Introduction

This is a program for the calculation of the cantilever dynamics in contact-resonance scanning probe microscopy techniques such as piezoresponse force microscopy, electrochemical strain microscopy and others. It is based on the following publications:

[1] **A theoretical model for the cantilever motion in contact-resonance atomic force microscopy and its application to phase calibration in piezoresponse force and electrochemical strain microscopy**

Stephan Bradler, Stefan Renato Kachel, André Schirmeisen, and Bernhard Roling, Journal of Applied Physics **120**, 165107 (2016); http://dx.doi.org/10.1063/1.4964942

[2] **Amplitude quantification in contact-resonance-based voltage-modulated force spectroscopy**
Stephan Bradler, André Schirmeisen, and Bernhard Roling, Journal of Applied Physics **122**, 065106 (2017); http://dx.doi.org/10.1063/1.4998435

[3] **Piezoresponse force and electrochemical strain microscopy in dual AC resonance tracking mode: Analysis of tracking errors**
Stephan Bradler, André Schirmeisen, and Bernhard Roling, Journal of Applied Physics **123**, 035106 (2018); https://doi.org/10.1063/1.5004472

The model uses a detailed description of the cantilever, including:

- lever and tip mass
- lever and sample tilt
- two-dimensional contact dynamics
- contact and air damping

as well as the five excitation types:

- vertical sample displacement
- longitudinal sample displacement
- local electrostatic force
- distributed electrostatic load
- base excitation

Furthermore, the program includes some useful features, for example:

- Resonance curve calculation
- Automated resonance peak analysis
- Lever shape calculation
- Determination of model parameters from experiment
- Automated simulation for a range of contact stiffnesses
- Dynamically adjustable peak width and damping strength
- Additional parameters such as laser spot positioning and tracking error
- Customizable C++ source file

Implemented functions

Input and output:

The parameters are loaded from the file Input.txt (Functions *ExtractParameter*, *load_input* and *load_input_experimental* in the code). The output is written in the file Calculated cantilever dynamics.txt. The tables in the output are determined by the four parameters AdjustParametersFromExperiment, ResonanceCurve, ContactStiffnessVariation and LeverShape. A positive value will execute and output the corresponding analysis, 0 (or negative numbers) will skip this step. Additional analysis can be performed by modifying the source file. Usually it is a good idea to include your input parameters in the output file (Functions *list_parameters* and *list_parameters_*experimental in the code).

Calculation:

The actual calculation for a given set of parameters is done by the function *calculate_A_and_phi* (calling the short functions *sgn* and *q*) in the code. This function calculates the periodical lever motion and its first three derivatives, which are all complex quantities due to the damping. For details see [1]. The amplitude and phase of the signal are given by the first derivative. This is done for single frequencies and is thus insufficient for describing resonance enhancement. When calculating the amplitude and phase for a number of frequencies, we get a resonance curve, which also allows us to find the resonance peak. This is done in the function *calculate_resonance_curve*. In order to extract the properties of the resonance peak according to the DHO model, theoretical DART analysis is performed in the function *calculate_DHO*. Unfortunately, the DHO model is only an approximation of the resonance peak and the test frequencies influence the result, see [3]. This is why the test frequencies are adjusted until they are symmetric around the resonance frequency in the function *converge_DHO*. For practical measurements it is often important to calculate the sensitivity of the signal towards the excitation. The function *calculate_sensitivities* gives the apparent vertical displacement as calibrated using static displacement (in pm) in terms of the excitation strength for the different excitation types. For the case of vertical sample displacement this is equivalent to the absolute shape factor, see [2].

Optimizing input to match experiment:

In many cases, not all of the model parameters are known or easily assessable. This is why the following functions were written to automatically adjust input parameters until the predefined output parameters are matched: *AdjustContactDamping* and *AdjustAirDamping* adjust damping parameters to match experimental Q factors. *AdjustMasses* calculates the lever mass and tip mass. This function requires the resonance frequencies and Q factors for the first two free resonances. It includes calculation of the air damping coefficient and calls the function *Predict_ffree2*. In a similar way, *AdjustContactStiffness* calculates the vertical and longitudinal contact stiffness as well as contact damping coefficients. The function requires the masses to be known (for example adjusted) as well as the contact resonance frequency and Q factor and the ratio between vertical and longitudinal contact stiffness.

Input parameters

Table: Parameters in the input file with explanation. NA = not available.

Parameter name in code	Parameter name in papers	unit	Explanation/function
L, H, w	L, H, w	m	Lever length, tip height, lever width
zeta, psi	ζ, ψ	radian	Lever angle, sample angle
k	k	N/m	Static lever stiffness
mT, mL	$m_T, m_L\ (m)$	kg	Tip mass, Lever mass
eta	η	1/s	Air damping coefficient
k1, k2	k_1, k_2	N/m	Vertical (1) and longitudinal (2) contact stiffness
g1, g2	γ_1, γ_2	Ns/m	Vertical (1) and longitudinal (2) contact damping coefficient
d1, d2	d_1, d_2	m	Vertical (1) and longitudinal (2) sample displacement
f0	f_0	N	Local electrostatic force
VACxDV	$V_{AC} * (V_{DC} - V_{surf})$	V^2	Used to calculate q(x)
u0	NA	m	Displacement at the cantilever base
epsilon_r, LaserPosition	ε_r, NA	-	Relative permittivity (i.e. 1 for air), laser spot position (i.e. 1 for tip end)
Df, TE	$\Delta f, TE$	Hz	Frequency spacing, tracking error
fStart, fStop, fStep	NA	Hz	Frequencies for resonance curve
AdjustDf	NA	-	Adjust Df in terms of the peak width
AdjustQAir, AdjustQContact	NA	-	Adjust damping coefficients to match defined Q factor
Precision, IntegrationSteps	NA	-	relative Precision in iterations, Steps for the numerical integration of q(x); suggest 1.0e-7 and 10000 to be safe
AdjustParmsFromExp, ResonanceCurve, ContactStiffnessVariation, LeverShape	NA	-	These define which analysis will be performed. A positive value means yes, 0 or a negative value means no. For ContactStiffnessVariation, the entered value defines the range.
ffree1, ffree2, fcr	NA	Hz	measured resonance frequencies: 1st free, 2nd free, (1st) contact
Qfree1, Qfree2, Qcr	NA	-	measured Q factors: 1st free, 2nd free, (1st) contact
csr	NA	-	contact stiffness ratio k2/k1
Min_k1, Max_k1	NA	N/m	Search range for k1. Used when adjusting k1 from experiment.

The program

The program (C++ source file) has three parts: (i) The header is just for defining everything. (ii) The main function determines what the program actually does. (iii) The functions are repeatedly called by the main and each other.

The main function does the following:

1. Create output file and header
2. Load parameters and write them in output file
3. If Active: Calculate model parameters from loaded experimental input, write results in output file
4. Find the resonance peak. If active: Write resonance curve in output file
5. Define a table for DHO parameters and sensitivities towards different excitation types
6. Calculate and list those parameters. If active: for different contact stiffness values
7. If active: Calculate the lever shape at the resonance frequency and write it in the output file

How to use the program

The program is meant to be a flexible tool. A lot can already be achieved by changing the input (Input.txt). A typical application might be the following:

If you want to calculate the sensitivity in an ESM or PFM experiment, just put the parameters in the parameter file. You likely won't know the masses, contact stiffness and damping parameters, but these can be automatically calculated from the measured resonance properties. During a scan, the contact resonance frequency varies, which can be described by the contact stiffness variation. You can then compare the simulated correlations between resonance frequency and sensitivity with the experimental correlation between resonance frequency and apparent amplitude. This can give you a clue which excitation type is the most likely, but beware of other correlations caused by contact angle or inhomogeneous material. Note that the method also applies to higher bending modes. Only the free resonance frequencies should always be the actual first and second free resonance frequency, otherwise the masses may be incorrectly adjusted. For more information, see [2].

If you want to do something else, feel free to adjust the source file. In most cases, modifying the main function should be enough. For example, you can easily create a loop in which you vary one parameter and see how it influences the DHO parameters.