(Electro)chemically induced stress effects in porous silicon nanostructures

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Stress effects are relatively well identified and studied in the case of bulk mono-, poly-crystalline and amorphous silicon. High stress values can provoke structural deformations and defects at the near-interface (near-surface) regions without remarkable changes of physical properties of the bulk silicon substrates. However, if at least one of the dimensions of the substrates (for example, at least thickness, in the case of thin films) becomes comparable or less than that of the stress affected near-interface region, it can lead to significant modifications of almost all physical properties of such low dimensional structures. Therefore, study of stress ant its influence on the properties of the low dimensional structures are of the first importance.

The low dimensional (1D, 0D) silicon nanocrystallites constituting porous silicon nanostructures (see figure 1) obtained by electrochemical dissolution (anodization in HF based solutions) [1] of monocrystalline silicon substrates are strongly affected by stress appearing after their formation. We present the nature of the initial stresses and stress induced structural relaxation effects in an as-prepared nanostructured porous silicon taking into account recent X-ray diffraction and Raman scattering results. An amazing stress relaxation effect in porous Si/SiC heterostructure formed by the anodization process is also reported.

We describe the stress evolution when the chemical composition of the Si nanocrystallites surface and pores inside the nanostructured porous layers is modified. In particular, the influence of nanocrystallites hydrogen coverage, low temperature oxidation and pores filling with ethanol on nanoscale stress level is studied by micro-Raman scattering spectroscopy. As an example, figure 2 shows the influence of the ethanol filling the nanopores of meso-porous Si on Raman peak position. The observed peak shift indicates on decrease of the initial tensile stress on 200 MPa. After complete ethanol evaporation from the pores, Raman peak returns back to its initial position corresponding to the nanocrystallites state before ethanol condensation inside the pores. Thus, the effect seems to be reversible indicating on its elastic nature.

The influence of the stress effects ensured by low temperature oxidation on optical and mechanical properties of porous Si nanostructures were observed by IR reflective spectroscopy and 3D topography profilometer (see figure 3), respectively. Oxidation induced anisotropic stress relaxation effect is simulated (figure 4) by finite element software taking into account anisotropic mechanical properties of the meso-porous silicon nanostructure.

[1] A. Halimaoui, in *Properties of porous silicon*, edited by L. T. Canham (INSPEC, The IEE, London, United Kingdom, 1997), p. 12.

Figure 1. SEM cross-sectional view of a porous Si nanostructure formed by electrochemical anodization of bulk monocrystalline Si substrate.

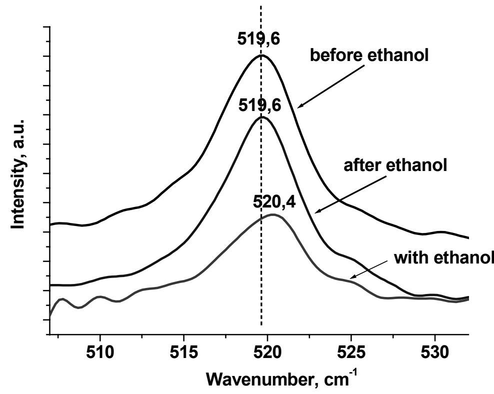

Figure 2. Stress effect on the Raman scattering spectrum of meso-PS layers resulting from filling of pores with ethanol at ambient temperature and pressure.

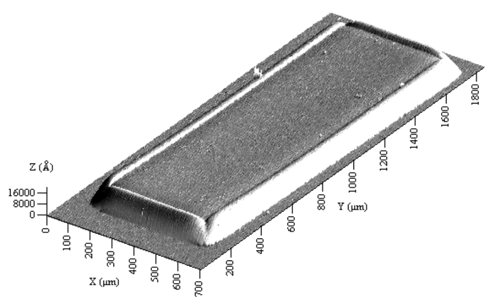

Figure 3. 3D profilometer picture showing oxidation induced anisotropic stress relaxation in a patterned meso-porous silicon nanostructure

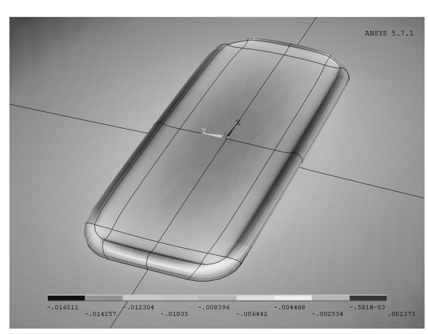

Figure 4. 3D finite element simulation of the oxidation induced stress relaxation effect in a patterned meso-PS nanostructure