Two-phase microfluidics: thermophysical fundamentals and engineering concepts

V V Kuznetsov\textsuperscript{1,2}
\textsuperscript{1} Institute of Thermophysics Siberian Branch of Russian Academy of Sciences
\textsuperscript{1} 1, Academician Lavrentyev Av., Novosibirsk, 630090, Russian Federation
\textsuperscript{2} Novosibirsk State University, 2, Pirogova Str., Novosibirsk, 630090, Russian Federation

E-mail: vladkuz@itp.nsc.ru

Abstract. Thermophysical fundamentals and engineering concepts of the two-phase microfluidic devises based on controlled liquid decay are discussed in this paper. The results of an experimental study of the explosive evaporation at a thin film heater of the MEMS devise in application to thermal inkjet printing are presented. The peculiarities of homogeneous nucleation and bubble growth in the liquid subjected to pulse heating are discussed. Using experimental data a simple equation suitable for predicting the growth rate of a vapor bubble in a non-uniformly superheated liquid was obtained and used to complete a mathematical model of the self-consistent nucleation and vapor bubbles growth in the induced pressure field. The results of numerical calculations according to the proposed model showed good agreement with the experimental data on a time of nucleation and duration of the initial stage of an explosive evaporation of water.

1. Introduction
The revolutionary development of novel micro and nanotechnologies in different fields of the engineering occurs at the past twenty years [1]. Microfluidic devices based on these technologies get a very wide range of the applications due to significant advantages over their conventional counterparts, including fast response time and high intensity of the heat and mass transfer. Using advances in two-phase microfluidics the promising devices were developed including microchannel heat sinks and MEMS devices based on the controlled decay of metastable liquid. Difficulties encountered in development of the two-phase microfluidics is caused by qualitative changes in the regularities of fluid and heat flows with phase change due to the reduction of channels size and are poorly understood [2].

A promising direction in the development of two-phase microfluidics is the MEMS devices based on controlled explosive decay of the liquid micro volumes, including thermal inkjet printheads [3]. In these printheads, the ink droplet is ejected from a microfluidic chamber as the result of liquid pulsed heating and explosive evaporation arising, see figure 1. It is well-known that the condition for transition to the explosive boiling is achievement of the temperature of limit overheating

\[ T_{\text{lim}} / T_c = 0.905 + 0.095 \cdot (T_s / T_c)^6, \]

where \(T_s\) is saturation temperature and \(T_c\) is critical temperature [4]. The problem of this temperature achievement (313.14 °C for water at atmospheric pressure) is the exponential growth of density fluctuations near spinodal line and a sharp decrease in the nucleation waiting time. It determines the possible time for explosive evaporation occurrence less then 2–3 microseconds. The regularities of explosive evaporation on a flat microheater were considered in
[5–7], but the initial stage of an explosive evaporation, which determines the efficiency of droplet ejection, is poorly understood because of its short duration.

In present paper the thermophysical fundamentals of two-phase microfluidic devices based on the controlled decay of metastable liquid are considered. The results of an experimental study of the explosive evaporation at a thin film heater of the MEMS devise in application to thermal inkjet printing are presented. The theoretical model of explosive evaporation at a multilayer thin film heater which can be used for design of the two-phase microfluidic device based on the controlled decay of metastable liquid is proposed and discussed.

2. Experimental study of the explosive evaporation in two-phase microfluidics

A necessary condition for the stable realization of an explosive boiling in two-phase microfluidics is rapid removal of the heat from a heat release zone immediately after the onset of nucleation. Therefore design of the microheater, which provides fast heating of the liquid as far as rapid heat dissipation after heat release shutdown, is of paramount importance to ensure the stable operation of the MEMS devises. For design of thin film microheater (resistor), the numerical calculations were carried out using 3–D heat equation for multilayer resistor immersed in a liquid. It was found that the multilayer thin film resistor with optimized material and thickness of the layers has the necessary properties. In this case, the perspective is the use of thin film resistor made from tantalum-aluminum alloy as heat release layer and additional layers of another material to provide a thermal interface with the substrate of quartz glass and electrical insulation of the resistive layer. These layers were made by sequential PECVD process of layering deposition of the silicon dioxide, TaAl alloy (resistive layer), silicon nitride and silicon carbide on the glass substrate according to [8]. During microheater manufacturing the hard silicon carbide was used as the outer layer. The heater area equals to $1.1 \times 10^{-8}$ m$^2$. Numerical calculations defined the layer thicknesses, which permit multiple high growth rate of liquid temperature without microheater destruction. The example of temperature profile calculations for multi-layer microheater at time $3.3 \, \mu$s from a heating start is shown in figure 2. As can be seen, the maximum temperature in the microheater corresponds to the resistive layer, and the choice of layer thicknesses allows us to achieve the necessary compliance of heat fluxes to the liquid and heat regulating layer below the resistive layer.

Key features of the experimental test section and measuring procedure are summarized here, and most details are available in a prior publication [7]. Studies of the initial stage of explosive evaporation of the water and alcohols are conducted using the thin film heater immersed in the cuvette with working liquid. Single rectangular pulses of a current are supplied to the resistive layer and effective heat flux reaches $2.2 \, \text{GW/m}^2$ at the temperature growth rate of 700 MK/s. Effective heat flux
is defined as the electric power divided on the microheater area. In order to register a nucleation the optical technique based on measuring the intensity of the laser beam reflected from the mirror surface of the heater, pulsed laser and digital video camera are used. The inverted and normalized optical signal from a photodiode corresponds to the specific surface area of the heater occupied by vapor bubbles. Heat flux to the liquid, liquid temperature and its growth rate were determined by numerical solution of the 3–D heat equation for multilayer microheater.

The experiments show that before initiation of an explosive evaporation the surface temperature of heater significantly exceeds the saturation temperature and the liquid is in metastable state. At initial stage of an explosive boiling, the bubbles are uniformly distributed on the surface and their number is small, see figure 3. The observed duration of an explosive evaporation is less than 350 ns, and as a result of the spontaneous nucleation in superheated layer the microbubbles form a vapor film on a heater surface. Pressure in the vapor film exceeds significantly the pressure in a surrounding fluid, which leads to ejection of the ink droplet in ink–jet printhead.

3. Modeling of the explosive evaporation in two-phase microfluidics

The reason for the bubbles incipience during explosive evaporation is the homogeneous nucleation in the superheated liquid layer. The model of homogeneous nucleation is well known [9]. This model defines the critical work of the nucleation as follows:

$$W_0 = 16\pi \sigma^3 / 3(p_s - p_l)^2(1 - \rho_v / \rho_l)$$

(1)

where \(\sigma\) is the surface tension, \(p_l\) is the liquid pressure, \(p_s\), \(\rho_v\), and \(\rho_l\) are the saturation pressure, vapor density and liquid density accordingly; as far as nucleation frequency:

$$J = N_1 B \exp(-G)$$

(2)

The nucleation frequency is governed by Gibbs number derived from the nucleation critical work \(G = \Psi W_0 / kT\). Here \(N_1\) is the molecules number by volume unit, \(B\) is the kinetics coefficient, \(k\) is the Boltzman constant and \(\Psi\) is the parameter which shows the reduction of critical work of a nucleation due to poor surface wettability. To determine kinetics coefficient \(B\) the Kogan’s approach [10] was used. Then total number of the bubbles generated near the heated surface during the time \(\tau\) equals to:

$$N_b(\tau) = \int_0^\tau \left\{ J[T(t,x,y,z), p_l] dV \right\} dt$$

(3)

For high heat fluxes the overheated layer thickness in a liquid is much less than the longitudinal microheater size. Therefore one can assume that the temperature varies mostly along the coordinate \(z\).
with normal orientation to the heater surface and the number of bubbles can be presented as follows:

\[ N_b(\tau) = S_h \int_0^{\infty} \int_0^{\infty} J[T(z,t), p], dz \left( 1 - \bar{S}_h(\tau) \right) dt, \]  

(4)

where \( S_h \) is the heater area and \( \bar{S}_h(\tau) \) is specific surface area of the heater occupied by vapor bubbles.

Measured dependence of the number of bubbles \( N_b \) on heater surface on the surface temperature is shown in figure 4 for the bubbles size larger than one micron. Points in figure 4 are the number of bubbles as function of surface temperature. Figure 4 shows also the calculated number of the bubbles at different liquid pressures for \( \Psi = 1 \) as the lines denoted as 1 - 4. The calculations were done using equation (4) for liquid temperature profile showed in figure 2 while neglecting the influence of the specific surface area of the heater occupied by vapor bubbles. The line 5 in figure 4 shows the calculation of the number of bubbles for \( \Psi = 0.25 \). One can see that the bubbles arise at lower liquid superheat than it predicted by the theory of homogeneous nucleation with \( \Psi = 1 \). It is connected with the reduction of the critical work of a nucleation due to poor surface wettability for water. In case of ethanol, the measured temperature of nucleation is in a good agreement with the prediction according to homogeneous nucleation theory for \( \Psi = 1 \).

The important feature of a nucleation at the microheater is pressure growth near its surface during the bubbles incipience and growth. It follows from figure 4 where the bubbles number grows with the temperature not as quick as homogenous nucleation theory predicts at initial pressure 1 bar (line 1). For instance, at the temperature of 320 °C the observed bubbles number corresponds to the calculated value in the pressure range from 20 up to 50 bar. The reason of this trend is nucleation suppression due to bubbles growth and pressure increasing. To account this phenomenon when calculating explosive boiling the two-zone model of self-consistent nucleation and vapor bubbles growth in the pressure field induced by growing bubbles was proposed in [7]. In this model arising bubbles increase the pressure near the heater and the bubble nucleation takes place under magnified pressure \( p_l \) which is defined by the second deviation from total volume of vapor generated during the time \( \tau \) as well as by inertia of the attached liquid mass as follows:

\[ p_l = p_{le} + 8 \rho l / S_h \pi^{3/2} \left( d^2 V_b / d\tau^2 \right), \]  

(5)

were \( l \) is the heater transverse size and \( p_{le} \) is the pressure far from the heater.

The total vapor volume generated at the microheater surface during the time \( \tau \) is determined by number of bubbles and their volumes. The volume of semi-spherical bubble at the time \( \tau \), if it was generated at the moment \( t \), equals to \( V_b(\tau - t) = 2\pi R_b^3(\tau - t)/3 \), where \( R_b(\tau - t) \) is the bubble radius. Considering that the bubbles are generated through homogeneous mechanisms, the vapor volume generated near heater surface and specific surface area of the heater occupied by vapor bubbles during time \( \tau \) are as follows:

\[ V_b(\tau) = S_h \int_0^{\infty} \int_0^{\infty} J[T(z,t), p], dz \left( 1 - \bar{S}_h(\tau) \right) dt, \]  

(6)

\[ \bar{S}_h(\tau) = S_h(\tau)/S_h = \int_0^{\infty} \int_0^{\infty} J[T(z,t), p], dz \pi R_b^3(\tau - t)(1 - \bar{S}_h(\tau)) dt. \]  

(7)

The nucleation occurs in short run that is much less that the liquid heating time. Thus, in the first approximation, the task of liquid temperature calculation for determination of the \( J \) function is independent on the nucleation problem solution. Hence, the temperature of the microheater surface and distribution of the liquid temperature can be determined from the solution of heat equation, see figure 2.

To solve the equations (1), (2), (5) – (6) we need in the model of bubble growth near the spinodal
The bubble growth rate in overheated liquid is yielded by Rayleigh's equation as follows:

\[
R_b \frac{d^2R_b}{d\tau^2} + 1.5\left(\frac{dR_b}{d\tau}\right)^2 = \frac{p_1(R_b) - p_1(\infty)}{\rho_l},
\]

where \( p_1(R_b) = p_v - 4\mu_l/R_b \cdot dR_b/d\tau - 2\sigma/R_b \) is the pressure at the bubble wall, \( p_1(\infty) \) is the pressure in near heater area and far from the bubble, \( p_v \) is the vapor pressure and \( \mu_l \) is the liquid viscosity. Right after nucleation, the vapor pressure equals to saturation pressure at surrounding liquid temperature and is compensated by the capillary pressure. During bubble growth the vapor pressure is reduced as a result of bubble wall cooling due to intensive evaporation. Therefore the bubble growth rate near a spinodal line is essentially smaller than that for the inertia controlled stage of bubble growth:

\[
\frac{dR_{bs}}{dt} = \sqrt{\frac{2(p_v - p_1(\infty))}{3\rho_l}}.
\]

Figure 5 shows the experimental data on dependence of the bubble radius on time during the nucleation in water at reduced heat pulse energy. For this case the number of bubbles is small and we can neglect the neighboring bubbles interaction. The analysis of this data shows that the rate of bubble growth can be approximated by modified equation (9) as follows:

\[
\frac{dR_b}{d\tau} = \frac{dR_{bs}}{dt} g(\tau - t),
\]

were the function \( g(\tau - t) \) can be fitted as exponential function \( g(\tau - t) = g_0 \cdot e^{-(\tau - t)/\tau_r} \). Here \( \tau_r \) is the characteristic time depending on physical properties of the liquid and vapor. For water one can use the reasonable approximation \( g_0 = 0.45, \tau_r = 3.9 \mu s^{-1} \) for calculation of the rate of bubble growth, see figure 5.

The proposed model of homogeneous nucleation and bubbles growth near spinodal line at the flat microheater consists of the equations (1), (2), (5)–(6) and heat equation for multilayer microheater immersed in the liquid. These equations were solved numerically to predict the regularities of an explosive evaporation in two-phase microfluidic devise. Figure 6 shows the dependences of the specific surface area of the heater occupied by vapor bubbles on time which were obtained for water in

\[
\begin{align*}
\text{Figure 5.} & \quad \text{The dependence of the bubble radius on time during the nucleation in water.} \\
\text{Figure 6.} & \quad \text{The dependences of the specific surface area of a heater occupied by vapor bubbles on time.}
\end{align*}
\]
the calculation (line) and in the experiment (points). One can see that account of the pressure growth near a heater surface and experimentally determined equation for the bubble growth rate near a spinodal line allow to predict reasonably the time of nucleation and the duration of an initial stage of water explosive evaporation in the MEMS devise with multilayer microheater.

4. Conclusions
Presented results show high efficiency of the two-phase microfluidic devise based on controlled liquid decay. The design of multi-layer microheater for two-phase microfluidics was proposed using numerical simulations. It allows receiving the abnormally high growth rate of the temperature for the liquid micro volume. The regularities of initial stage of the explosive evaporation of water on the heater with an external silicon carbide layer when exposed to high-intensity heat pulses were established. Based on experimental data the equation for the bubbles growth rate near a spinodal line was proposed. It allows us to complete the mathematical model of self-consistent nucleation and growth of the vapor bubbles in induced pressure field. The results of numerical calculations of the water explosive evaporation according to the proposed model show good agreement with the experimental data on the time of nucleation and duration of the initial stage of explosive evaporation in the MEMS devise with multilayer microheater. Presented results reveal the basic regularities of the explosive evaporation in two-phase microfluidics with pulsed heating. It allows us to create more efficient two-phase microfluidic devices based on the controlled liquid decay, including thermal ink jet prinheads.

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