6)$$

has the density (actual grand potential density)

$$\hat{w}[\rho] = \hat{f} - \mu_c \rho = \hat{f}_0 + \frac{\lambda}{2} \left(\frac{d\rho}{dx} \right)^2 - \left(\mu_c^0 - \lambda \frac{d^2 \rho}{dx^2} \right) \rho, \quad (7)$$

implying that, in the bulk, $\hat{w} = \hat{w}_0$, i.e. \hat{w}_0 is the bulk grand potential density.

Given the form of $\hat{w}_0(\rho)$, the solution of Eq. (5) provides the equilibrium density profile $\rho(x)$:

$$x = \sqrt{\frac{\lambda}{2}} \int_{\rho_V}^{\rho} \frac{d\rho}{\sqrt{w_0(\rho) - w_0(\rho_V)}} + \text{const}. \quad (8)$$

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