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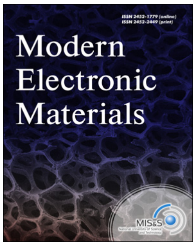

Stress topology within silicon single-crystal cantilever beam

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Abstract
Flexural elastic deformations of single-crystal silicon have been studied using microspectral Raman scattering. Results are reported on nano-scaled sign-changing shifts of the main peak of the microspectral Raman scattering within the single-crystal silicon cantilever beam during exposure to flexural stress. The maximum value of Raman shift characteristic of the 518 cm^{-1} silicon peak at which elasticity still remains has been found to be 8 cm^{-1} which corresponds to an applied deformation of 4 GPa. We report three-dimensional maps of the distribution of internal stresses at different levels of deformation up to irreversible changes and brittle fracture of the samples that clearly show compression and tension areas and an undeformed area. A qualitative explanation of the increase in the strength of the cantilever beam due to its small thickness (2 μm) has been provided that agrees with the predictions of real-world physical parameters obtained in SolidWorks software environment with the SimulationXpress module. We have defined the relative strain of the beam surface which was 2% and received a confirmation of changes in the silicon lattice parameter from 0.54307 nm to 0.53195 nm by the BFGS algorithm.

Introduction

Raman spectroscopy (RS) of semiconductor materials and devices delivers valuable data on phonon frequencies, electron state energies, electron-phonon interactions, carrier concentration, impurity concentration, crystalline structure, crystal orientation, temperature and mechanical stresses. RS' capabilities are finding ever greater demand due to the significant complexity of technical solutions (beam and ion implantation doping etc.) of new generation electronics devices especially in nanoelectronics and nano- and microelectromechanical devices (NEMS and MEMS). As the working dimensions decrease, elastic stresses develop that affect significantly the operational and functional parameters of new micro- and nanoelements.

Micro-Raman spectroscopy (MRS) allows studying localized mechanical stresses in multilayer elements of ICs. For example, an IC containing 240 × 50 nm^2 silicon nitride (Si_3N_4) strips separated from the silicon substrate by SiO_2

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and polycrystalline silicon nanolayers, 10 nm in thickness and 9.4 μm in width, exhibited a Raman shift of about ± 4 cm^{-1} [1]. This confirms the practical value of this control and diagnostic tool. In highly integrated solar cells on the basis of single or polycrystalline silicon doped with B or Al, MRS and microphotoluminescence with a resolution of up to 500 nm revealed interaction of optical phonons with compression or tension stress caused defects that had never been found using any other methods before [2].

The effect of single-axis compression stress on the Raman shift in single crystal silicon was studied [3]. Stresses in an approx. 3″ 600 nm thick film were produced by pressing to the surface of large radius cylinders (0.5-1 m). For 0.5 m radius the shift caused by laser excitation at $\lambda = 325$ nm with a 9 nm penetration depth into silicon was 0.4 cm^{-1}. The distribution of Raman shift is quite illustrative and informative unlike infrared and electron microscopies and X-raying which are also used. MRS was used [3] to study the surface of a Si(111) plate nanostructured and amorphized with ultrashort excimer laser pulses. The stresses were represented as microdistributions of Raman shift suggesting localization of hexagonal Si (510 cm^{-1}) and α-Si (490 cm^{-1}).

The effect of elastic deformations on the phonon spectrum typical of sodium chloride was studied [4] using computer simulation with a molecular dynamics method. The calculations were made for two crystal deformation modes: uniform tension/compression and pure shift. It was shown that these deformations cause transformation of the phonon state density whereas the localized oscillation modes, the so-called discrete breathers, only depend on the former deformation type (uniform tension/compression) and shift deformation does not influence them. The authors [4] noted that it is elastic deformation that shows itself during the study of mechanical properties of single crystals by indentation under $0.1 \leq P \leq 1$ N load when the indenter trace forms.

Below we will analyze our results on the sign-variable shifts of the main combination scattering peak (518 cm^{-1}) in single crystal silicon and the topology of elastic stresses during localized deformations of up to 4 GPa obtained using nanosized selected area spectral analysis.

Experimental

We carried out nanoscale studies of sign-variable shifts of the 518 cm^{-1} combination scattering peak typical of a silicon cantilever beam during exposure to flexural stress.

To study the distribution of the micro- and nano-deformations in the cantilever beam we used a confocal microscope and an OmegaScope Raman microspectrometer integrated with an AIST-NT atomic force microscope (Zelenograd City). The confocal microscope was used to select an area for precision positioning of the semiconductor laser excitation radiation on the deformed cantilever beam.

The MRS study was carried out at $\lambda = 473$ nm, 25 mW, with a special resolution of 425 nm. The spectral resolution of the microspectrometer was 0.8 cm^{-1}.

Flexural deformations were detected with the confocal microscope. The measurement area on the cantilever beam was chosen using the confocal microscope (10 ×) with a 0.28 digital aperture. This optical resolution allowed us to achieve precision visualization and select an area for plotting hyperspectral Raman shift distribution maps for different cantilever beam flexure.

The reference material for MRS stress distribution study was single crystal Si(100) having one clear Raman line at 518 cm^{-1}. The test object was a cantilever beam with microscopic sizes typical of cantilevers: $135 \times 35 \times 2$ μm^3.

To study flexure deformations of single crystal silicon we used two cantilevers of the same type: semi-contact fpN11 with a rigidity of 5.3 N/m. One of the cantilevers (the test one) was installed into an ACM AIST-NT SmartSPM holder. The other cantilever was used as a thrust and rigidly fixed on a scanator (Figure 1a). We moved the second cantilever at a microscopic scale in the desired direction to produce flexural deformations of the fixed cantilever beam. The scanator movement speed was preset in software. We set the movement step taking into account the minimum resolution of Raman spectral lines and hardware spectral resolution (0.8 cm^{-1}). The step was 20 μm. the actual flexure of the cantilever beam is shown by its confocal image (Figure 1b).

The maximum stroke of the beam free end was more than 100 μm. During all the deformation measurements the beam remained elastic as confirmed by it recovery after unloading. The greatest beam flexure was achieved at a 4.5 GPa pressure.

Micro-Raman spectra were mapped with an AFM indexer [5]. The hyperspectral data for the 518 cm^{-1} peak typical of silicon were obtained with a 100 × objective, 0.7 digital aperture. Note that the cantilever scanning area in the AFM (100 × 100 μm^2) is much greater than the transverse size of the cantilever beam. This allowed us to form an array of 900

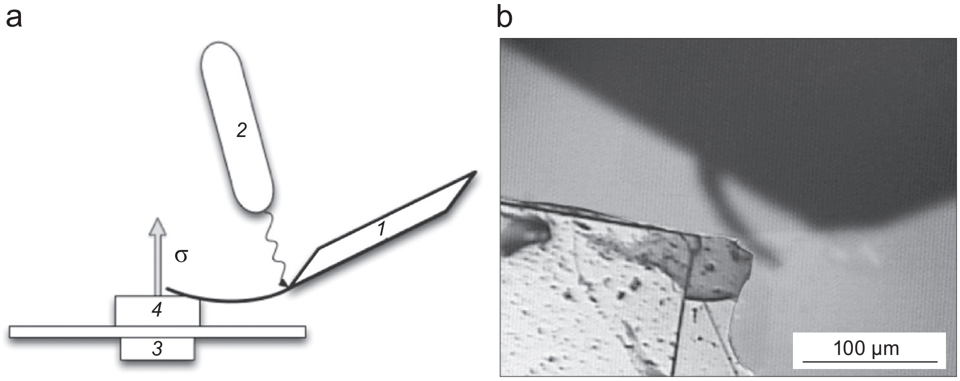

Figure 1 (a) Schematic of flexural deformation of a cantilever beam and (b) its confocal microscope image: (a): (1) cantilever beam (first), (2) source and laser excitation radiation, (3) scanator with sample holder, and (4) thrust of cantilever (second).