Modeling approach for CVD-Diamond based mechanical structures

P. Schmid, M. Adamschik, S. Ertl, P. Gluche and E. Kohn

Department of Electron Devices and Circuits, University of Ulm
89069 Ulm, Germany, schmid@ebs.e-technik.uni-ulm.de

ABSTRACT

In this study, mechanical structures based on polycrystalline diamond films grown on silicon substrate are investigated. In contrast to all-silicon MEMS, additional problems arise due to the unusual properties of diamond. These effects are investigated by modeling diamond-based micro-mechanical devices and comparing the results to measurements on processed devices.

All simulations were carried out using the standard simulation tool ANSYS and measured modeling parameters.

Keywords: Diamond, CVD, Stress

INTRODUCTION

Diamond is well suited for sensor and actuator applications because of its outstanding mechanical and thermal properties (see table 1) [1]–[7]. Especially the almost strain independent elasticity, the high fracture strength and hardness, together with a high thermal conductivity makes it an ideal material for mechanical micro structures. The resistivity of diamond ranges from 10 mΩcm up to $10^{14}\Omega$cm, depending on doping. It can therefore be used as an insulator, semiconductor and almost metal-like conductor, allowing the fabrication of various all-diamond devices. Since boron-doped diamond also shows a piezoresistive effect [8], piezoresistors can be fabricated to read out the strain signal. In addition, diamond is chemically inert and can thus be used in hazardous environments or in bio-medical applications. Diamond devices can operate at very high temperatures without degradation of device performance [2], [9].

The Chemical Vapor Deposition (CVD) technique allows growth of high quality diamond films with mirror-like surface finish on Si-substrate [10], [11], making it compatible to standard silicon MEMS-technologies and even suitable for monolithic integration with Si circuits.

However, the largely different properties (like Young's modulus or thermal expansion coefficient) of diamond and the substrate material silicon cause problems not observed in all-silicon MEMS. Especially additional stress components are incorporated in the diamond film itself due to the special growth conditions. The diamond CVD-process on silicon consists at least of two distinctly different growth steps [10], [11], a nucleation and an outgrowth step, resulting in a layered film with individual sub-layers of different properties. Stress in diamond films is also highly dependent on the desired film quality (nano-crystalline, random oriented or highly oriented (HOD)) [12], [13]. In this investigation, mainly highly-oriented diamond films, which consist of textured and 100-oriented grains, were used. These high quality films exhibit properties, which are comparable to monocrystalline diamond [10], [11].

Table 2: Modeling parameters

	Diamond	Silicon
Young's modulus	750 GPa	170 GPa
Poisson ratio	0.07	0.27
Therm. exp. coeff.	see fig. 3	

In this study, the influence of the different material parameters and the built-in stress on the performance of diamond-based MEMS is investigated. The following examples of diamond devices are chosen:

- The influence of the small Young's modulus of the silicon substrate on the strain distribution, when used as a suspension for diamond cantilevers
- The influence of the diamond film / Si interfacial stress developed during growth due to thermal contraction on the performance of a diamond membrane pressure sensor
- The influence of the built-in stress of diamond cantilevers on the threshold voltage of diamond micro-switches

All simulations were carried out using the standard ANSYS software. The results are compared to measurements on processed devices. Since the material parameters of polycrystalline diamond films are highly dependent on the growth process, data found in the literature (especially for Young's modulus) must be used with caution. Therefore most of the parameters used for the simulations were measured or determined by fitting modeling results of test structures to measurement results. A summary of the parameters used is shown in table 2.

Table 1: Properties of diamond compared to silicon

	Silicon (mono)	Silicon (poly)	Diamond (ideal)	Diamond (poly)
Therm. Conduct. [W/cmK]	1.5	0.3-1.2	20	4-15
Young's modulus [GPa]	190	$\leq$170	1050	$\leq$850
Fracture Strength [GPa]	1.4	$\leq$1.2	10.3	$\leq$4.8
Hardness [Mohs]	7		10	
Debye Temp. [°C]	350		1830	

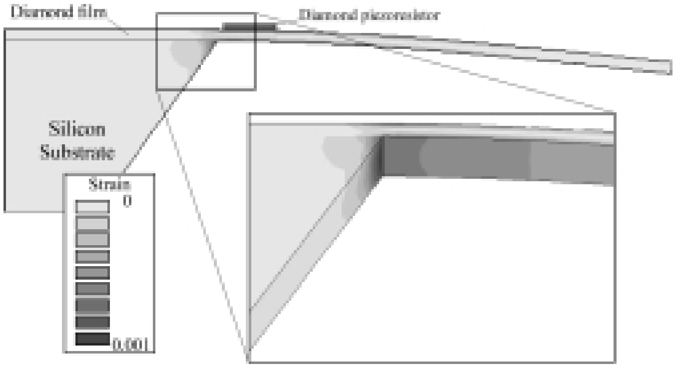

Figure 1: Strain distribution in a diamond cantilever on silicon substrate

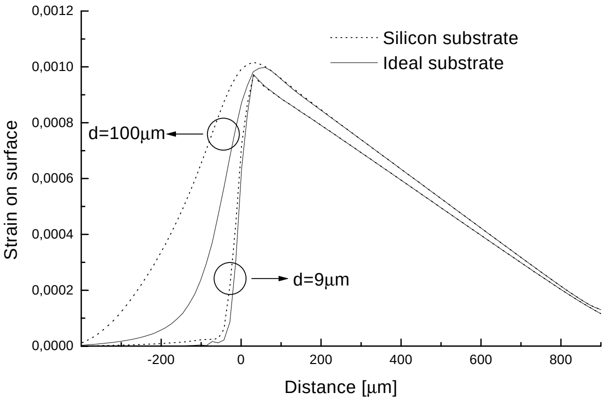

Figure 2: Surface strain of diamond cantilever on silicon and ideal substrate (film thickness 9 μm and 100 μm)

DIAMOND CANTILEVERS

Due to the relatively small Young's modulus of silicon, the substrate material, which serves as a suspension for the free standing diamond structures (e.g. cantilevers), is distorted, when the cantilevers are bent. This distortion may influence the strain distribution in the diamond films and therefore the performance of the devices. Since diamond piezoresistors on the surface of the cantilever are used to read out the device signal, especially the surface strain distribution is important. Figure 1 shows a cross-section view of the structure. The modeled strain distribution is also shown in this figure. As can be seen, the silicon is distorted due to the high Young's modulus of the diamond film. Figure 2 compares the strain distribution of a diamond film on silicon and on an ideal, i.e. non-deformable, substrate for different diamond film thicknesses. As can be seen, the strain distribution on the surface of the film is only slightly influenced by the substrate material, even for thick diamond films. Thus the output signal of such devices is not influenced by the substrate material.

At higher temperatures however, at which diamond may still be fully elastic [2], the silicon suspension may already show plastic deformation. Therefore, for these high temperature applications, different concepts have to be developed, e.g. using SiC substrates.

DIAMOND MEMBRANES

Diamond films are usually grown at a temperature of approx. 700°C. Due to the largely different thermal expansion coefficients of diamond and silicon (see figure 3), the diamond film is distorted when cooling the samples from the growth temperature to R.T. In case of a diamond membrane, this effect is shown in figure 4.

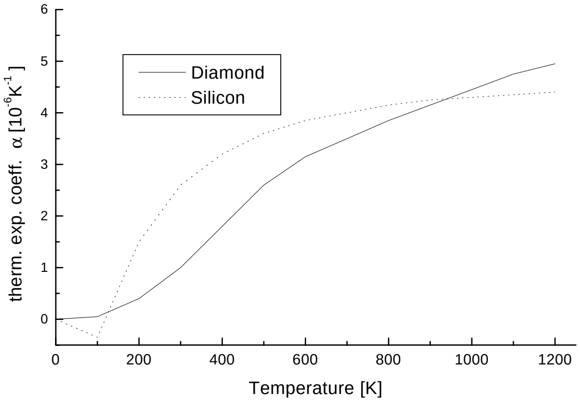

Figure 3: Thermal expansion coefficients of diamond and silicon (after [1])

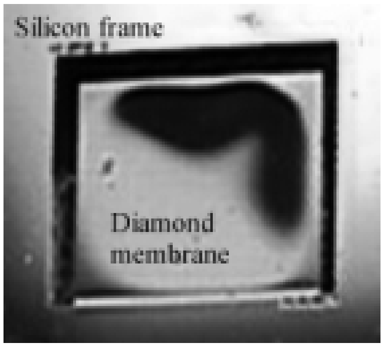

Figure 4: Diamond membrane on silicon substrate

This strong bending leads to a hysteresis when deflecting the membrane, e.g. when used as a pressure sensor. The strain distribution in such a membrane pressure sensor for zero applied pressure is shown in figure 5. The modeling and measurement results of the pressure-deflection behaviour of the sensor are shown in figure 6. For the simulation, only the stress component due to the thermal contraction was considered (by modeling the cooling process according to the thermal expansion coefficients shown in figure 3), other stress components were neglected. As can be seen, the simulated results agree quite well with the measured characteristics, proving that the main stress component for this case is caused by thermal contraction of the substrate. Especially, non-uniform stress components in the film itself would lead to an asymmetric hysteresis curve, which is not observed.

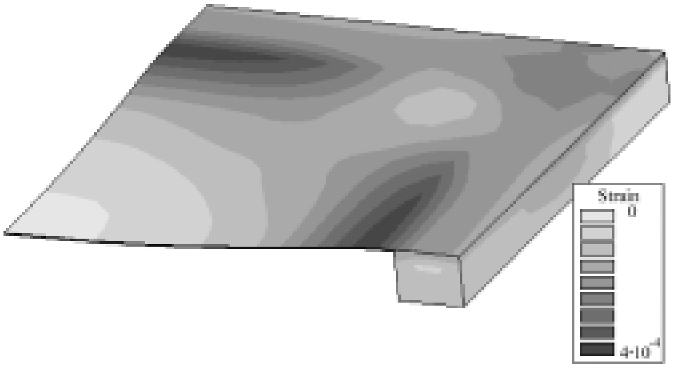

Figure 5: Strain distribution in a distorted membrane pressure sensor for zero applied pressure (pressure decreasing)

DIAMOND MICROSWITCHES

In this section, the influence of the built-in stress in free-standing diamond cantilevers is discussed. As an example, diamond microswitches are chosen. Figure 7 shows the cross section of such a device. The cantilever is deflected by an electric field across the air gap. Due to the built-in stress in the diamond film, the cantilever is strongly bent, as can be seen in figure 8. This effect influences the threshold voltage of the device. The voltage dependent deflection of the switch was modeled, with and without the effect of built-in stress. The simulation procedure is iterative, since the deflection influences the electric field distribution in the air gap and therefore electrical and mechanical simulations are strongly coupled. The built-in stress distribution was obtained by fitting the simulation to the measured bending curve.

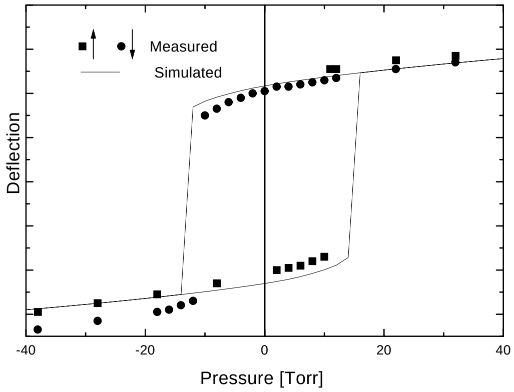

Figure 6: Modeled and measured characteristics of a diamond membrane pressure sensor

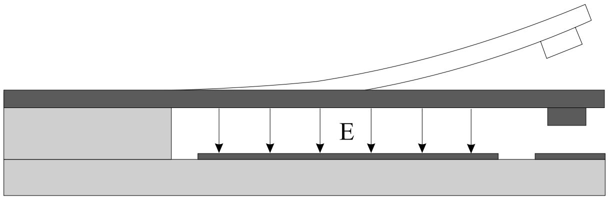

Figure 7: Cross section of a diamond microswitch

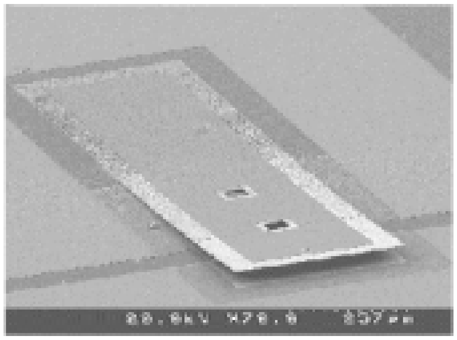

Figure 8: Bending in a diamond microswitch device

The simulation results are shown in figure 9. The measured threshold voltage is also given, showing that the characteristics of the device can be well modeled by this simple approach.

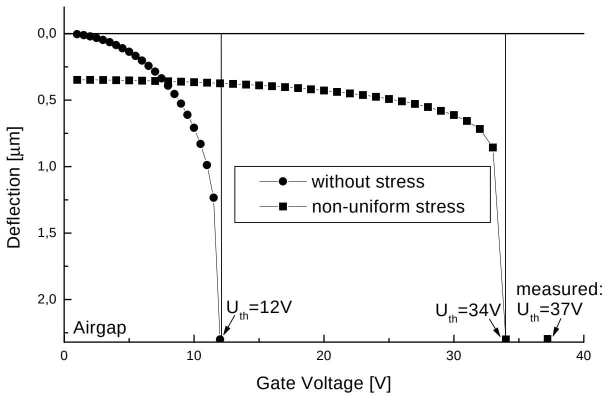

Figure 9: Modeled characteristics of a diamond microswitch with and without non-uniform built-in stress

SUMMARY

Micromechanical devices based on CVD-grown diamond have been modeled and measured to investigate the problems of this promising technology related to the special properties of polycrystalline diamond. It has been shown that though the properties are complicated, not fully reproducible yet and not fully understood in detail either, the characteristics of these devices can be modeled to the first order by using approaches, where only one parameter is dominating.

REFERENCES

[1] O. Madelung, "Semiconductors", Springer, 1991

[2] M. Werner, S. Klose, F. Szücs, Ch. Moelle, H.J. Fecht, C. Johnston, P.R. Chalker, I.M. Buckley-Golder, "High temperatures Young's modulus of polycrystalline diamond", Diamond Rel. Mat. 6 (1997), 344-347

[3] "Handbook series on semiconductor parameters", World Scientific Publishing Co. Pte. Ltd., 1996

[4] "MEMS Material Database", WWW, URL: http://mems.isi.edu/mems/materials/, Jan. 1999

[5] De Beers Industrial Diamond Division, "Properties of Diamond"

[6] H. Verhoeven, A. Flöter, H. Reiß, R. Zachai, D. Wittorf, W. Jäger, "Influence of the microstructure on the thermal properties of thin polycrystalline diamond films", Appl. Phys. Lett. 71 (10), 1997, 1329-1331

[7] P. Gluche, M. Adamschik, A. Vescan, W. Ebert, F. Szücs, H.J. Fecht, A. Flöter, R. Zachai, E. Kohn, "Application of highly oriented, planar diamond (HOD) films of high mechanical strength in sensor technologies", Diamond Rel. Mat. 7, 1998, 779-782

[8] O. Dorsch, K. Holzner, M. Werner, E. Obermeier, R.E. Harper, C. Johnston, P.R. Chalker, I.M. Buckley-Golder, "Piezoresistive effect of boron-doped diamond thin films", Diamond Relat. Mater. 2, 1993, 1096-1099

[9] E. Kohn, W. Ebert, A. Vescan, "Devices at High Temperatures – Status and Prospects", Israel Journ. of Chemistry, Vol. 38, 1998, 105-112

[10] A. Flöter, H. Güttler, G. Schulz, D. Steinbach, C. Lutz-Elsner, R. Zachai, A. Bergmaier, G. Dollinger, "The nucleation and growth of large area, highly oriented diamond films on silicon", Diamond '97 Conference, Edinburgh, UK, 1997

[11] S.D. Wolter, T.H. Borst, A. Vescan, E. Kohn, "The nucleation of highly oriented diamond on silicon via an alternating current substrate bias", Appl. Phys. Lett. 68 (25), 1996, 3558

[12] J. Michler, Y. von Kaenel, J. Stiegler, E. Blank, "Complementary application of electron microscopy and micro-Raman spectroscopy for microstructure, stress and bonding defect investigation of heteroepitaxial chemical vapor deposited diamond films", J. Appl. Phys. 83 (1), 1998, 187-197

[13] Y. von Kaenel, J. Stiegler, J. Michler, E. Blank, "Stress distribution in heteroepitaxial chemical vapor deposited diamond films", J. Appl. Phys. 81 (4), 1997, 1726-1736