European Network on New Sensing Technologies for Air Pollution Control and Environmental Sustainability - *EuNetAir*

COST Action TD1105

WGs & MC Meeting at SOFIA (BG), 16-18 December 2015

New Sensing Technologies for Indoor Air Quality Monitoring: Trends and Challenges

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DEVELOPING A THEORY FOR PREDICTIVE MODELING OF ACOUSTIC SENSORS IN ENVIRONMENTAL APPLICATIONS

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WG2

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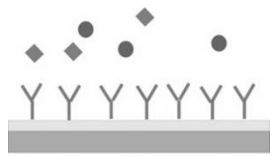
Scientific context and objectives in the Action

Background: Predictive modeling of acoustical sensors for environmental applications and healthcare

- **Brief reminder of MoU objectives:** WG2
- Area of research: Acoustic resonators for sensor applications in the air and liquids



- **SAW-based sensors**:

SH-SSW (surface shear waves with horizontal polarization): sensing in the air and liquid phase

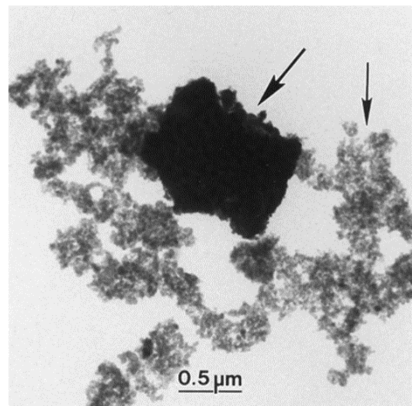
- **BAW types:**

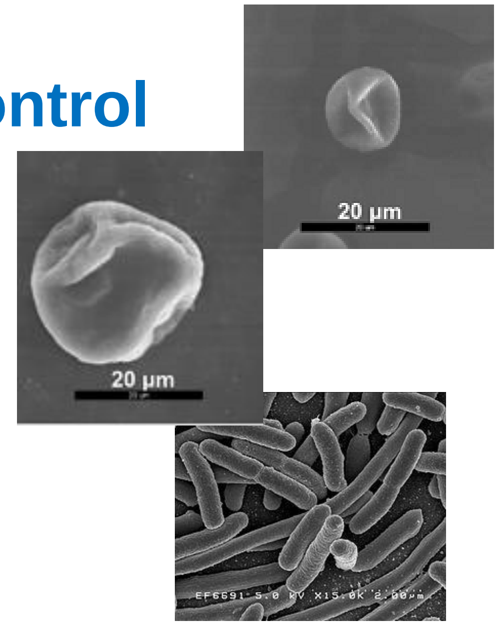
QCM-D Quartz Crystal Microbalance with dissipation (humid air, aerosols, liquids)

Current research activities :Theoretical modelling of SAW-based and QCM-D sensors

Current research topics / Problem statement

- Acoustic **biosensors for healthcare**
- **Acoustic sensors for environmental control**
- **Goal1:**
- Air quality control





- The system :
- Microparticles and NPs
- Mineral,organic and bioorganic dust (bacteria and viruses), dispersed in water

Environmental applications

- Goal 2: Control of clean water quality

Problem statement: Microplastic litter pollution

- Third Conference The Ocean of Tomorrow projects: What results so far for healthy and productive seas and oceans?
- 11 November 2015, Brussels (EC Conference)

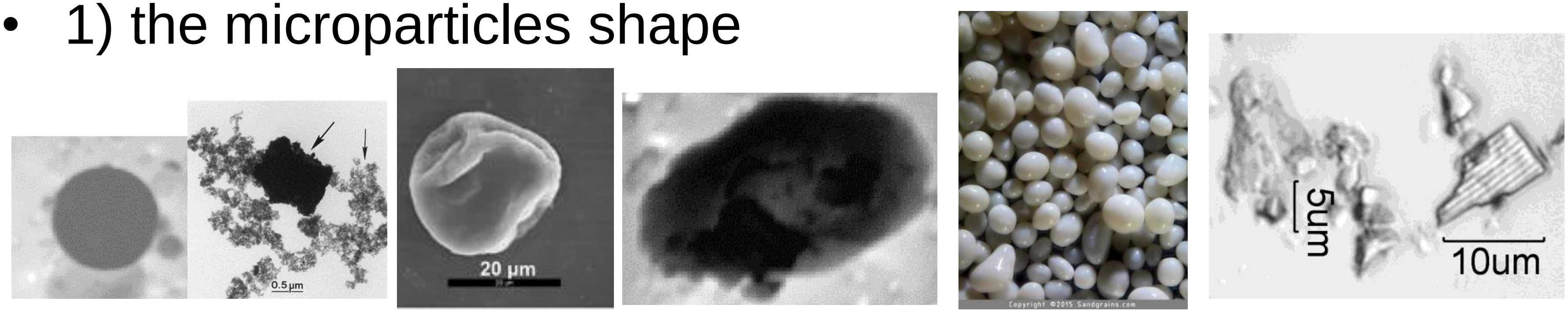
Brief list of ongoing research topics

- **Predictive modeling of SAW-sensors and QCM-D**
- Analytical and numerical results for the phase velocity change of SAW (SH-SSW) sensor characteristics for organic (polymer) sensing coatings. The 'missing-mass" effects in liquid phase operation. Gravimetrical sensitivity enhancement.

- Analytical and numerical results for the shift in the resonance frequency and dissipation of QCM-D sensors for dispersions of microparticles and NPs in liquids

Predictive modeling in QCM-D research (Microparticles and NPs dispersed in liquids)

- Results in QCM-D: analytical formulae and numerical calculations for change in the resonance frequency and the dissipation to determine
- 1) the microparticles shape



The collection of microparticles (airborne and/or precipitated):

Spherical ash particle, carbon particles, pollen particle (allergic agent), irregular shape soil particle, fine sand grains, precipitated diatoms fragments) (‘white-rain’’)

- 2) the pollution level (the concentration of NPs in water microdroplets)

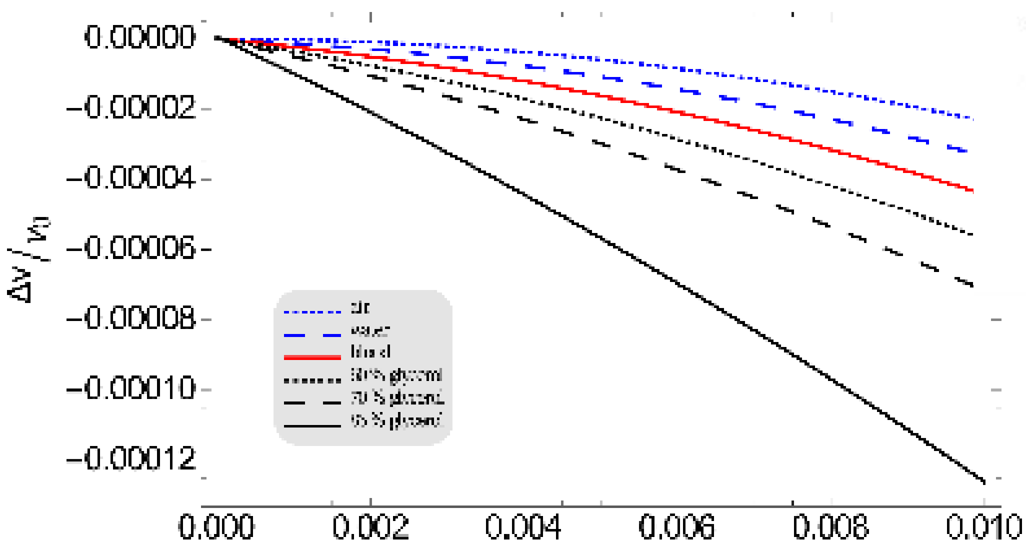
Predictive modeling of SAW-sensors response in liquids

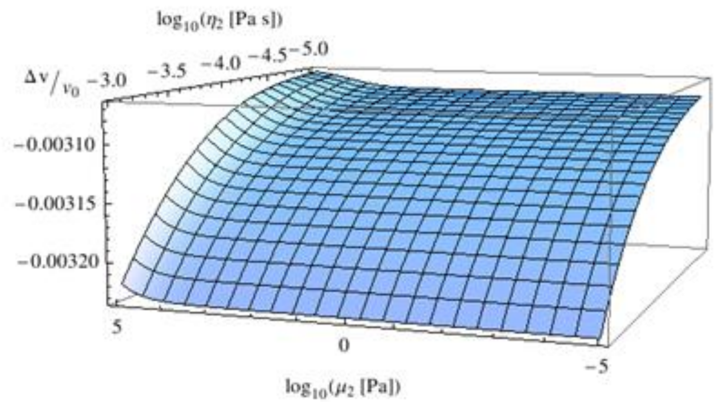
The ’missing mass”effect in viscous liquids

Modeling SH-SSW sensors response (Δv/v)

Varying polymer coatings

Towards the higher mass sensitivity

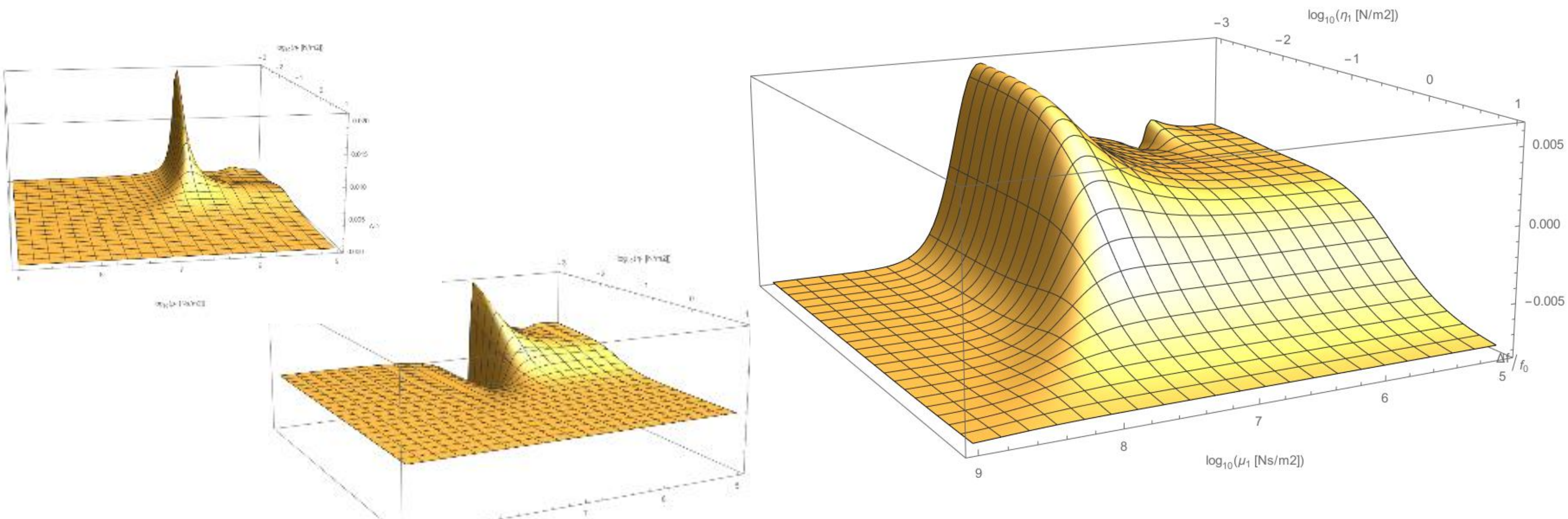




Voinova, Vikström (2015, submitted)

Modeling the QCM-D response:

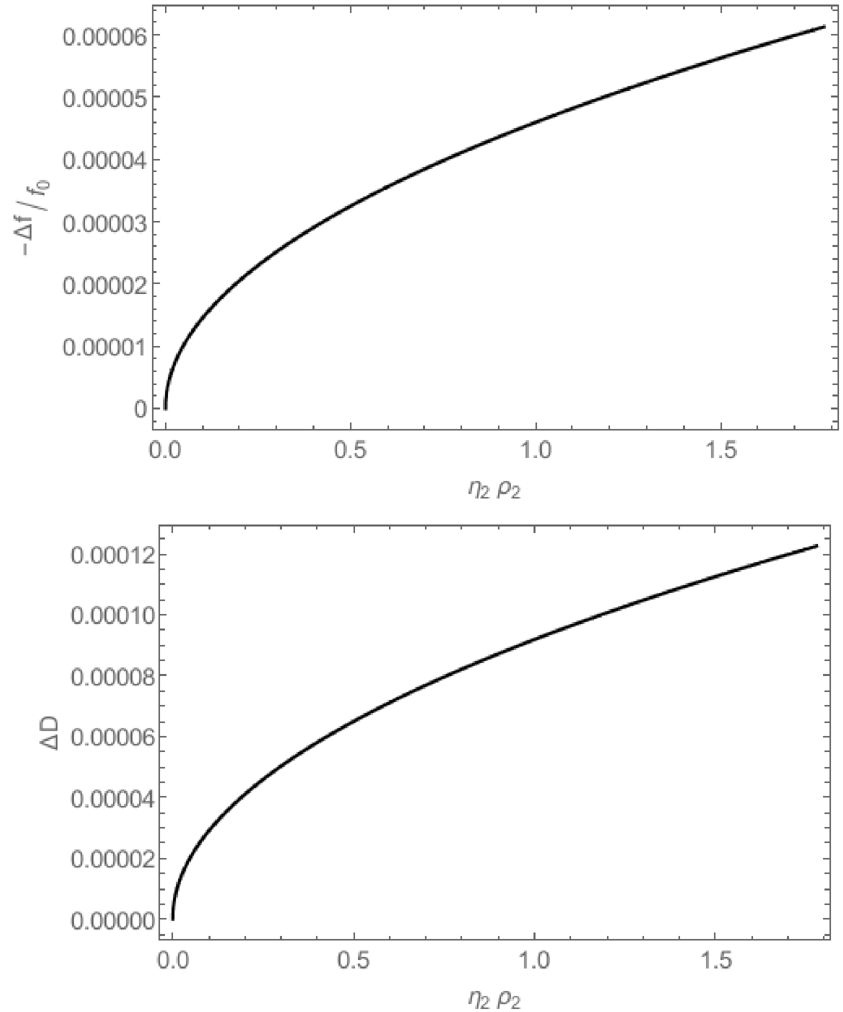
Coated QCM operating in a liquid phase
Varying polymer coatings (viscoelastic layers)
Predicted ’missing mass’’ effect in liquid phase



Numerical results for the change in the resonance frequency and dissipation of coated QCM-D operating in viscous liquids

Modeling of QCM-D response operating in viscous liquids

Figure 1



A bare QCM-D, operating at a frequency *f*=1 MHz, in a liquid phase. Both the frequency shift and the dissipation depend on the product of the viscosity and the density of the liquid.

Modeling the QCM-D response in dispersed microparticle/NPs systems

Pollutant model particles:

Gold NPs

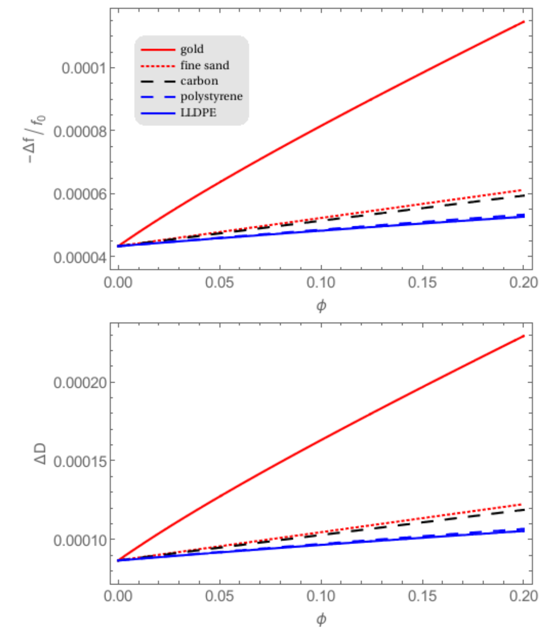
Fine sand grains

Carbon NPs

Polystyrene

LLDPE polymer

Figure 2

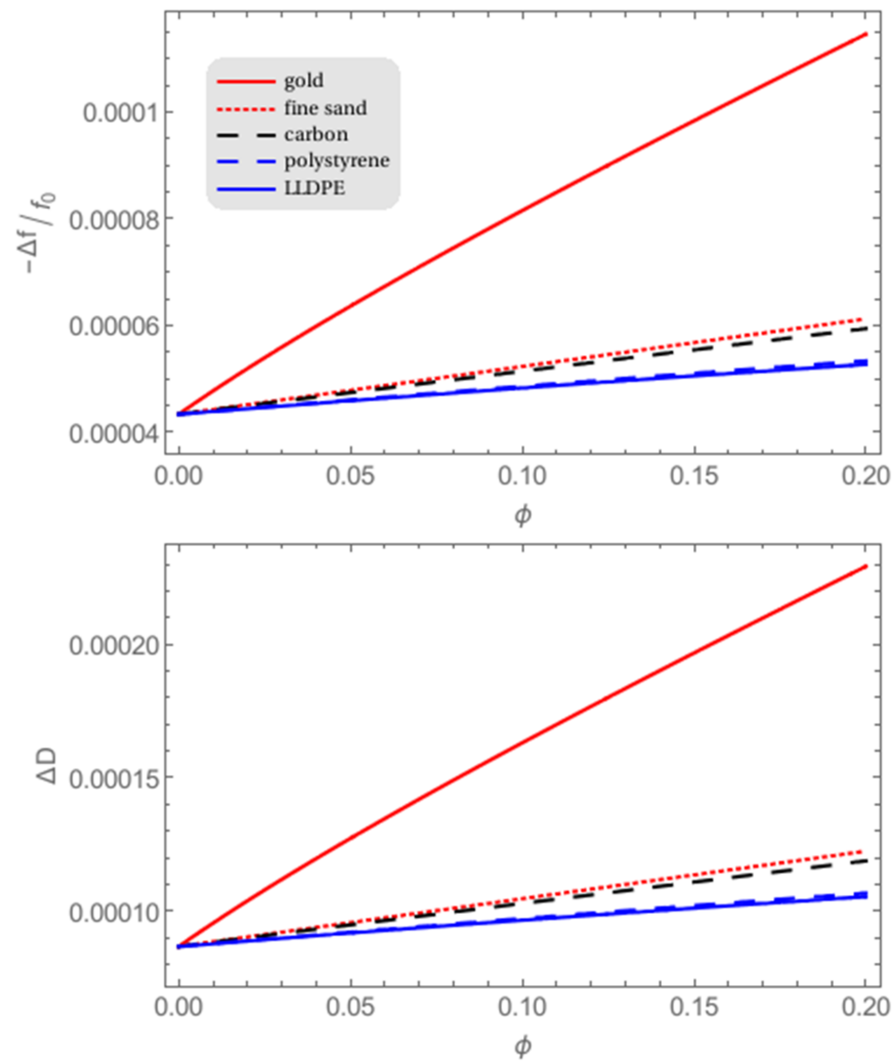


Modeling QCM-D
The system: NPs dispersed in water

Figure 2
A bare QCM-D, operating at a frequency *f*=1 MHz, in water containing by spherical (shape factor α=2.5) nanoparticles at different (low) concentrations ϕ. The nanoparticles affect the effective viscosity (as given by Einstein's expression) and density of the contaminated water. The plot shows the effect of spherical nanoparticles of different material.

For these materials and low concentrations, the relative change in the viscosity-density product is small (linear behavior)

Figure 2



EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

Modeling the QCM-D response in water dispersions

Microplastic (PVC) particles pollution

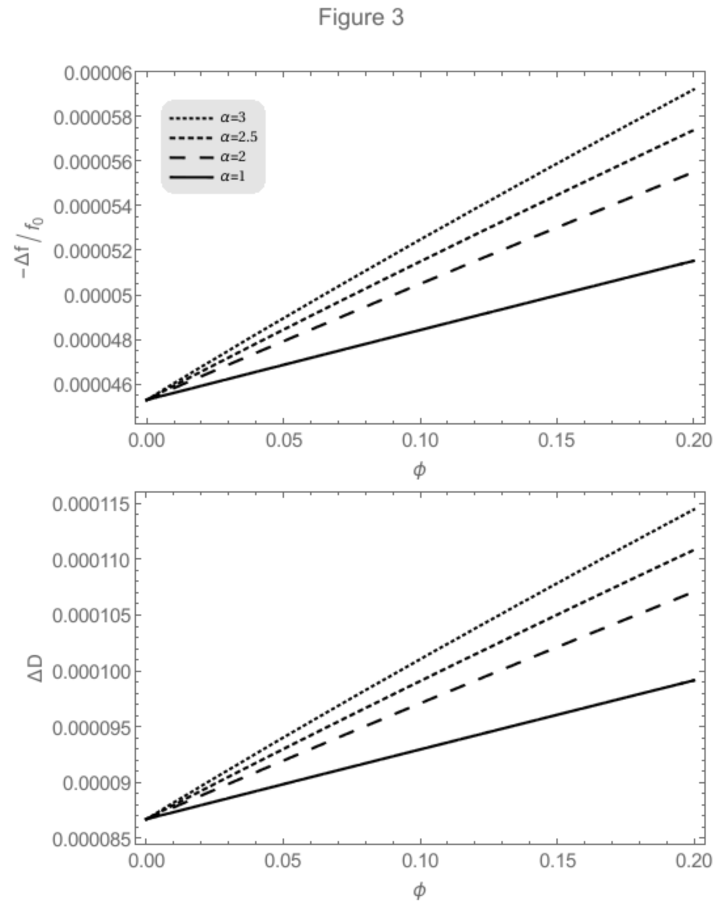


Figure 3
A QCM-D coated with a 10 nm PMMA-film, operating at a frequency *f*=1 MHz, in water contaminated by rigid PVC nanoparticles at different (low) concentrations ϕ. The nanoparticles affect the effective viscosity (as given by Einstein's expression) and density of the contaminated water. The density of rigid PVC is known, and the plot shows different shape factors α (α=2.5 corresponds to spherical nanoparticles).

Modeling QCM-D response in water colloids

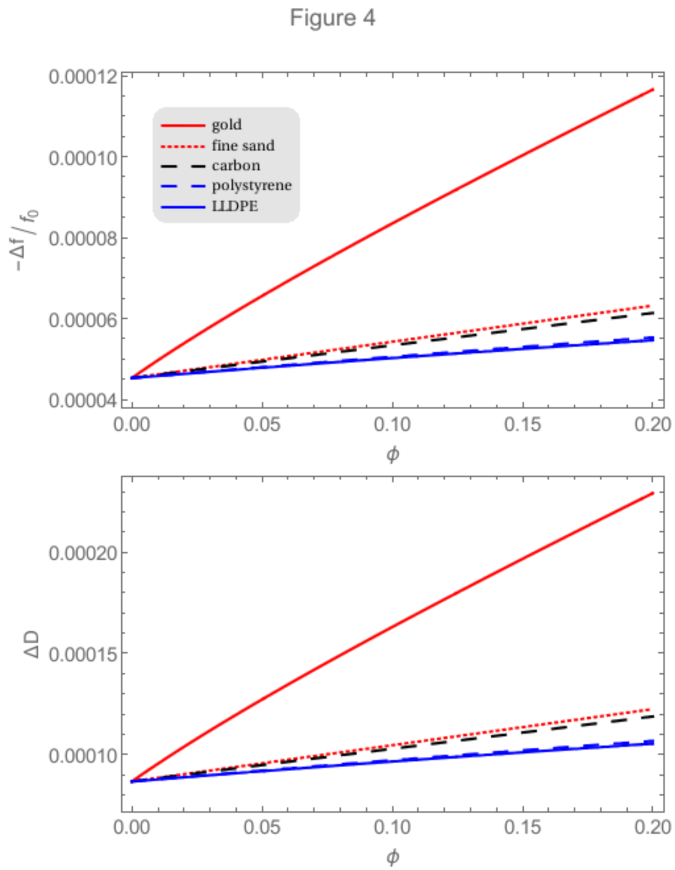
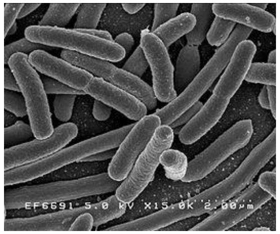


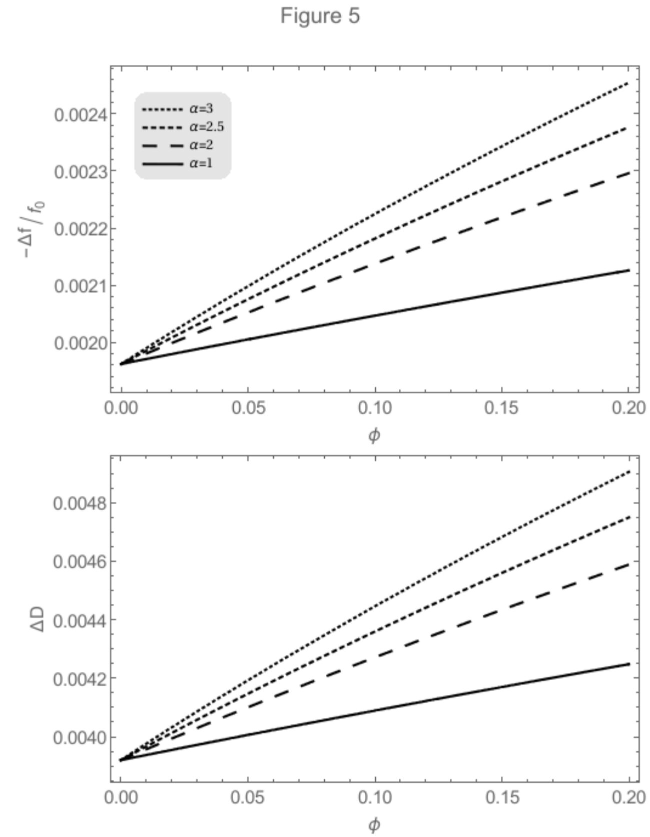
Figure 4

A QCM-D coated with a 10 nm PMMA-film, operating at a frequency *f*=1 MHz, in water containing spherical (shape factor α=2.5) nanoparticles at different (low) concentrations ϕ. The nanoparticles affect the effective viscosity (as given by Einstein's expression) and density of the water colloid. The plot shows different nanoparticle materials (specified by the nanoparticle mass density).

Modeling of QCM-D in water dispersions

- **Pollutant: model bacteria (E.Coli)**





- **Figure 5**
- A QCM-D coated with a 10 nm PMMA-film, operating at a frequency f=1 MHz, in glycerol containing E-coli bacteria at different (low) concentrations ϕ. The bacteria affect the effective viscosity (as given by Einstein's expression) and density of the glycerol colloid. The density of E-coli bacteria is known, and the plot shows different shape factors α.

Modeling the QCM-D response in water-glycerol dispersions

- Pollutant model NPs:
- Gold NPs
- Fine sand grains
- Carbon NPs
- Polystyrene
- LLDPE

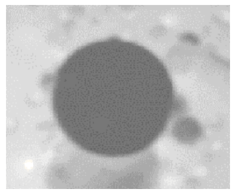


Figure 6

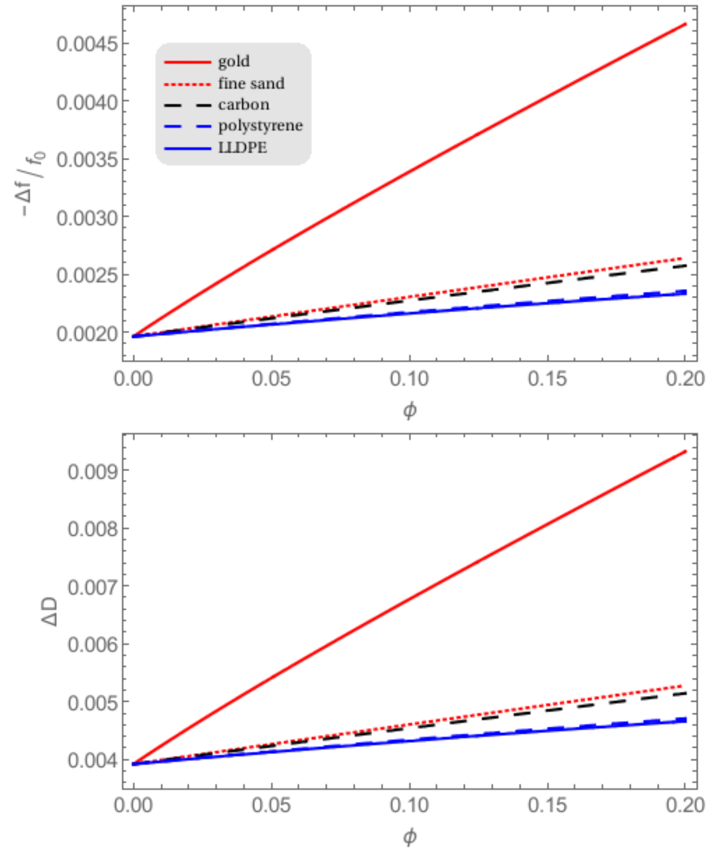


Fig.6. A QCM-D coated with a 10 nm PMMA-film, operating at a frequency f=1 MHz, in glycerol containing spherical (shape factor α=2.5) nanoparticles at different (low) concentrations ϕ. The nanoparticles affect the effective viscosity (as given by Einstein's expression) and density of the glycerol colloid. The plot shows different nanoparticle materials (specified by the nanoparticle mass density)

Modeling the QCM-D response in water dispersion. The NPs packing effect

Figure 7

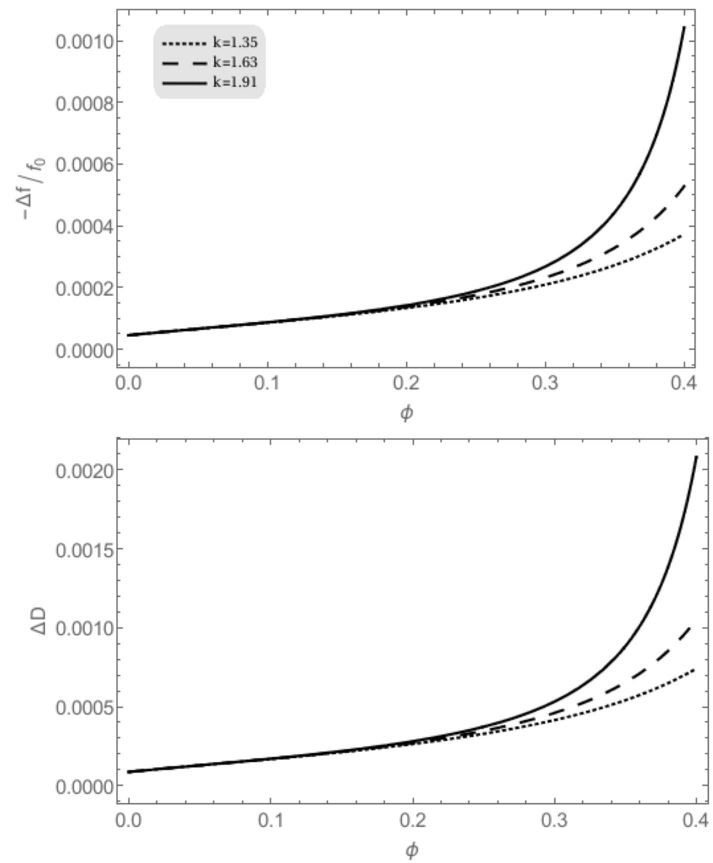


Figure 7

A QCM-D coated with a 10 nm PMMA-film, operating at a frequency *f*=1 MHz, in water containing spherical (shape factor α=2.5) gold nanoparticles at different concentrations ϕ (including high concentrations). The plot shows different packing factors *k.*

QCM-D modeling response

Model particles: fine sand grains

Water dispersion

Figure 8

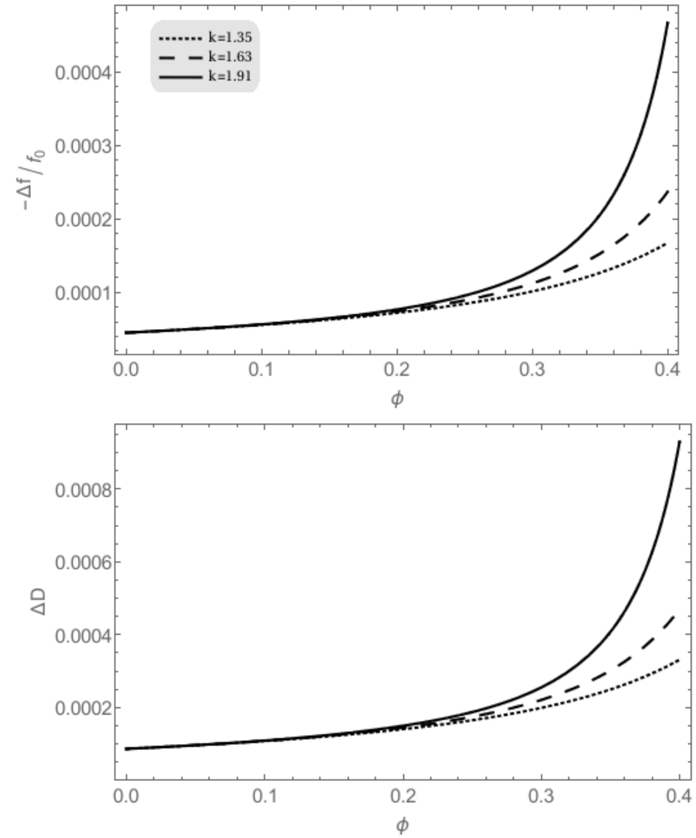
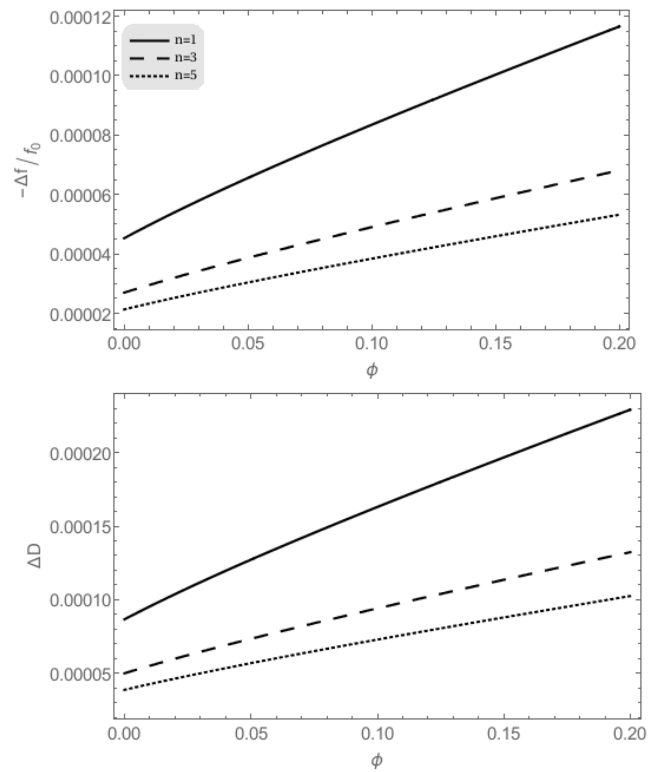


Figure 8
A QCM-D coated with a 10 nm PMMA-film, operating at a frequency f=1 MHz, in water containing spherical (shape factor α=2.5) fine sand grains at different concentrations ϕ (including high concentrations). The plot shows different fine-sand packing factors *k*.

Modeling the QCM-D in water dispersions The higher harmonics

Figure 9



- **Figure 9**
- A QCM-D coated with a 10 nm PMMA-film, operating at a frequency *f*=1 MHz, in water containing spherical (shape factor α=2.5) gold nanoparticles at different (low) concentrations ϕ. The nanoparticles affect the viscosity (as given by Einstein's expression) and density of the water colloid. The plot shows different overtones.
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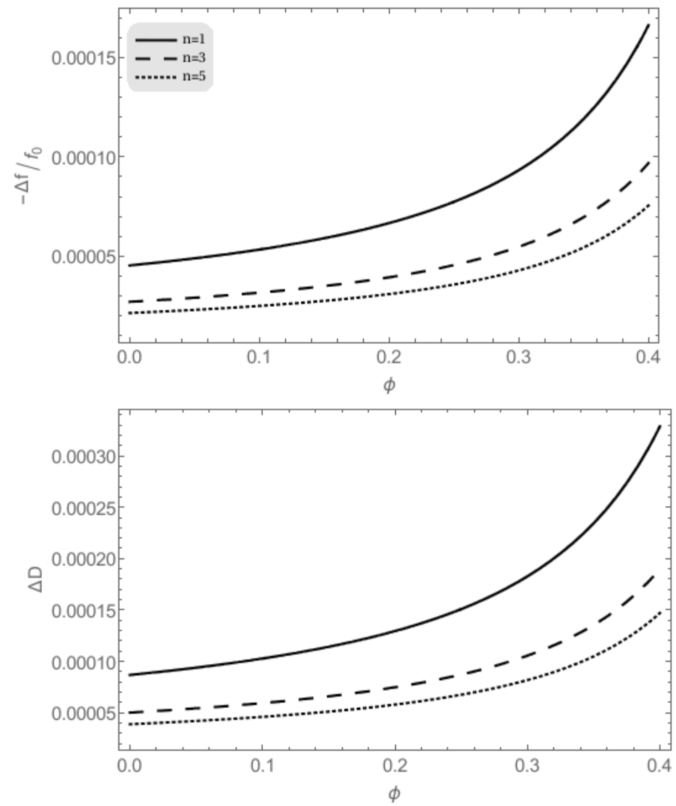
Modeling QCM-D response Microplastic NPs (PVC) water dispersions

Figure 10



- Fig.10. A QCM-D coated with a 10 nm PMMA-film, operating at a frequency *f*=1 MHz, in water contaminated by spherical (shape factor α=2.5) rigid PVC nanoparticles at different concentrations ϕ (including high concentrations). We assume the packing factor *k=1.50*. The plot shows different overtones

SUMMARY

- SH SSW: viscous loading amplifies the mass sensitivity: ‘missing mass” effect is revealed (described before for the coated QCM resonators operating in liquid environments)
- QCM-D: a new theoretical model for analysis of microparticles dispersed in liquid phase is developed.
- In the future practical applications, the general analytical expressions derived for the SSW- and QCM-D characteristics may be used as a basis software for the sensors improvement.

SUMMARY

- Predicting modeling: from the physico-mathematical analysis of the acoustical impedance derived for both SSW and QCM-D sensors we obtain the measurable characteristics $(\Delta v, \Gamma, \Delta f, \Delta D)$ as a function of the concentration of pollutant microparticles in water droplets. For non-spherical particles, the correction for the shape factor may be deduced from measurable characteristics

The analytical formulae in parallel with numerical calculations open a way to quantitative interpretation of the experimental measurements of aerosols, colloids, biological colloids to determine the level of pollution (mineral particles, dust, bioorganic dust, NPs).
In the future practical applications, the general analytical expressions derived for the SSW- and QCM-D characteristics may be used as a basis software for the sensors detection of pollutants in the humid air and water microdroplets.