Design optimisation of silicon-based MEMS sensors dedicated to bioaerosols monitoring

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***Abstract*— Due to recent paradigm changes for the monitoring of air pollution, assessing human exposure to (bio)-aerosols with low-cost sensors is expected to be of growing importance. In this context, our work subsequently investigates the development of Si-based gravimetric instruments. Thus particle-resonator interactions are considered to provide a particle detachment criteria as well as geometrical features ensuring performances both in terms of sensitivity and uniform resonator response. Analytical and numerical methods have been carried out and confronted to experimental results.**

***Keywords*— MEMS mass sensor; Bioaresol; Design Method**

I. Introduction

As human beings spent almost 90% of their time indoors, they are exposed to various exogenous and building-endogenous particulate pollution for which no guidance values are available. Worse, it is not currently possible to define such values as particles are a very heterogeneous mixture both in terms of size and chemical and microbiological compositions. These, however, play a predominant role in the type of health effects induce by exposure.

Microbiological particles include fungal spores, which are the most numerous and most diversified living particles of the air that we breathe. Indeed airborne fungal spores are ten to hundred times more abundant than pollens. Besides, spores, like mycelial fragments or fungal metabolites, are known to induce various diseases such allergies, infection, food poisoning or irritations in both outdoor and indoor environments. In 2012, Hulin [1] demonstrated a correlation between the development of atopic asthma in children and the detection of molds in the home. In this context, efforts are needed to supervise fungal aerosols concentrations. Unfortunately, current recommended instruments are based on gravimetric methods and are not appropriate for personal mass concentration tracking because of their limited performances, sizes, price... The development of portable, lower-cost bioaerosols sensors may bring new promising opportunities to apprehend exposure and conceive strategies to reduce it [2].

Microfabrication techniques allow downscaling while reducing cost and are widely used together in various engineering applications such as realization of MEMS [3-6], Packaging [7, 8], ultrasonic [9], gravimetric sensor [10], transducers and other acoustical applications (egg. BAW and SAW) [11]. Many miniature mass sensor systems using microfabrition techniques have been developed in the last recent years. These devices are not designed for aerosol measurement but for very low weight elements such as volatile organic compound. Two types of devices have been developed: acoustic resonator and Micro Electromechanical Systems (MEMS). Piezoelectric transducer formed of thin films of ZnO or AlN, are already used as gas sensors. They are composed of bulk or surface waves acoustic resonators [12]. Thanks to surface functionalization, these devices can achieve sensitivity as low as 0.05 fg/m[13][14][15]. The advantages of MEMS compared to acoustic resonators are their low-cost and easier fabrication. Moreover, nanofabrication techniques enable to reduce their size to the nanometer scale and achieve ultimate weight resolution as low as the attogram[16][17][18][19]. And yet resonator with plane deformation can achieve high resonance frequency and high quality factor [20][21][22][23]. But few sensors have been fabricated specifically to measure solid particles [24][25]. In first reference, authors use FBAR as particle sensor and reach very good sensitivity. The disadvantage of such a device is that the response of the resonator is highly dependent to localization of the deposited particle. It's why some authors [24] propose the use of thermally actuated Silicon MEMS resonators with piezoresistive detection. The shear deformation mode is less dependent to particle localization, but their sensitivity is still limited to few nanograms due to their weak quality factor and their weak resonance frequency. To increase the sensitivity authors shrink the size of MEMS devices [25], but the active detection zone is in the same time reduced.

Therefore, we chose to develop silicon resonator-based MEMS microbalance (as that presented in figure 1) which combines high performances with simple micro fabrication techniques. In this paper, we focus attention on how to design this MEMS-based gravimetric sensors for micro-sized fungal bioaerosols. However, dealing such a topic means:

- making good use of particle-sensor interactions to establish operating conditions;
- optimizing resonator geometry and deformation mode to provide the best sensitivity as well as a uniform response.

II. Resonator conception and design

Based on MEMS oscillating structures, gravimetric sensors rest on the use of an self-sustained oscillator made of: a transduction system, a resonator and a oscillator amplifier. Taken together, these devices detect additional masses on the resonator surface by recording all change in their resonance frequency. As a result, looking at potential improvements implies substantive work on optimizations of particle-sensor interactions and mechanical aspects. Both are proposed herein.

A. Determination of the operating conditions

Prerequisite for measuring particle mass, the particle capture and adhesion on a working resonator surface is the result of a competition between detachment mechanisms (rebound, rolling, sliding...) and adhesive forces which are assessed thanks to elastic contact models. Described in the literature for out-plane mode sensors [28], this kind of examination may also be used for bulk-mode resonators. Thanks to a thermodynamical model and contact angle measurements (on different surfaces and different particles mat) the adhesion energy of fungal aerosols has been evaluated. Assuming quasi-static situations, the adhesion moment has been evaluated taking into account an asymmetric JKR-pressure distribution over the particle-resonator contact area and compared to the inertia force moment to satisfy:

$$M_{ad} > M_{inertia} \tag{1}$$

where $M_{inertia}$ is inertia force moment, which is proportional to the resonator displacement amplitude and to the square of the resonance frequency ω^2. Regarding M_{ad}, this term corresponds to the adhesion moment, which depends on the adhesion energy and on the particle radius [29]. From a particle monitoring perspective, facing (1) means working with a MEMS-microbalance resonance frequency inferior to a critical value which depends on both adhesion energy and particle geometry. In other words, the design of the resonator should be achieved in accordance with this criteria.

The particle-resonator adhesion, while necessary, is not sufficient to ensure a relevant measurement of mass since the response of the resonator depends not only on the physical mass of the deposited particle but also on the particle-surface interactions. As mentioned in [30] [31] [32], an inappropriate dimensioning of microbalances might suggest the detected particles appear to be with a negative mass by recording an increase in the resonance frequency. In order to prevent such a surprising situation, the dependence between the frequency shift of the resonance frequency and the added mass should be studied more in detail. In the case where a particle stacked to the resonator surface has a rotation movement around as sketched in the figure 2 the behavior of a sparse particle on a resonator can be derived from fundamental dynamic law (equation (2)) and from kinetic moment theorem (equation (3)):

$$m_{phys}(\ddot{U} - R\ddot{\theta}) = -F_f - f_{el} \tag{2}$$

$$I\ddot{\theta} = (-F_f - f_{el})R - M_{a} \tag{3}$$

where m_{phys} and *R* are respectively the particle mass and radius when F_f and f_{el} represent frictional and effective elastic forces between the particle and the resonator surface. Lastly, *I* is the inertia moment, and $\ddot{U}$ is the resonator acceleration where the particle is attached. For harmonic operating modes ($\ddot{U} = -\omega^2 U$, $\ddot{\theta} = -\omega^2\theta$), such a trivial theoretical model leads to define an effective mass for the particle as the mass the resonator feels particles through. This effective mass can be defined by rewriting the fundamental dynamic law as below:

$$-m_{eff}\,\omega^2 U = -F_f - f_{el} \tag{4}$$

By combining equation (2) and (3), we can find effective mass is function of pulsation and its expression is:

$$m_{eff}(\omega) = \frac{m_{phys}(\omega)}{1 + \frac{m_{phys}(\omega)R^2}{I}\frac{\Psi^2}{\Psi^2 - 1}} \tag{5}$$

Regarding Ψ, it is defined as a normalized pulsation: $\Psi = \frac{\omega}{\Gamma^*}$ with $\Gamma^* = \sqrt{\frac{6\pi W_{ad} R^2}{I}}$ (6) where W_{ad} is the work of adhesion between particles and resonator.

Equation (5) highlights frequency shift is not only a function of the geometric and physical parameters of the resonator and the particles added but also a function of the interactions between them. As shown in figure 3 which presents the ratio $m_{eff}(\omega)/m_{phys}$ against the normalized pulsation, the rotational degree of freedom of a spherical particle leads the resonator feels a load to be the same as, larger than or smaller than the physical particle mass. The subsequent impact of that observation is that a relevant and consistent measure of mass ($m_{eff}(\omega) \approx m_{phys}$) only happens when $\omega << \Gamma^*$ what limits usable frequency band.

In the case of Aspergillus niger conidia, adhesion energy has been determined by contact angle measurements (CAM) and varies from 100 to 120 mJ.m^{-2}, consistent with previous works on mechanical properties of Asp. Niger [33] [34]. The corresponding values of Γ^* in are in the order of a few GHz. Yet if we consider the adhesion criteria giving by the equation (1), the MEMS resonator should be designed to exhibit resonance frequency inferior to 10 MHz to avoid particle detachment. Then the normalized pulsation Ψ should be about 0.01, for this value the effective mass is almost equal to physical mass, so it ensures a relevant measure of mass.

B. *Performance criteria*

With the aim to find the most appropriate structures for the particle mass sensing, different resonator families (elliptic- and rectangular-shaped devices) are numerically investigated (Table 1). Thanks to *COMSOL Multiphysics* software, the impact of the geometrical features on sensitivity is studied. This sensitivity is commonly defined as:

$$S = \frac{f_{res}}{2m_{eff,res}} \qquad (6)$$

To illustrate, different mode sensitivities may be plotted versus respectively the aspect ratios (Figure 5) and the eccentricity of the resonators (Figure 6). As seen in these figures, resonance mode impacts more the sensitivity of rectangular-shaped resonators than that of elliptic ones. Moreover and in spite of lower initial sensitivities, circular structures performances may be improved by increasing the eccentricity and therefore the effective detection zone. Seen through the lens of gravimetric sensors development, the extensional mode of a square-shaped resonator seems, however, to be the most appropriate since it presents the best sensitivity (0.13 Hz/pg).

TABLE I. GEOMETRICAL PROPERTIES OF STUDIED RESONATORS

	Elliptic	**Rectangular**
Minor axes/Shortest side (µm)	**375 and 500**	**750 and 1000**
Eccentricity/Ratio aspect	*0* **to** $\sqrt{3}/2$	**1 to 2**

Although equation (6) allows in selecting geometries, it is interesting to note that for a given frequency shift this relation does not take into account how the added mass is distributed over the resonator surface. If this distinction seems meaningless for the monitoring of gases, it is of critical importance for aerosol particles which each have a precise location on the surface. Assuming previous operating conditions are met, any particle on the resonator surface induces a downward frequency shift, due to the change in the kinetic energy of the system. If that added mass Δm does not change the resonance mode ($\Delta m << m_{eff,res}$), the use of Rayleigh-Ritz theorem leads to express the punctual sensitivity of the resonator where the particle is attached as:

$$S_{punc}(x_p, y_p) = \frac{\Delta f}{\Delta m}(x_p, y_p) = \frac{f_{res}}{2m_{eff}} U_m{}^2(x_p, y_p) \qquad (7)$$

where f_{res} and $m_{eff,res}$ are respectively the resonance frequency and the effective mass of the resonator $U_m(x_P,y_P)$ is the mode shape normalized to 1 at the position (x_P,y_P). If $u(x,y,t)$ is the resonator displacement, $U_m(x,y)$ can be defined by: $u(x,y) = a_m U_m(x,y)e^{i\omega t}$. From (8), it is seen the frequency shift induced by added mass depends on the mode shape - or in other words the mechanical properties of the resonator - and the position of the particle.

Such a definition of the sensitivity also deserves attention on our part since it allows considering the dispersion of sensitivities for each structure. It consists in a histogram displaying relative frequencies of punctual sensitivities when bins tend towards zero. Thus, this quantity may be used to know the surface proportion of the resonator which exhibits the same punctual sensitivity. In this respect, Figure 6 presents relative frequencies of punctual sensitivities of a square-shaped resonator for different deformation modes. On this occasion, such an analysis shows first that since the particle-to-surface adhesion is considered as punctual (JKR- contact zone area << A_{eff}), resonators owns rather a Hz/ng-sentivity to particle mass than a Hz/pg one as proposed with (6). Then if extensional mode presents a narrower range of sensitivities (to get an uniform mass sensor is to develop is to design a sensor which its sensitivity density is a Dirac), the Lamé mode maximum is obtained for a lightly bigger sensitivity. Besides this can also improved by considering the second- or the third-order with a sensitivity of 130 Hz/ng.

III. CONCLUSION

Particle-resonator interactions are moved to the center stage of the discussion. In this way limiting rolling-detachment conditions (derived from the Johnson-Kendall-Roberts model) enables the determination of an operating frequency range up to 10 MHz while providing geometrical features for an adequate design basis for the resonator. Thus, it appears rotational degree of freedom may significantly impact on the mass sensed by the resonator. But, we have demonstrated that for frequency inferior to the critical value of 10MHz, the designed resonator gives a relevant measure of mass. We have also demonstrated that a good sensitivity as well as the best uniformity are obtained for extensional mode of square resonator.

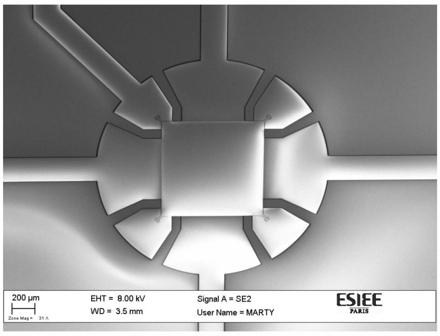

Fig.1. Optical image of silicon MEMS microbalance for aerosol measurement.

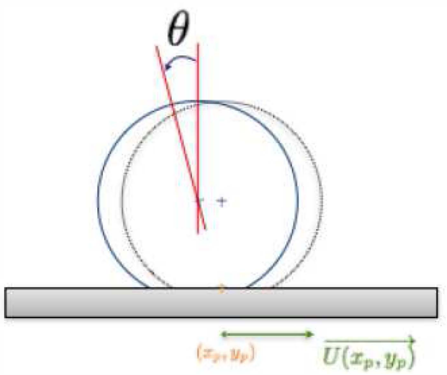

Fig. 2. Schematic of rotational movement of attached particle on resonator surface.

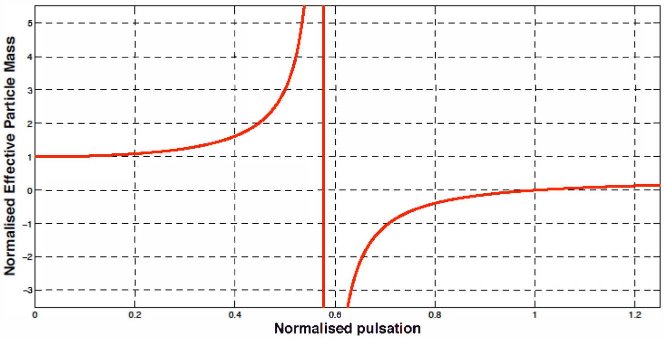

Fig. 3. Normalized effective particle mass against normalized pulsation for a spherical particle ($m_{phys}R^2 = \frac{5}{2}I$)

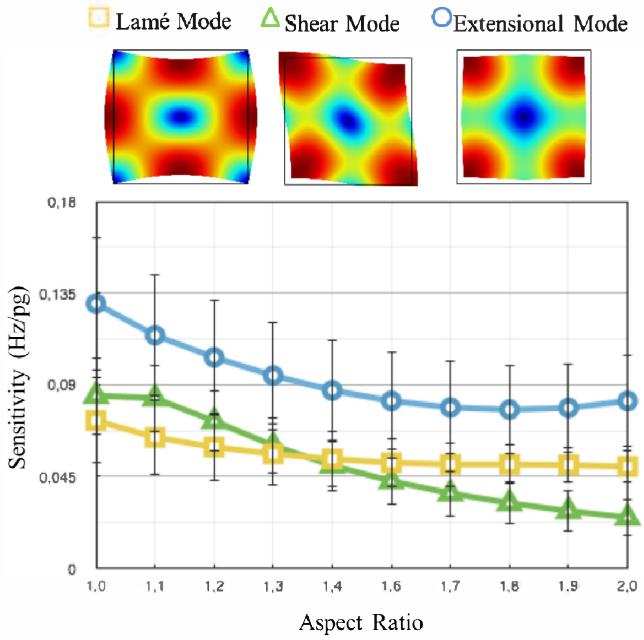

Fig. 4. Mode sensitivities against the aspect ratio of a rectangular-shaped resonator. Its shortest side is of 750 µm.

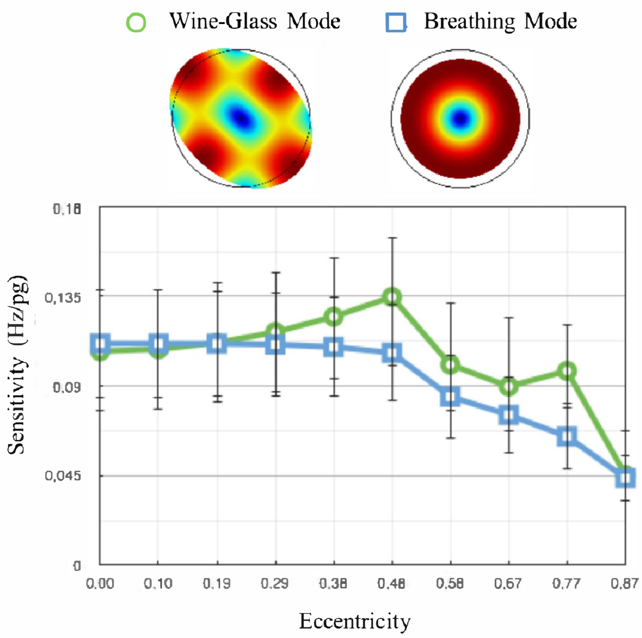

Fig. 5. Mode sensitivities against aspect ratio of an elliptic-shaped resonator. Its minor axe is of 375µm

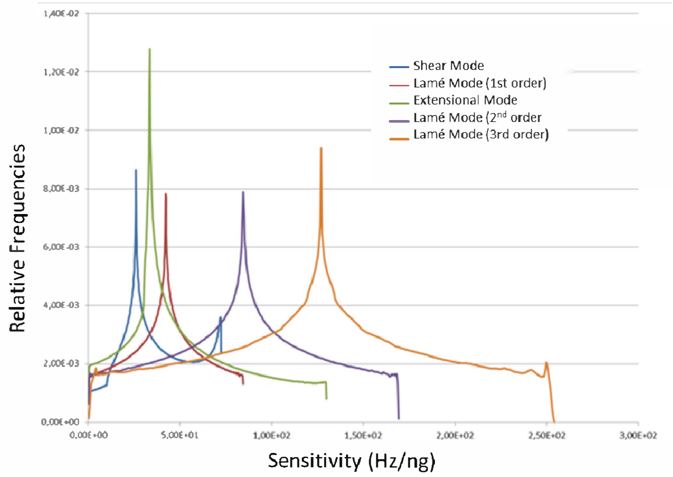

Fig. 6. Distribution of punctual sensitivity for different deformation modes (Side length =1 000 µm).

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