Dynamics in Microfluidic Systems with Microheaters

S. aus der Wiesche, C. Rembe, C. Maier and E. P. Hofer

Department of Measurement, Control and Microtechnology MRM
University of Ulm, D-89069 Ulm, Germany
stefan.aus-der-wiesche@e-technik.uni-ulm.de

ABSTRACT

The physics of nucleation, boiling, bubble growth and collapse in thermal microactuators will be presented. The boiling process exhibits an equivalence to a phase transition of second order and this leads, in contrast to classical nucleation theory, to spatial extended nuclei. The dynamics of the resulting bubbles which grow from such extended nuclei is quite different from the dynamics of common vapor bubbles. However, a simple nucleation criterion can be given. The mathematical modeling and simulation of thermal microactuators is studied. The finite-volume-method is used to solve the coupled constitutive equations, i.e. the electrical potential equation for the heater, the nonlinear heat diffusion equation, and the three dimensional Navier-Stokes equation. Due to a hydrodynamic instability, the resulting bubble flow is found to be appreciable different from the corresponding perfect potential flow. The theoretical results agree well with experimental facts.

Keywords: microfluidic systems, microheaters, boiling nucleation, bubble dynamics

INTRODUCTION

Microheaters offer a large potential for industrial and scientific applications. The bubble ink jet is the most important commercial example. Furthermore, microheaters can act as pressure sources in micropumps, or microdrop valves, or can be the key actuators in micro reaction chambers. The use of thermal microheaters in the bubble inkjet technology is illustrated in Figure 1.

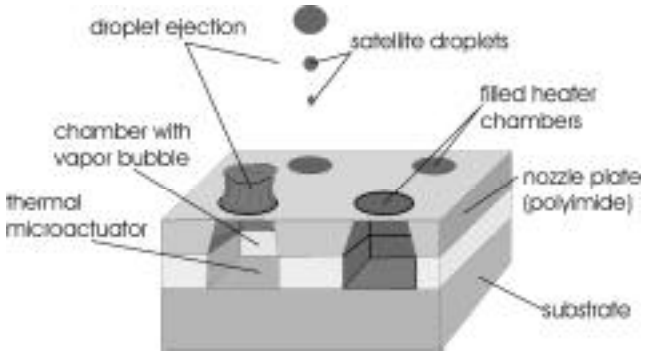

Figure 1: Microheaters used in bubble inkjets.

The principle of microheaters where the rapid heating of a liquid caused by an electrical pulse generates vapor bubbles as pressure source is quite simple, however, there are many unsolved questions about modeling and simulation of the nucleation dynamics, the bubble dynamics, and the hydrodynamics in such microfluidic systems. In the recent decade, many authors have studied the phenomenon of evaporation and vapor bubble dynamics in thermal microactuators [1-3]. Neverless, the physical background is not sufficiently understood, especially, the nature of nucleation at the thermodynamic limit of superheating, the so-called spinodal [4].

The aim of this paper is twofold. As preliminary part the relevant physics of boiling near the spinodal will be summarized and used to discuss the nucleation process as it is appropriate for thermal microactuators. In the main part the mathematical simulation of the bubble dynamics of microfluidic systems with thermal microactuators as pressure sources is discussed.

As important result of the underlying nucleation theory, boiling above thermal microheaters exhibits an equivalence to a phase transition of second order. This leads, in contrast to classical nucleation theory, to spatial extended nuclei and, therefore, the resulting bubble dynamics is quite different from common bubble dynamics.

NUCLEATION THEORY

Nucleation and boiling above thermal microheaters lies beyond common equilibrium thermodynamics due to the extreme superheating of the liquids (e.g. ink, or for simplicity, water). In fact, the liquids are superheated up to the thermodynamic limit, the spinodal. Consequently, a description of boiling near the spinodal requires a different treatment than common thermodynamics could even give. The rigorous theory can be found in detail in [5]. In this section the relevant results of such an approach are briefly summarized.

Thermodynamic basis

In order to discuss nucleation near the spinodal, it is convenient to consider typical isotherms of a fluid in the pressure-volume-diagram as shown in Figure 2. The spinodal is the boundary between the metastable and the unstable region. Ordinary boiling begins at point A and a superheated liquid would be represented by point B.

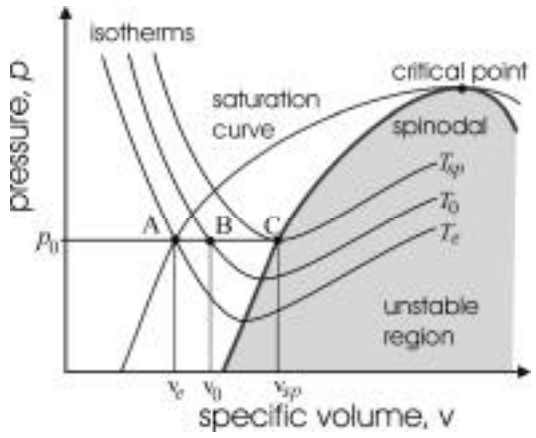

Figure 2: Isotherms of a fluid in the *p*-v-diagram.

At point C the spinodal is reached. All points on the spinodal can be interpreted as the continuation of the critical point because long wave fluctuations become important at this curve [5,6]. Whereas classical nucleation theory considers only critical nuclei which are small in extend but large in degree, as exemplified by small vapor bubbles in a liquid [4,7], near the spinodal the critical nuclei were built up by long wave perturbations. Therefore, the expression for the free energy *F* of the metastable liquid at fixed temperature must be generalized by

$$F(\mathrm{v}) = \frac{1}{\mathrm{v}_0} \int_V \left(f(\mathrm{v}) + \kappa (\nabla \mathrm{v})^2 \right) dV \qquad (1)$$

because smooth variations of the specific volume v, which is a function of the position **x** must be considered. In (1), v_0 is the average specific volume, *f* the free energy per molecule, and κ is a phenomenological coefficient which describes physically the additional gradient energy contribution due to the nonuniformness of the system. The condition $dF = 0$ for the free energy in case of a stable or an unstable equilibrium remains valid, and, therefore, one gets with expression (1) from a variational principle the specific volume distribution which corresponds to the unstable, critical nucleus. Introducing the dimensionless specific volume *Y* and the normalized length *X*

$$Y \quad \frac{\mathrm{v} - \mathrm{v}_0}{\mathrm{v}_{sp} - \mathrm{v}_0}, \quad X \quad x\sqrt{\frac{\mathrm{v}_{sp} - \mathrm{v}_0}{\kappa}\xi}, \qquad (2)$$

respectively, where the coefficient ξ is proportional to the third derivative of *f* (v), the critical work *R* to built up a critical nucleus in an isotropic liquid can be expressed as

$$R = \frac{2\pi}{\mathrm{v}_0}\sqrt{\frac{\kappa}{\xi}}\left(\mathrm{v}_{sp} - \mathrm{v}_0\right)^{3/2} \int_0^{\infty} X^2 Y^3 dX \,. \qquad (3)$$

From (3) it is obvious that the critical work *R* decreases with increasing superheating and vanishes at the spinodal. From (2) it follows also that the spatial extent of the critical nucleus increases with increasing superheating but the degree of perturbation decreases. In fact, the correlation length of the system increases up to optical wave lengths and the phase transition near the spinodal exhibits an equivalence to a phase transition of second order. In other words, a critical phenomenon is present [5].

Nucleation criterion

From the above thermodynamic basis, it follows that the nucleation above thermal microheaters cannot be understood by considering the classical nucleation theory. The nucleation will occur as critical phenomenon and this implies an interesting universal behavior expressed through simple scaling laws for the critical exponents of the thermodynamic variables [6]. Calculation of the nucleation rate of formation of critical nuclei leads to the conclusion that for practical interest reaching of the spinodalian temperature must be the criterion for homogeneous nucleation at normal pressure.

Bubble growth in early stages

Another important consequence concerns the early stage of bubble growing. Since the critical nuclei near the spinodal are spatially extended the initial bubble nuclei must be considered as spatial extended, too. In Figure 3 the vapor bubble growth above a typical microheater is shown.

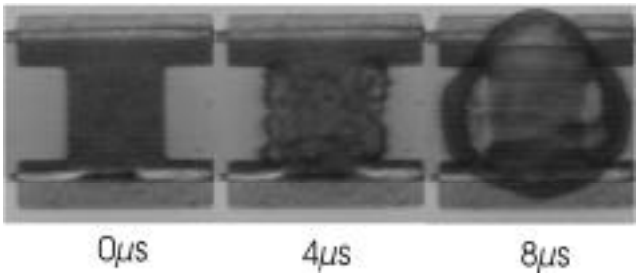

Figure 3: Vapor bubble growth above a microheater.

The visualization has been performed with the stroboscopic technique described in detail in [8]. In contrast to classical boiling the vapor bubbles grow from extended nuclei. The rapid phase change process looks like common film boiling but, in fact, the underlying mechanisms are quite different as mentioned in the previous subsections.

SIMULATION OF BUBBLE DYNAMICS

In this section, the simulation of the bubble dynamics above microheaters will be discussed. The special aim of the simulations is the understanding of the early stages of bubble growth including the prediction of the time point of nucleation.

Governing equations

The physics of the microheater can be subdivided into three parts, namely, the problem of calculation of the electric field distribution in the resistor, the solution of the thermal problem of heat conduction, and, finally, the resulting bubble growth which is in fact a two-phase flow.

In the static case the equation for the electric potential ϕ reads as

$$\mathrm{div}(\sigma\ \mathrm{grad}(\phi)) = 0 \qquad (4)$$

with the electric conductivity σ which is a function of position and temperature T. The heating power rate P due to dissipation in a resistor is given by

$$P = \mathbf{j} \cdot \mathbf{E} = \sigma (\ \phi)^2 . \qquad (5)$$

where **j** and **E** represent the current density and the electric field vectors, respectively. This must be inserted into the heat conduction equation

$$c\rho \frac{fT}{ft} = \mathrm{div}(\lambda\ \mathrm{grad}(T)) + S \qquad (6)$$

where the thermal conductivity λ, the density ρ, and the specific heat c are functions of position and temperature.

The resulting bubble flow obeys the governing equations of fluid dynamics for two-phase flows. Because of their complexity, in general, in the following simulation of the liquid phase will be treated as incompressible and the resulting bubble flow will be discussed in the framework of gas bubble dynamics, i.e., the mass flux due to the evaporation will be neglected.

Physical algorithm

The simulation of the above governing equations of the microheater can be simplified if the physical process is taken into regard. At first, the coupling between the electric equations (4), (5) and the temperature equation (6) is found to be very weak. Therefore, the elliptic electric potential problem (4) can be solved separately. After this, the heating source S for the heat conduction equation (6) is known. Due to the short time scale (μs) the convection in the liquid layer can be neglected which leads to a pure parabolic heat conduction problem (6). It follows from the nucleation criterion from the above section that the time point of reaching the spinodalian temperature of the liquid gives the time point of nucleation. After this, the heating process is neglected and the bubble dynamics can be discussed as pure two-phase flow problem. In fact, in general even this would be too complex. Therefore a simple geometry is assumed, i.e. bubble dynamics in a semi-infinite incompressible liquid bounded by a rigid wall will be discussed. In addition, the simulation of the non-spherical flow is concentrated only to the resulting flow pattern and the simple gas bubble model is used.

Mathematical algorithm

All the governing equations can be expressed in the form of balance equations

$$\frac{f}{ft}(r_i \rho_i \varphi_i) + \mathrm{div}(r_i \rho_i \varphi_i \mathbf{v}_i - r_i \Gamma\ \mathrm{grad}(\alpha\varphi_i)) = S \qquad (7)$$

where r_i stands for volume fraction of phase i, ρ_i stands for any conserved property of phase i, such as enthalpy or momentum, $\mathbf{v}_i$ stands for the velocity of phase i, Γ stands for the appropriate exchange coefficient, and S stands for the appropriate source terms [9,10]. Because of this the same integration technique for the governing equations can be chosen. This was be carried out using the commercial program PHOENICS which provides solutions of differential equations having the form (7).

Integration of (7) over a topological cartesian control volume discretized in space leads to a set of algebraic equations. Due to the cartesian symmetry of the micro heater geometry in case of solving the electric and the heat conduction problem, a stretched but pure cartesian grid was chosen. Whereas in case of simulating the bubble flow, a staggered-grid was generated using oblate spheroidal coordinates [11]. For all calculations an appropriate unit system were chosen. The temperature dependence of the variables was taken into consideration with polynomials in T. The two-phase flow was treated explicitly by the Interphase Slip Algorithm (IPSA).

RESULTS

Time point of nucleation

Using the nucleation criterion given in this paper and calculating the temperature distribution in a liquid layer above the micro heater leads to the time point of nucleation.

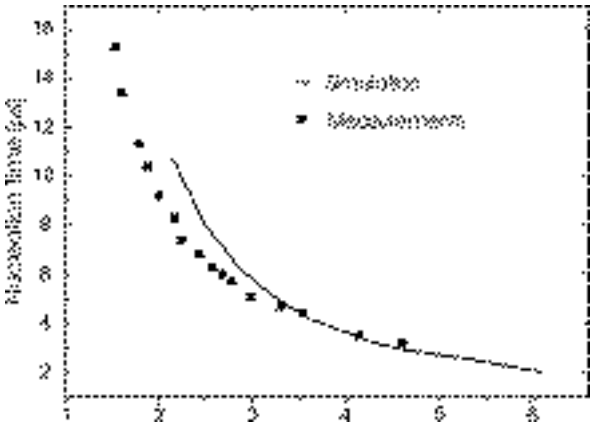

Figure 4: Nucleation time and heating power [12].

The chosen liquid was water with a spinodalian temperature of about 312°C. The variation of the time point of nucleation in dependence of the heating power of the micro heater is shown in Figure 4. The simulation results are compared with experimental observations using high speed cinematography and show very good agreement.

Non-spherical bubble dynamics

Assuming the gas bubble model, i.e. neglecting the mass flux due to the evaporation of the superheated liquid into the growing vapor bubble, simplifies the two-phase flow problem enormously. Since the bubble nuclei are spatially extended and film boiling is not present, the resulting flow pattern may be approximated by the flow caused by an expanding flat gas bubble. The spherical flow would be appropriate in case of small nuclei at time $t = 0$ whereas an oblate spheroidal flow may be an idealization for the bubble flow caused by spatially extended nucleus.

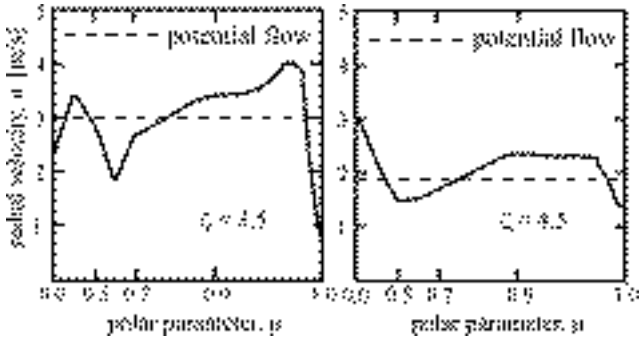

Figure 5: Velocity profiles of the bubble flow.

In spherical coordinates the cavity shapes are isobaric surfaces. This fails for the other, non-spherical potential flows. Due to this hydrodynamic instability the resulting bubble flow is found to be appreciable different from the idealized potential flows.

Introducing the dimensionsless oblate spheroidal coordinates [11]

$$\begin{matrix} x \\ y \\ z \end{matrix} = c\sqrt{1-\mu^2}\sqrt{1+\zeta^2}\begin{matrix} \cos\omega \\ \sin\omega \\ \end{matrix} \qquad (8)$$
$$z = c\mu\zeta$$

the idealized potential flow can be compared with the numerical results, as shown in Figure 5. The roughing of the bubble surface leads to an important consequence for the evaporation of the superheated liquid surrounding the vapor bubble. Due to the enlargement of the surface the mass flow will increase and this will start another – hydrothermal - instability mechanism, as explained further in [13]. Note also that in the early stages of bubble expansion strong pressure differences occur at the heater surface. This leads to mechanical stress comparable with cavitation effects not only in the collapsing but even in the growing stage of bubble dynamics.

CONCLUSION

The physical modeling of the phase transition near the spinodal is given. As a result the spatial extent of a critical nucleus in an extremely superheated liquid increases with increasing superheating. A simple nucleation criterion could be derived also. Based on this, the simulated time points of nucleation agree well with experimental facts. The resulting bubble flow was obtained numerically. For comparison reasons the solution of the idealized potential flow was calculated also, having large differences to the numerical solution which had to be expected, because a hydrodynamic instability excluded the potential flow pattern. This is an indication of the necessity of the numerical algorithm presented in this paper.

REFERENCES

[1] R. R. Allen, J. D. Meyer, W. R. Knight, “Thermodynamics and Hydrodynamics of Thermal Ink Jets”, Hewlett Packard Journal, Vol. 36, 21-27, 1985

[2] A. Asai, “Three-Dimensional Calculation of Bubble Growth and drop Ejection in a Bubble Jet Printer”, J. Fluids Eng., Vol. 114, 638-641, 1992.

[3] W. Runge, “Nucleation in Thermal Ink-Jet Printers”, Proc. IS&T 8th Int. Congr. Adv. In Non-Impact Printing Techn., 1992

[4] S. J. D. van Stralen, R. Cole, “Boiling Phenomena. Volume 1 and 2”, Hemisphere, Washington, 1972

[5] S. aus der Wiesche, C. Rembe, E. P. Hofer, ”Boiling of superheated liquids near the spinodal”, Heat and Mass Transfer (in press), 1999

[6] L. D. Landau, E. M. Lifshitz, “Statistical Physics”, Pergamon Press, 1982

[7] J. I. Frenkel, “Kinetic Theory of Liquids”, Dover Publications, New York, 1955

[8] Rembe, C., aus der Wiesche, S., Beuten, M., Hofer, E.P, “Investigations of nonreproducible phenomena in thermal ink jets with real high speed cine photomicrography”, Proceedings of SPIE EUROPTO Series, Vol. 3409, Electronic Imaging: Processing, Printing, and Publishing in Color, Zurich, 1998,

[9] S. R. de Groot, P. Mazur, “Non-equilibrium thermodynamics”, Dover Publications, New York, 1984

[10] see, for instance, “The PHOENICS beginner’s guide, CHAM, London, 1991

[11] H. Lamb, “Hydrodynamics”, Cambridge University Press, 1997

[12] E. P. Hofer, C. Maier, C. Rembe, S. aus der Wiesche, E. Kohn, M. Adamschik, P. Gluche, “A New Diamond Micro Heater for Inkjet Printheads”, Proc. IS&Ts NIP 14, 72-75, Toronto, 1998

[13] H. S. Lee, H. Merte, “The Origin of the Dynamic Growth of Vapor Bubbles related to Vapor Explosions”, Journal of Heat Transfer, Vol. 120, 174-182, 1998