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Simulation model and droplet ejection performance of a thermal-bubble microejector

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ABSTRACT

The present study investigates simulation model and droplet ejection performance of a thermal-bubble microejector. This model is achieved by coupling an electric-thermal model and flow model with bubble dynamics equations. We simulate the bubble nucleation and the bubble growth, to predict the droplet ejection process. The model is validated by comparing prediction results with experimental data. Especially, in forming one droplet, the results show that the ejection volume increases linearly with the thermal energy, and the variation range of the pulse width is within ~0.2 μs. Moreover, the effects of the geometry of the nozzle, reservoir and thin-film resistance, applied current and pulse width on satellite droplets creation, droplet speed and volume are presented.

1. Introduction

Depositing nanovolume of chemical or biochemical species with high precision and high reliability is today the major interest in various fields of applications. The functionalization of DNA chips is certainly the most challenging one. During the last 10 years, many studies have been devoted to the development of miniaturize systems enabling the ejection of small droplet but most of them suffer from a lack of flexibility due to the difficulty to integrate high density arrays of individually addressable ejectors.

Thermal ejection is a good candidate to achieve simultaneously high density integration and individual actuation. This paper proposes a thermal ejection micro-array [1] enabling in situ oligonucleotide synthesis on DNA chips. It consists in a micro-array of individually addressable ejectors which eject nucleotides on a glass slide. The microejector is fabricated using monolithical silicon technologies. The microejector consists of three main elements, which are the supporting membrane, the resistance heater with the diode matrices for addressing and the SU8 nozzle.

The working principle of the microejector is based on a thermal-bubble inkjet printing. A very short electric pulse is applied to a resistive heater to generate a high heat flux. If the surface temperature of the liquid is higher than the nucleation temperature, a vapor bubble is formed at the surface of the passivation layer. Sudden formation of the vapor bubble generates a pressure impulse, the rapid growth of the bubble expels a small liquid drop from the nozzle exit. After the applied current is removed, the temperature and pressure of the vapor decrease quickly, once the bubble collapses, the nozzle refills due to capillary forces for the next ejecting.

The operating cycle of a thermal-bubble microejector is shown in Fig. 1. The operating cycle is divided into three phase: (1) the liquid is heated until bubble nucleation; (2) the bubble growth and collapse with droplet ejection; (3) refill of the reservoir.

Three main problems should be resolved in designing thermal-bubble jet: bubble nucleation condition (temperature), the nucleation mechanism and ejection performance including the elimination of satellite droplets.

The nucleation mechanism [1,2] and the nucleation temperature [3,10] have been studied by a number of researchers. They have suggested that the homogeneous nucleation is the primary mechanism for bubble nucleation in a thermal-bubble jet. The nucleation temperature increases as the heat rate increases.

Asai et al. [4] presented a one-dimensional numerical model of bubble growth and collapse in a side-shooter printhead. The bubble pressure was predicted by the Clausius–Clapeyron equation with the ideal gas law. He also developed a three-dimensional numerical model [5] to predict the droplet motion using the volume-of-fluid (VOF) method, where the interface was tracked by the liquid volume fraction. The simulation results showed a good agreement with the experimental observations. Moreover, he developed a model of nucleation probability [6] based on the

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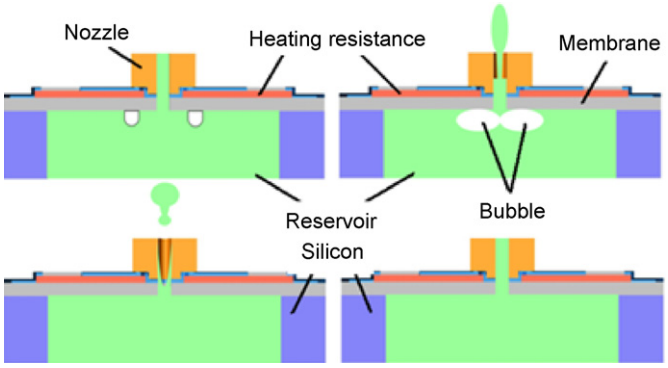

Fig. 1. Schematic representation of the operating cycle, phase 1: bubble nucleation, phase 2: bubble growth and collapse with droplet ejection, phase 3: refill of the reservoir.

classical nucleation theory and used it to simulate the initial bubble growth process. The initial bubble nucleation time is within 0.01 μs.

Sen and Darabi [7] used a two-dimensional fluid flow model coupled to the heat transfer model to predict the droplet ejection process. The free surface between the ink and the air was tracked using volume of fluid method by the level-set (LS) formulation. The bubble growth was simulated by the Clausius–Clapeyron equation with the ideal gas law.

Recently, Suh and Son [8] predicted the ejection process in a top shooter printhead through tracking the liquid–vapor and liquid–air interfaces method by LS formulation. The formulation was modified to include the effect of phase change at the liquid–vapor interface and was extended to treat the contact angle condition at an immersed solid surface.

Deng et al. [9] have studied the bubble nucleation temperature and the bubble dynamics in DNA solutions. The experimental results showed that the bubble nucleation temperature increased with the DNA concentration, and also increased with the heat flux. Based on classical thermodynamics model for nucleus formation, the simulation results revealed that the bubble nucleation temperature increased with an increase in DNA concentrations, which was consistent with experimental observations.

Although, there are a number of experimental and numerical investigations on the bubble nucleation and bubble growth in thermal-bubble jet, there is very limited information on the typical working conditions of a thermal jet. In this paper, we present a two-dimensional axisymmetric thermal-bubble model simulates bubble nucleation and bubble growth to predict the ejection process and reveal the typical working conditions of the microejector. The method is based on the phase field formulation. Furthermore, the droplet ejection performance of the microejector also is presented. These numerical simulations are performed using COMSOL Multiphysics.

2. Theory and method

The physical behavior of a heating flow is driven by the interface dynamics. The simulation model is achieved by coupling an electric-thermal model and flow model with bubble dynamics equations. The electric-thermal model deals with the heat transfer process in the liquid and solid. The fluid dynamic behavior of drop ejection in an incompressible, Newtonian fluid is governed by the Navier–Stokes equations. Bubble dynamics theory is used to simulate the nucleation and growth of the vapor bubbles. The bubble interface dynamics of a two-phase flow are governed by the Cahn–Hilliard equation.

2.1. Electric-thermal model

A heat transfer model is used for calculating the temperature distribution in liquid and solid before the bubble is generated. The governing equation of transient heat transfer with inner heat source is

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q_{dc} \tag{1}$$

where T is temperature, ρ density, C_p heat capacity, k thermal conductivity, Q_{dc} the heat input to the heater per unit volume per unit time.

2.2. Flow model

The liquid velocity field in the reservoir and the droplet velocity field are described by the incompressible Navier–Stokes equations:

$$\rho \frac{\partial u}{\partial t} + \rho u \nabla \cdot (u) = \nabla \cdot [-pI + \eta_L(\nabla u + (\nabla u)^T)] + \rho g \tag{2}$$

$$\nabla \cdot u = 0$$

where ρ is the fluid density, u the fluid velocity, p pressure, μ the viscosity, g gravity.

2.3. Bubble dynamics

It is observed that nucleation bubble instantaneously covers the surface of the heater in ~0.01 μs, the vapor bubble pressure is estimated very high, which can reach ~12 MPa. Once the vapor is nucleated, the vapor pressure is calculated by the Clausius–Clapeyron equation:

$$P_{sat} = P_{amb} \exp\left[\frac{wQ_{vap}}{R}\left(\frac{1}{T_b} - \frac{1}{T}\right)\right] \tag{3}$$

where P_{sat} is the saturated bubble pressure, R the gas constant, w the molecular weight, Q_{vap} the heat of vaporization, T_b the boiling temperature of the liquid at ambient pressure. The properties of water at its boiling point are used: $T_b = 100\,^{\circ}\mathrm{C}$, $w = 18 \times 10^{-3}\ \mathrm{kg\,mol^{-1}}$ and $Q_{vap} = 2.26 \times 10^6\ \mathrm{J\,kg^{-1}}$. The ideal gas law is expressed as

$$P_{sat} V = nRT$$

where V is the bubble volume, n the number of moles of gas. The mass flux leaving the liquid surface leads to an increase in pressure of the vapor. The pressure exerts a force on the liquid surface and the vapor region begins to expand. The mass flux can be evaluated from the conductive heat flux, which can be approximated by the following expression:

$$\dot{m} = -\left(\frac{M_w}{\Delta H_{vl}}\right) n \cdot K_v \nabla T_v \approx C_{\rho_L} \frac{(T - T_{sat})}{T_{sat}} \tag{4}$$

where M_w is the molecular weight of the vapor, ΔH_{vl} is the enthalpy of vaporization and C is a constant ($\mathrm{m\,s^{-1}}$). The mass flux is generated by the bubble growth. So, the mass flux appears in the energy Eq. (1) as

$$\rho C \frac{\partial T}{\partial t} + \rho C_p (u \cdot \nabla) T = -\nabla \cdot (-k \nabla T) - \left(\frac{\dot{m} \delta \Delta H_{vl}}{M_w}\right) \tag{5}$$

2.4. Phase field method

The bubble interface is tracked using the volume of fluid (VOF) technique. The equations governing the interface dynamics of a two-phase flow can be described by the Cahn–Hilliard equation.