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Acoustofluidics 3: Continuum mechanics for ultrasonic particle manipulation

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Although ultrasonic particle manipulation is performed in fluids, the adjacent solid material and its modelling play an important part in the design of such devices, as the impedance difference between liquids and solids is not very large. The modelling of the solid is done in the framework of linear elastodynamics, which is described by the displacement field, the strain field and the stress field. These quantities are related by kinematical relations, local linear momentum conservation and constitutive laws. Also material damping is important and can be modelled in the framework of linear viscoelasticity. Because of the finite size of the devices, resonant modes are important to analyse. In addition some of the elements behave as mechanical structures obeying specific equations that take into account the structural boundaries. A practical example is given, which shows the full complexity of device modelling, which is preferably done using the Finite Element Method.

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A Introduction

Ultrasonic manipulation is performed in a fluid volume. This volume is either partially (manipulation in droplets[1] or flow-through channels,[2–6]) or fully bounded by solid bodies.[7] Because the impedance of these solid boundaries is finite, a pressure field in the fluid will necessarily give rise to motion and deformations of the solid surrounding it. Therefore the modelling of these surroundings is important in order to understand the system as a whole. In particular resonances and damping of the various modes encountered and used in the fluid are influenced by the neighbouring materials including the container, the transducers used to excite the acoustic modes and possible glue layers that attach the transducer to the container. The harmonic motion of the structural elements at resonance, given the scale of typical devices, will have MHz frequencies as has the pressure variation in the fluid. The resulting strains normally are small, such that the solid motion can be treated in the framework of linear elasticity. The present article will start with the basic theory in three dimensions. Then the motion of structures is introduced in particular plates which are the most relevant elements used in particle manipulation systems. Then the solid is coupled to the fluid. Practical systems need to be solved using the Finite Element Method (FEM) which is able to take care of complicated shapes. The article ends with an example of an ultrasonic cavity as used for ultrasonic manipulation.

B Linear elastodynamics

In contrast to the description of the behavior of a fluid, a solid has a defined reference configuration. Referring to Fig. 1: a solid body is moving from its reference configuration λ_0 to the current configuration λ. The position of a material point P with respect to a coordinate system with base vectors $\boldsymbol{e}_i$ ($i = 1,2,3$) is $\boldsymbol{X}$ in the reference configuration and $\boldsymbol{x}$ in the current configuration. The displacement vector $\boldsymbol{u}(x_i,t)$ which is dependent on the position $\boldsymbol{x}$ and time t is defined as

$$\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{X} = u_i\boldsymbol{e}_i. \quad (1)$$

The summation convention is used for repeated indices. For the limiting case of small deformations and rotations, the basic equations of linear elasticity describe the relevant quantities: the strain

Foreword

In this third paper of 23 in the tutorial series of Acoustofluidics in Lab on a chip, Jürg Dual and Thomas Schwarz presents linear elastic continuum mechanics to model microdevices designed for acoustic cell and particle manipulation. Since acoustofluidic resonators both encompass fluid and solid material, and the difference in impedance is not very large, the influence of the solid material is very important for the behaviour of the resonator. The modelling of the solid is done using linear elastodynamics which is further described as well as a tool for modelling the material dampening of the solid using linear viscoelasticity. This paper presents an important theoretical toolbox for understanding and modelling the solid part of an acoustic particle manipulator.

tensor γ_{ij} which describes the local deformation and the stress tensor σ_{ij} which describes the local state of stress. Both γ_{ij} and σ_{ij} are symmetric second rank tensors. The linear constitutive law connects the two and is therefore in general a tensor of rank 4. A detailed explanation can *e.g.* be found in ref. 8.

For a given displacement field $u_i(x_j,t)$ the strain tensor γ_{ij} is computed using the kinematical relations

$$\gamma_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right), \tag{2}$$

where ",$_j$" means taking the derivative with respect to x_j. For small deformations and rotations $u_{i,j} \ll 1$ is assumed.

$$\gamma_{11} = u_{1,1} \tag{3}$$

is the longitudinal strain in the x_1 direction. This corresponds to the normalized length change of a material line element that extends in the direction of $\boldsymbol{e}_1$.

$$\gamma_{12} = \frac{1}{2}\left(u_{1,2} + u_{2,1}\right) \tag{4}$$

is the shear strain in the 1–2 plane, corresponding to half of the change in angle between two material line elements extending in the directions of $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$, respectively.

Using the summation convention the volume strain is given by

$$\gamma_{ii} = \gamma_{11} + \gamma_{22} + \gamma_{33}. \tag{5}$$

With the components of the stress tensor σ_{ij} we can formulate the local linear momentum equation, where a superposed dot corresponds to the time derivative:

In the direction x_1:

$$\sigma_{11,1} + \sigma_{12,2} + \sigma_{13,3} = \rho\ddot{u}_1, \tag{6}$$

or in indicial notation for the direction x_i:

$$\sigma_{ij,j} = \rho\ddot{u}_i. \tag{7}$$

Here ρ is the density. Body forces are neglected, because of the linearity of the theory and because the focus here is on the high frequency ultrasonic motion.

An isotropic linearly elastic material is fully described by two material constants E, G or λ and μ, where E and G are Young's and shear modulus, respectively, and λ and μ are the Lamé constants, respectively.

$$\sigma_{ij} = \lambda\gamma_{kk}\delta_{ij} + 2\mu\gamma_{ij}. \tag{8}$$

δ_{ij} is the unity tensor (Kronecker symbol).

$$\delta_{ij} = \left\{\begin{array}{l} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{array}\right\} \tag{9}$$

λ and μ are related to E and G by

Jurg Dual

Jürg Dual has been Full Professor of Mechanics and Experimental Dynamics in the Center of Mechanics of the Institute of Mechanical Systems at the ETH in Zurich since October 1, 1998. Since 2008 he also has been President of the University Assembly of ETH in Zurich. Jürg Dual was born on May 14, 1957 and studied mechanical engineering at the ETH Zurich. He then spent two years on a Fulbright grant at the University of California in Berkeley, where he graduated with a M.S. and a M.Eng. degree in mechanical engineering. He then received his Dr.sc.techn. degree at the ETH Zurich under the guidance of Prof. Dr. M. Sayir at the Institute of Mechanics. For his dissertation he was awarded the Latsis Prize of the ETH Zurich in 1989. After one year as visiting assistant professor at Cornell University, Ithaca, NY, he returned to the ETH Zurich as assistant professor. He is a Fellow of the ASME, member of the SATW (Swiss Academy of Technical Sciences) and Honorary Member of the German Association for Materials Research and Testing. His research focuses on wave propagation and vibrations in solids as well as micro- and nanosystem technology. In particular he is interested in both basic research and applications in the area of sensors (viscometry), nondestructive testing and ultrasonic manipulation of cells and particles. In his research, experimentation is central, but must always be embedded in corresponding analytical and numerical modeling. As mechanics is a very basic science, it is particularly attractive for him to interact with neighbouring disciplines like bioengineering, materials science or micro- and nanosystem technology.

Thomas Schwarz

Thomas Schwarz received the M.Sc. degree in electrical engineering from the Dresden University of Technology in 2007. He is currently pursuing the Ph.D. degree at the Institute of Mechanical Systems, ETH, Zurich. During his studies he focused on precision and microengineering. Currently, his main research area is ultrasonic manipulation within microfluidic systems.

$$\mu = G = \frac{E}{2(1+\nu)},$$
$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} = 2G\frac{\nu}{1-2\nu}. \tag{10}$$

ν is Poisson's ratio.

Using E and ν the inverse of eqn (8) can be easily obtained, *e.g.* for γ_{11}

$$\gamma_{11} = \frac{1}{E}(\sigma_{11} - \nu(\sigma_{22} + \sigma_{33})). \tag{11}$$

Combining eqn (2), (7) and (8) we obtain

$$\sigma_{ij,j} = (\lambda + \mu)u_{k,ki} + \mu u_{i,kk} = \rho \ddot{u}_i. \tag{12}$$

These are three coupled differential equations that need to be solved together with initial conditions for displacement and velocity

$$u_i(x_j,0) = g_i(x_j),\ \dot{u}_i(x_j,0) = h_i(x_j). \tag{13}$$

For the boundary conditions, the displacement $\boldsymbol{u}$ and the stress vector $\boldsymbol{t} = \boldsymbol{\sigma}\cdot\boldsymbol{n}$ are relevant, where $\boldsymbol{n}$ is the outward unit normal vector of the boundary surface of the solid. Either the stress vector or the displacement can be prescribed on the boundary in normal and tangential directions. For interface conditions, the associated field variables are not prescribed, but are determined from solving the coupled equations. Conditions for both displacement and stress vector then need to be imposed. As an example, for the interface of an inviscid, quiescent fluid with the solid structure we have

$$\boldsymbol{u}_{\mathrm{nS}} = \boldsymbol{u}_{\mathrm{nF}},\ \boldsymbol{t}_{\mathrm{nS}} = -p\boldsymbol{n},\ \boldsymbol{t}_{\mathrm{tS}} = 0, \tag{14}$$

where the indices n and t relate to the normal and tangential directions, respectively, F and S relate to the fluid and solid, respectively, and p is the pressure in the fluid. The first of eqn (14) is sometimes formulated as a velocity or acceleration boundary condition. Note that because of zero viscosity, no boundary condition applies for the tangential motion of solid and fluid.

There exists a unique solution to these equations, if all the equations (eqn (12)–(14)) are set up properly.[9]

Eqn (12)–(14) cannot be solved in a straightforward manner. They can, however, be simplified using the Helmholtz decomposition[10]

$$u_i = \varphi_{,i} + \varepsilon_{ijk}\psi_{k,j} \tag{15}$$

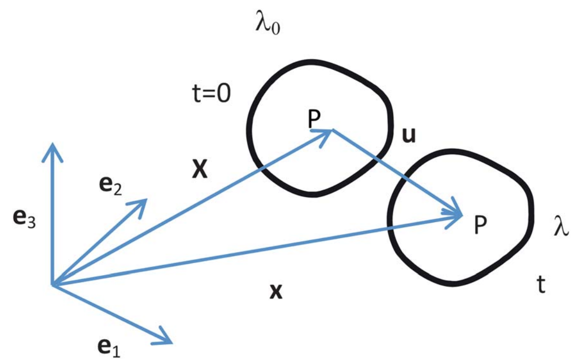

Fig. 1 A solid body moving from its reference configuration λ_0 to the current configuration λ.

where a scalar displacement potential φ and a vector potential $\boldsymbol{\psi}$ with zero divergence have been introduced as well as the permutation tensor ε_{ijk}. ε_{ijk} is +1 when i,j, k are even permutations of 1,2,3, and −1 for odd permutations and 0 otherwise. When eqn (15) is inserted into eqn (12) it is seen that two types of waves exist, which satisfy the classical wave equations

$$\varphi_{,ii} = \frac{1}{c_1^2}\ddot{\varphi},\ \psi_{k,ii} = \frac{1}{c_2^2}\ddot{\psi}_k, \tag{16}$$

with wave speeds

$$c_1^2 = \frac{\lambda + 2\mu}{\rho},\quad c_2^2 = \frac{\mu}{\rho}, \tag{17}$$

where c_1 and c_2 correspond to the wave speeds of the primary and secondary waves, respectively. The terms come from geophysics and result from the fact that $c_1 > c_2$ and hence the primary wave arrives first. They are often abbreviated as P- and S-waves, respectively. For plane waves in isotropic materials, P-waves are longitudinal, while S-waves are transverse.

Typical values are $c_1 = 6300$ m s^{-1} and $c_2 = 3140$ m s^{-1} for aluminium and $c_1 = 2650$ m s^{-1} and $c_2 = 1080$ m s^{-1} for PMMA, respectively.

For single crystal silicon (SCSi), the situation is more complicated as it is anisotropic. Therefore the wave speeds are dependent on the direction of propagation and the constitutive law must be replaced by[11]

$$\sigma_{ij} = c_{ijkl}\gamma_{kl},\ \gamma_{ij} = s_{ijkl}\sigma_{kl}. \tag{18}$$

The 4th order tensors c_{ijkl} and s_{ijkl} are the stiffness and the compliance tensor of the material, respectively. They are symmetric with respect to the indices i and j, as well as k and l, due to the symmetry of $\boldsymbol{\sigma}$ and $\boldsymbol{\gamma}$. They are also symmetrical with respect to index pairs ij and kl, because for elastic materials a strain energy exists, which is given by

$$U = \frac{1}{2}\sigma_{ij}\gamma_{ij} = \frac{1}{2}c_{ijkl}\gamma_{ij}\gamma_{kl}. \tag{19}$$

In general therefore an anisotropic elastic material is characterized by 21 independent material constants.

For a specific material the stiffness and compliance tensors reflect the symmetries of the material. SCSi is a crystalline cubic material where all 3 coordinate axes taken parallel to the crystal axes are equivalent. For easier readability sometimes a different representation is introduced (Voigt notation), which reflects the symmetries of the quantities. As seen in the first part of eqn (20) double indices running from 1 to 3 each are replaced by one single index running from 1 to 6.

$$\begin{pmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{pmatrix} = \begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{pmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & c_{44}\end{bmatrix}\begin{pmatrix}\gamma_1\\ \gamma_2\\ \gamma_3\\ \gamma_4\\ \gamma_5\\ \gamma_6\end{pmatrix}. \tag{20}$$

The corresponding components of the stiffness tensor for SCSi in the notation of eqn (20) are

$$c_{11} = 165.7\ \mathrm{GPa},\ c_{12} = 63.9\ \mathrm{GPa},\ c_{44} = 79.6\ \mathrm{GPa}. \tag{21}$$

While the analytical treatment of wave propagation in such materials is quite involved and beyond the scope of the present tutorial, for a numerical vibrational analysis of an anisotropic structure only the material properties are changed when compared to the isotropic solution.[11]

The two types of waves for the isotropic material interfere and get reflected at boundaries and interfaces to yield the modes of vibrations of the system. It must be noted that in general a P-wave is reflected as both a P-wave and an S-wave. The same is true for an incident S-wave. At interfaces a part of the energy is transmitted, another part is reflected depending on material properties and incident angle. In addition, interface waves exist at free boundaries (*e.g.* Rayleigh waves) and at interfaces (*e.g.* Stoneley waves).[10]

C Deformations of structures

If one or two dimensions of a structure are much smaller than the third, there exist a number of models that allow simple modelling of the behaviour, which take into account the stress free boundary conditions and are based upon certain assumptions regarding the displacement distribution. These assumptions have originally been made by physical insight, they can also be made in a rigorous way using matched asymptotic expansions.[12] These models can be grouped as:

- beam (length $\gg$ cross-sectional dimension) with longitudinal, torsional and bending motion,
- plate (flat structure, thickness $h \ll$ other dimensions) with longitudinal, bending, shearing and twisting motion,
- shell: as plate, except that the middle surface has a curvature.

In view of the applications to micromanipulation where often a cover is used above and/or below a chamber or channel, we focus here on bending vibrations of thin plates as an example for structural models.

In the modelling of plates it is customary to refer all quantities to the middle surface and the coordinate system has its axis located at this middle surface in the reference configuration. For simplicity we consider a displacement $w(x_1,t) = u_3(x_1,x_3{=}0,t)$ of the middle surface in the x_3 direction independent of x_2 (Fig. 2).

The bending motion is analyzed in the context of the Kirchhoff plate theory, which is equivalent to the Euler–Bernoulli beam theory.[8] The displacement assumption is that plane cross-sections orthogonal to the middle surface in the reference configuration remain plane and orthogonal to the middle surface during deformation.

For a homogeneous, isotropic, linearly elastic plate of unit width, small strains, small deformation and wavelengths which are large with respect to the thickness h of the plate the following equations are valid:

Displacement assumption

$$u_1 = -w_{,1}x_3. \tag{22}$$

Constitutive law relating bending moment and curvature

$$M_2 = \int_{-h/2}^{+h/2} \sigma_{11}\mathrm{d}x_3 = -\frac{E}{(1-\nu^2)}\frac{h^3}{12}w_{,11}. \tag{23}$$

Angular momentum equation

$$-Q_3 + M_{2,1} = 0. \tag{24}$$

Linear momentum equation

$$f_3 + Q_{3,1} = \rho h\ddot{w}. \tag{25}$$

Here M_2 is the bending moment, Q_3 the shear force, both per unit width and f_3 the load per unit area. Please note that shear deformation has been neglected in the kinematic equation (eqn (22)) and rotatory inertia has been neglected in the angular momentum equation eqn (24).

$E/(1 - \nu^2)$ is called the longitudinal plate modulus which results from the assumptions of plane strain ($\gamma_{22} = 0$) and negligible transverse normal stress ($\sigma_{33} = 0$).

Combining eqn (23)–(25) we obtain

$$\frac{E}{(1-\nu^2)}\frac{h^3}{12}w_{,1111} + \rho h\ddot{w} = f_3. \tag{26}$$

In order to solve eqn (26) we consider harmonic solutions with an angular frequency ω of the type

$$w = w_0 e^{i(\omega t - kx_1)}, \qquad k = \frac{\omega}{c}, \tag{27}$$

where k is the wavenumber and c the phase speed. If w satisfies eqn (26), for $f_3 = 0$ we obtain

$$c^2 = \sqrt{\frac{Eh^2}{12\rho(1-\nu^2)}}\,\omega = c_3 j_2 \omega, \tag{28}$$

where c_3

$$c_3 = \sqrt{\frac{E}{\rho(1-\nu^2)}} \tag{29}$$

is the longitudinal wave speed in the plate and j_2

$$j_2 = \sqrt{\frac{h^2}{12}} \tag{30}$$

is the radius of inertia of the cross-section.

The phase speed c is a function of frequency, therefore bending waves are dispersive. This dispersion is called geometric dispersion and is a function of the ratio of plate thickness h to wavelength λ. Using $\omega = ck$ we obtain:

$$c = c_3 j_2 k,\ \omega = c_3 j_2 k^2. \tag{31}$$

The dispersion relation is plotted in Fig. 3 for the Kirchhoff plate theory and the Mindlin plate theory. The deviations between the two theories are due to rotatory inertia and transverse shear deformation, which must be taken into account for about $j_2 k > 0.1$.

Note that in general for plate vibrations with $w(x_1,x_2,t)$, the differential equation is

$$D(w_{,1111} + 2w_{,1122} + w_{,2222}) + m\ddot{w} = f_3, \tag{32}$$

where

$$D = \frac{Eh^3}{12(1-\nu^2)}, \qquad m = \rho h. \tag{33}$$

D is the plate bending stiffness and m is the mass per unit area of the plate.

As an example let us consider vibrations of a plate that are independent of x_2, with pinned–pinned boundary conditions (*i.e.* zero displacement and zero bending moment) at $x_1 = 0$ and $x_1 = L$. We assume

$$w(x_1,t) = f(x_1)e^{i\omega t}. \tag{34}$$

After insertion into eqn (32) we get

$$f_{,1111} - k^4 f = 0, \tag{35}$$

with the solution

$$f = a_1\sin(kx_1) + a_2\cos(kx_1) + a_3\sinh(kx_1) + a_4\cosh(kx_1). \tag{36}$$

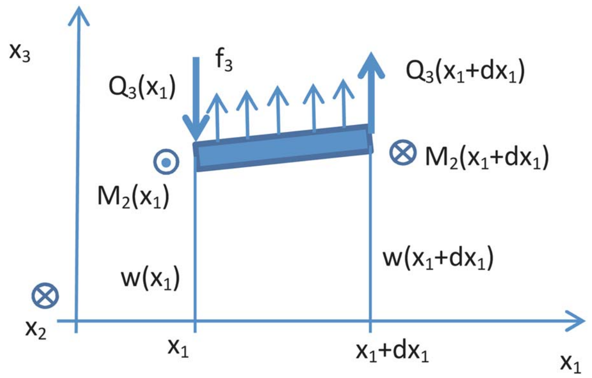

Fig. 2 Infinitesimal element of a plate (length dx_1 and unit width) with stress resultants shear force Q_3 and bending moment M_2.

a_1 to a_4 are obtained from the application of the boundary conditions

$$f(0) = f(L) = f_{,11}(0) = f_{,11}(L) = 0. \quad (37)$$

Because the differential equation is of forth order, we need four boundary conditions. This yields a 4×4 homogeneous system of equations for the unknowns a_1 to a_4, the determinant of which must vanish for a nontrivial solution to exist, resulting in

$$\sin(kl) = 0, k_nL = n\pi. \quad (38)$$

For the corresponding eigenfrequencies f_n one obtains using eqn (31)

$$f_n = c_3 j_2 \frac{n^2}{2}\frac{\pi}{L^2}. \quad (39)$$

For other boundary conditions, the solution is more complicated.

For example, for clamped–clamped (zero displacement and zero rotation at both ends) we have[10]

$$k_nL = 4.73, 7.85, 10.99, 14.14, \ldots \quad (40)$$

Note that the resonance frequencies are proportional to $1/L^2$ and increase with n^2.

Material damping can easily be incorporated into the equations, if we restrict ourselves to harmonic motion. According to the theory of linear viscoelastic materials[13] and for small damping, the plate material is described by a complex Young's modulus E^*

$$E^* = E_0(1 + i\varphi). \quad (41)$$

Here φ is the loss tangent, which characterizes the intrinsic damping. E_0 is the elastic part. Similarly complex values can be introduced into the Lamé constants of eqn (8).

For metals φ is about 0.01–0.0001 and E^* is nearly independent of frequency. For plastic materials, damping is much larger, depends on temperature and a strong frequency dependence might be present. For a given device, the intrinsic damping might strongly affect the pressure amplitudes that can be achieved in an ultrasonic manipulation device. Glue layers are of particular relevance in this context.

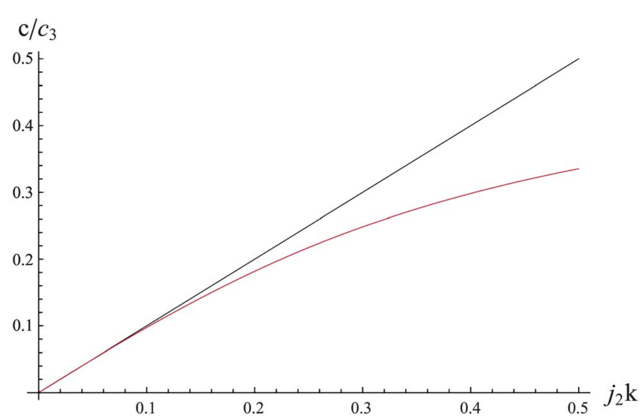

Fig. 3 Normalized dispersion curve (phase speed c *vs.* wavenumber k) for bending waves in a plate according to the Kirchhoff plate theory (black) and according to the Mindlin plate theory (red).[10]

D Fluid structure interaction at the device level

When a fluid is in contact with a solid, fluid structure interaction takes place. Both the field equations in the solid and in the fluid must be satisfied, as well as the boundary conditions. In addition, at the interface, certain conditions must be satisfied, depending on how the fluid is modeled. For an inviscid fluid the interface conditions are given in eqn (14).

At the interface the normal displacements must be equal, the normal stress of the solid must be equal to the negative of the pressure in the fluid, and the shear stress in the solid must vanish, if the fluid's viscosity is neglected.

If the cavity becomes very small, the viscosity might become important. Then the tangential part of the stress vector must be set equal to the viscous stress in the fluid and the tangential velocities must also be equal. The boundary conditions in eqn (14) must therefore be replaced by

$$\boldsymbol{u}_F = \boldsymbol{u}_S, \boldsymbol{t}_F = \boldsymbol{t}_S. \quad (42)$$

A harmonic tangential motion of the surface will give rise to a viscous boundary layer of thickness δ in the fluid. It is given by[14]

$$\delta = \sqrt{\frac{2\eta}{\rho_F \omega}}, \quad (43)$$

where ρ_F and η are density and viscosity of the fluid, respectively. For water at 1 MHz, δ is about 0.5 µm and less than 10^{-3} of the wavelength. Viscous effects at the boundary can be neglected, unless the cavity is comparable in size to δ.

In order to understand the physics of interaction between a harmonically vibrating surface and an inviscid fluid, two simple cases are given here.

In the first case, the solid moves without influence from the fluid. In the second case, there is a strong coupling between the two domains.

D.1 Acoustic radiation from a vibrating surface

Referring to Fig. 4 situations are considered, where the surface of a solid half

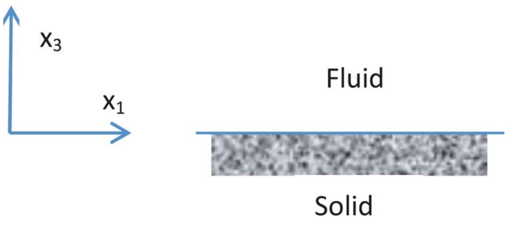

Fig. 4 Boundary between a fluid and a solid half space.

space ($x_3 < 0$) is vibrating harmonically with a given displacement distribution $u_3(x_1,0) = u(x_1)\exp(i\omega t)$. The fluid which occupies the half space $x_3 > 0$ does not influence the motion. We look for the solution in the fluid, which must satisfy

$$p_{,ii} = \frac{1}{c_F^2}\ddot{p} = -k_F^2 p, \qquad (44)$$

with the boundary condition at $x_3 = 0$ (ref. 15)

$$-\omega^2 \rho_F u_3 + p_{,3} = 0, \qquad (45)$$

where c_F and k_F are acoustic wave speed and wavenumber in the fluid.

(a) Constant displacement $u = u_0 e^{i\omega t}$

We obtain the solution by setting

$$p = p_0 e^{i(\omega t - k_F x_3)}, \qquad (46)$$

where we have assumed that there is no energy flowing back towards the surface (radiation condition). Eqn (46) satisfies (44) and the boundary condition yields

$$p_0 = -\frac{\rho_F \omega^2}{i k_F} u_0 = \rho_F c_F v_0, \qquad (47)$$

i.e. the pressure amplitude is equal to the characteristic impedance times velocity amplitude as expected by linear acoustic theory. Energy is radiated into the fluid.

(b) Sinusoidal displacement $u = u_0 \sin(k_{1x1})$, k_1 given

We assume a solution of the form

$$p = p_0 \sin(k_1 x_1) e^{i(\omega t - k_3 x_3)}, \qquad (48)$$

which satisfies eqn (44) if

$$k_3^2 = k_F^2 - k_1^2. \qquad (49)$$

We must discriminate between two cases:

(b1) $k_F > k_1$

i.e. the wavelength $\lambda_1 = 2\pi/k_1$ of the surface motion is larger than the wavelength in the fluid for the particular frequency. k_2 is a real number and we obtain a wave propagating away from the surface.

(b2) $k_F < k_1$

i.e. the wavelength λ_1 of the surface motion is smaller than the wavelength in the fluid for the particular frequency. k_3 is a purely imaginary number. When inserted into the assumption eqn (48), we obtain

$$p = p_0 \sin k_1 x_1 e^{-\alpha x_3} e^{i\omega t}, \quad \alpha = \sqrt{k_1^2 - k_F^2}. \qquad (50)$$

This is an exponentially decaying pressure field and no acoustic radiation occurs.

The fluid is pumped back and forth between neighbouring peaks and valleys of the surface motion. Therefore, for low frequencies, *i.e.* $f < c_F/\lambda_1$, no acoustic radiation occurs.

D.2 Acoustic radiation from a plate vibrating harmonically

We now combine the Kirchhoff plate equations in 2D with the acoustic solutions by looking at a situation, where a plate vibrates in contact with a fluid half space $x_3 > 0$ on one side.[16] The plate motion satisfies eqn (26), where f_3 is given by the fluid pressure.

The fluid satisfies eqn (44). The boundary condition at $x_3 = 0$ is

$$-\rho_F \omega^2 w = -p_{,3}. \qquad (51)$$

Note that the top surface of the plate is taken as $x_3 = 0$. With this boundary condition we now consider the full interaction between the sound field and the motion of the plate. This will result in a modified wave speed for the wave in the plate. Assuming a wave traveling in the $+x_1$-direction we look for solutions of the form

$$p = P(x_3) e^{i(\omega t - k_1 x_1)}, \quad w = w_0 e^{i(\omega t - k_1 x_1)}. \qquad (52)$$

k_1 is unknown and common to both fields. When inserted into eqn (44) we obtain for the fluid pressure:

$$P_{,33} + (k_F^2 - k_1^2)P = 0, \qquad (53)$$

resulting in

$$P = A e^{i\beta x_3} + B e^{-i\beta x_3}, \quad \beta^2 = \left(k_F^2 - k_1^2\right). \qquad (54)$$

As before we have to discriminate two cases, while keeping in mind that k_1 is now not constant, but a function of frequency.

(a) $k_F > k_1$

i.e. the wavelength of the plate motion is larger than the wavelength in the fluid for the particular frequency. We obtain a wave propagating away from the surface.

The radiation condition yields $A = 0$.

The boundary condition in eqn (51) at the plate yields B and after insertion into eqn (26) we obtain a modified dispersion relation

$$Dk_1^4 - \left(\rho h + \frac{i\rho_F}{\sqrt{\left(k_F^2 - k_1^2\right)}}\right)\omega^2 = 0. \qquad (55)$$

The solution k_1 must be obtained numerically. It is complex, representing the fact that the acoustic radiation will introduce an exponential decay of the traveling wave. It is called a leaky bending wave.

(b) $k_F < k_1$

i.e. the wavelength of the plate motion is smaller than the wavelength in the fluid for the particular frequency.

When combining eqn (51) and (26), we obtain as in section D.1 an exponential decay of the fluid motion into the fluid and a modified dispersion relation.

$$Dk_1^4 - \left(\rho h + \frac{\rho_F}{\sqrt{\left(k_1^2 - k_F^2\right)}}\right)\omega^2 = 0. \qquad (56)$$

In this case, the dispersion relation is only modified in a way, where the mass term is increased by fluid being pumped around.

This is the situation that one would like to have, if one wants to make a density sensor.

A special case of this is when $k_F \ll k_1$. We can then neglect k_F, neglect $\rho k_1 h$ when compared to ρ_F (thin plate) and get

$$k_1^5 = \frac{\omega^2 \rho_F}{D}. \qquad (57)$$

Physically speaking, all the stiffness is provided by the plate and all the mass is provided by the fluid.

In Fig. 5 the interaction between a silicon plate (thickness 100 μm) and water is shown by comparing the relative wavenumbers.

In a micromanipulation device, the assumption of the semi-infinite fluid domain is not valid. Therefore reflections from the solid adjacent boundary need to be considered.[17]

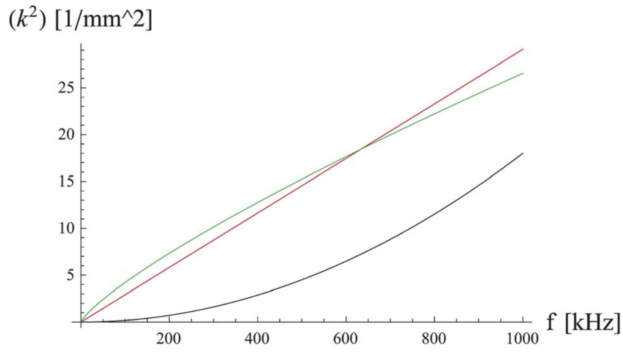

Fig. 5 Square of the wavenumber for waves in water (black), bending waves in plates without fluid (red, eqn (31)) and interacting bending waves (eqn (57)) (green).

D.3 Vibrations of devices for particle manipulation

For general geometries as they occur in particle manipulation devices, a numerical solution must be found, as there is no analytical solution available. The method used normally is the Finite Element Method (FEM).[18] In short, in the FEM the spatial domain is split up in standard subdomains, for which certain displacement assumptions are made. The displacements within the elements are expressed in terms of the nodal values, which correspond to the points, where an element connects with its neighbours. The elements are then assembled to yield a discretized version of the problem as shown in eqn (58).

$$[\boldsymbol{M}]\{\ddot{\boldsymbol{x}}\} + [\boldsymbol{D}]\{\dot{\boldsymbol{x}}\} + [\boldsymbol{K}]\{\boldsymbol{x}\} = \{\boldsymbol{F}\}. \quad (58)$$

Here $\boldsymbol{M}$ is the mass matrix, $\boldsymbol{D}$ the damping matrix, $\boldsymbol{K}$ the stiffness matrix and $\boldsymbol{F}$ the loading vector. $\boldsymbol{x}$ is the vector of the nodal displacements. These equations are then solved to yield a discretized solution, consisting of the nodal vector $\boldsymbol{x}$.

Eqn (58) contains the resonance frequencies and modes of the system. Often $\boldsymbol{D}$ is set to zero and then $\boldsymbol{M}$ and $\boldsymbol{K}$ are diagonalized to yield modes independent of each other corresponding to the modal coordinates $\boldsymbol{y}$. $\boldsymbol{D}$ is then taken as a diagonal matrix, *i.e.* damping is assigned to the modes individually. Each mode is then considered as a single degree of freedom system (SDOF). A necessary condition for this assumption is that the modes are separated sufficiently, *i.e.* the bandwidth of each mode must be smaller than the spacing between the frequencies of adjacent modes. For this simplification the quality factor (Q-factor) is a good parameter to quantify the damping of the particular mode. A SDOF system with mass m, stiffness k, damping δ and driving force f is described by the equation

$$m\ddot{y} + \delta\dot{y} + ky = f. \quad (59)$$

The resonance frequency ω_0 and quality factor Q are then defined as

$$\omega_0 = \sqrt{\frac{k}{m}}, \quad Q = \frac{m\omega_0}{\delta} = \frac{\omega_0}{\Delta\omega}, \quad (60)$$

where $\Delta\omega$ is the bandwidth. Q can also be seen as the ratio between the dissipated energy per cycle D_{tot} divided by $2\pi U$, where U is the maximum stored energy. In an ultrasonic manipulation system many damping mechanisms are present, each one will contribute to the resulting Q according to its activity level. As U is fixed we have

$$\frac{1}{Q_{\text{tot}}} = \frac{D_{\text{tot}}}{2\pi U_{\text{max}}} = \frac{1}{Q_{\text{fluid}}} + \frac{1}{Q_{\text{solid}}} + \frac{1}{Q_{\text{glue}}} + \frac{1}{Q_{\text{support}}}. \quad (61)$$

$1/Q_i$ correspond to the respective normalized damping energies D_i. For a solid described with a complex modulus (41), the contribution is

$$\frac{1}{Q_{\text{solid}}} = \varphi. \quad (62)$$

Examples of single-mode analysis of an experimentally determined acoustofluidic resonance have been given in ref. 15, 19 and 20.

The usual steps when applying the FEM are:

- Definition of the geometry.
- Definition of material properties.
- Choosing suitable elements for the spatial discretization. Important in this decision is whether structural elements (beams, plates, shells) or 3D brick elements are used. Also the approximation of the displacement functions within the element is an important consideration.
- Definition of boundary conditions, interface conditions and loading conditions (possibly depending on the element).
- Choosing the mode of analysis (*e.g.* harmonic analysis).
- Computation of the results.
- Analysis of the results and quality check.

E Example of a mechanical model of an ultrasonic cavity used for particle manipulation

The finite element modelling is a useful tool for the simulation of fluid structure interaction. A practical simulation is only possible by including the resonant cavity and the surrounding mechanical structure, which are coupled and therefore influence each other. The modelling helps to understand the response of the system and can be very useful for the design and optimization process. The frequency at which a strong pressure field is built up inside the fluid cavity which is suitable for particle manipulation can be determined.

The two dimensional simulation presented here was done with COMSOL Multiphysics 4.1 and represents the three dimensional situation where all quantities are independent of the third dimension. The resonating system model is a typical microfluidic device for ultrasonic manipulation.[20] It consists of the three parts shown in Fig. 6a. The main part consists of silicon, where a cavity for a fluid is etched inside. The system is sealed with a glass part at the top. The silicon

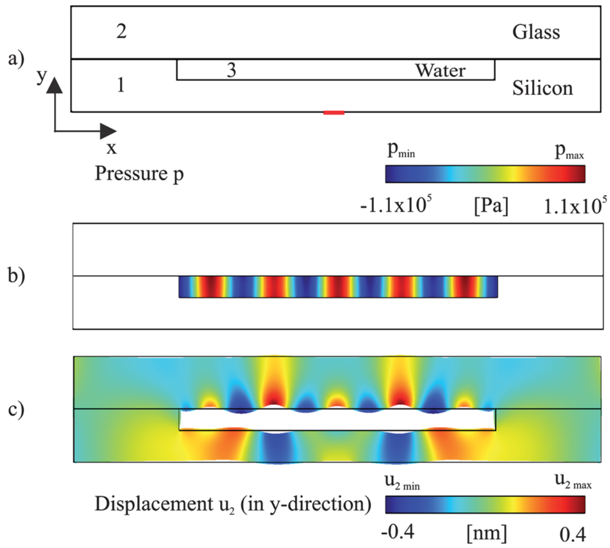

Fig. 6 (a) Model of a microfluidic device for ultrasonic manipulation, (b) pressure field in the fluid at a frequency of 2404 kHz, (c) displacement and deformation of the solid structure in the y-direction (deformation scaled by a factor of 10^5).

dimensions are 5 mm × 0.5 mm. The water filled cavity is 3 mm × 0.2 mm and the glass top has the dimensions 5 mm × 0.5 mm. The piezoelectric transducer, which is normally driving such a system, is omitted here for simplicity reasons. Therefore the excitation is done with a prescribed displacement amplitude of 0.1 nm in the y direction in the middle of the silicon bottom over a length of 0.25 mm (represented by the red part in Fig. 6a). This excitation amplitude leads to pressure amplitudes in the fluid which are comparable with the excitation achieved with a piezoelectric transducer.

The geometry is built in COMSOL using the above dimensions and produces the three domains 1–3 shown in Fig. 6a. To every domain, a material with its properties must be assigned. The following material properties have been used: water with a density of 998 kg m^{-3} and a speed of sound of 1481(1 + i/2000) m s^{-1}. Damping has been included with complex stiffness parameters for solids and complex wave speed for the fluid.[21] Silicon is an anisotropic material with stiffness parameters as given in eqn (21) and a density of 2330 kg m^{-3}. The damping of the silicon has been neglected as it is small compared to the other used materials. The glass has a Young's modulus of 63(1 + i/400) GPa, a Poisson's ratio of ν = 0.2 and a density of 2220 kg m^{-3}.

For the modelling of the water domain the pressure acoustic physics-module (acpr) has been chosen, where the dependent variable is the acoustic pressure p. The coupling for all cavity boundaries with the surrounding structure is defined with an acceleration a_n (acceleration denoted by (solid/lemm1) in COMSOL) normal to the interface which is coupled to the solid mechanics physics-module. The first boundary condition used here is equivalent to eqn (14), where the normal displacement is used instead of the normal acceleration.

The silicon and glass parts are represented with the solid mechanics physics-module (solid). There the dependent variable is the displacement field $\boldsymbol{u}$ with its field components u_1 and u_2. Two linear elastic material models are needed: one with anisotropic properties for the silicon and the other with isotropic properties for the glass. The boundary conditions used were as follows: at all outside boundaries a free displacement was implemented, with exception of the boundary for the prescribed displacement amplitude of 0.1 nm in the y direction. For the fluid structure interaction a boundary load was defined with a so-called"load defined as force per unit area" (acoustic load per unit area denoted by (acpr/pam1) in COMSOL) from the pressure acoustic physics-module. This boundary load is defined by COMSOL and can be understood as $-p\boldsymbol{n}$ as shown in eqn (14) which is equal to the normal stress vector $\boldsymbol{t}_{nS}$ in the solid.

The meshing was done automatically with about 13 500 "free quad" elements of equal size for all three domains. The maximum element size depends on the speed of sound of the used materials and the frequency and must be much smaller than the wavelength. A mesh convergence test, where the results with different element sizes are compared can be used to ascertain that the spatial discretization is sufficient. A frequency response analysis (frequency domain) was performed. In the simulation the PARDISO solver was used and "fully coupled" was applied as both fields (acoustic, solid) are influencing each other. The simulation was done parametric over a frequency range from 2–3 MHz in 1 kHz steps. As an example of the simulation one result at the frequency of f = 2404 kHz is represented in Fig. 6b and c. The pressure field in the fluid and the displacement and deformation of the solid structure in the y direction are presented. The deformation is scaled by a factor of 10^5.

A strong pressure field is created at this frequency and the system is in resonance, therefore the excitation is with 0.1 nm smaller than the maximum displacement of the solid with 0.4 nm. This result shows nicely the coupling between the two modules. The excitation of the system is done with the displacement of the silicon and is exciting the fluid cavity to resonance. The standing pressure wave inside the fluid cavity is strongly influencing the surrounding structure.

Conclusions

In this paper linear elastic continuum mechanics has been summarized and applied to a typical problem that occurs in ultrasonic manipulation devices. While some physical insight can be gained by studying simple systems, for an analysis of a practical device numerical tools like FEM are needed. It has been shown that for systems where the fluid used is a fluid with water like properties, the relatively small impedance difference results in motion for the whole system and not just for the acoustic cavity. When designing a device normally resonance frequencies are sought, because they have much stronger fields, which helps in the manipulation efficiency. These resonance frequencies and modes are influenced by all the components of the system. For the absolute value of the pressure maxima in the cavity also the damping of the resonance mode is important, which is normally difficult to model on first principles.

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