

# An improved modeling and simulation tool for arbitrary coated surfaces – FilmDoctor goes Mathematica

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It has recently been shown [1, 2] that some important questions about the stability of coated surfaces, like

- Where and when do Hertzian cone cracks appear?
- How to dimension a certain contact measurement like a scratch test such that I will increase the probability of coating delamination for proper adhesion measurement?
- How does time dependent and/or high temperature behavior influence the phenomenological observations on stability and reliability of coated surfaces?

often require the use of very complex, inhomogeneous, multi-body and sometime even non-linear contact modeling. A more general modeling tool box allowing to use existing contact problem solutions for layered material to be quickly adapted or even extended in a very flexible manner to such broader consideration would therefore be of great help to the coating community.

With the help of Wolfram Research the authors have developed such a toolbox by the means of a combination of the contact mechanics software FilmDoctor® [3] and the Computer Algebra System Mathematica® [4] via a so called MathLink communication system.

This work will now show how the MathLink interface provided by Mathematica can be used to access the FilmDoctor software package from the Mathematica software. These approach allows to combine the well known Mathematica software (with all the optimization algorithms and it's GUI) with the fast analytical solutions for contact experiments provided by the software FilmDoctor. This could help a lot in the field of surface optimization for new materials or material combinations, multi-layered and gradient structures and intrinsic stress design, because not only more work can be done with the help of the computer, but also the construction of distinct or extended models does need significantly less time. Subsequently, with respect to optimum coating designs especially for industrial applications, the tool box allows narrowing down the search vector field for better performance, which will save time and money for testing and building prototypes.

The second part will show examples and some principle limiting effects regarding contact measurement options and results possible to obtain. By the means of small FilmDoctor derivatives like TestOptimizer [5] and LifeTimePredictor such principle limits, like materials regions not being accessible on principle with certain tests or how to properly apply the options of multiaxial contact experiments [6], have been derived. It will also be show how these tools can be used for quick and effective test dimensioning allowing to design contact measurements which truly give what one is interested in.

- [1] N. Schwarzer, From interatomic interaction potentials via Einstein field equation techniques to time dependent contact mechanics, submitted to Material Research Express, accepted Jan 2014
- [2] N. Schwarzer, Endlessly Touchable – the Next Generation of Surface and Coating Optimization, [www.siomec.de/pubs/2013/001](http://www.siomec.de/pubs/2013/001)
- [3] [www.siomec.de/FilmDoctor](http://www.siomec.de/FilmDoctor)
- [4] [www.wolfram.com/mathematica](http://www.wolfram.com/mathematica)
- [5] [www.siomec.de/TestOptimizer](http://www.siomec.de/TestOptimizer)
- [6] N. Schwarzer, J. Mater. Res., Vol. 24, No. 3, March 2009, 1032 – 1036