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Supporting Information: Photoinduced cubic-to-hexagonal polytype transition in silicon nanowires†

S.P. Rodichkina[a,b], V. Lysenko[b], A. Belarouci[b], I. Bezverkhnyy[c], R. Chassagnon[c], M. Isaiev[d,e], T. Nychyporuk[b], V. Yu. Timoshenko[a,f,g]

[a] Lomonosov Moscow State University, Faculty of Physics, Leninskie Gory 1, 119991 Moscow, Russia.
[b] University of Lyon, Nanotechnology Institute of Lyon, UMR CNRS 5270, INSA de Lyon, F-69621, France.
[c] Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Universite de Bourgogne-Franche Comte, 21078 Dijon Cedex, France.
[d] Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Str., Kiev 01601, Ukraine.
[d] Laboratoire LEMTA, Faculte des Sciences et Technologies, CNRS UMR 7563, Universite de Lorraine, BP 70239, 54506 Vandoeuvre les Nancy Cedex, France.
[f] National Research Nuclear University 'MEPhI' (Moscow Engineering Physics Institute), PhysBio Institute, Kashirskoe sh. 31, 115409 Moscow, Russia.
[g] Lebedev Physical Institute of the Russian Academy of Sciences, Leninskiy Prospekt 53, 119991 Moscow, Russia.

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1 Simulation of temperature profile along SiNWs under photoexcitation

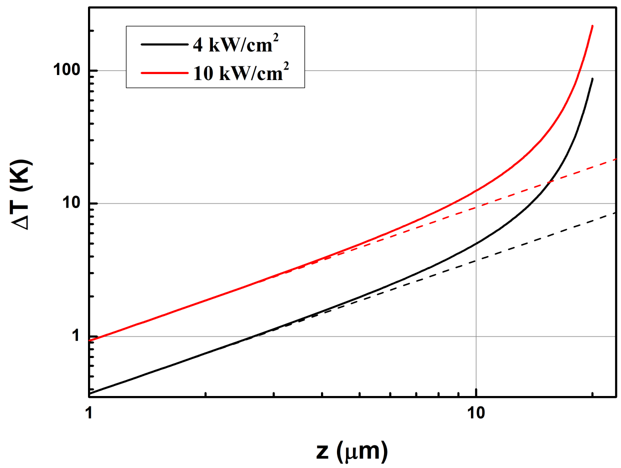

Fig. 1 Heating profile along SiNWs for the laser excitation intensities of 4 and 10 kW/cm^2, required for the LO-TO phonon splitting and hex-Si phase formation, respectively. The dashed lines show the linear $\sim z$ dependence.

Fig. 1 shows the simulated profile of ΔT along SiNWs under photoexcitation. The profiles were obtained by the finite element method, considering SiNWs as a homogeneous medium, heated at the top side by a heat flux with an area and intensity equal to that of the laser radiation, the SiNWs/c-Si interface was maintained at room temperature. The steady-state heat equation was solved in the three-dimensional case, z-axis was directed along SiNWs with $z = 0$ at SiNWs/c-Si interface and $z = 22$ μm at SiNWs tips, which were heated by the heat flux. From the figure one can see the linear dependence of ΔT on coordinate z for $z < 10$ μm, while the strong temperature gradient is observed in the upper part of SiNWs with $z > 10$ μm, which is responsible for the hex-Si phase formation in SiNWs. The values of the temperature gradient at SiNWs tips are equal to 50 and 100 K/μm for the laser intensities of 4 and 10 kW/cm^2, respectively. The effective thermal conductivity coefficient of SiNWs array, estimated at laser intensities < 4 kW/cm^2, is of about 0.8 W/(m K).

2 Role of the temperature gradient in c-Si $\rightarrow$ hex-Si phase transition in SiNWs

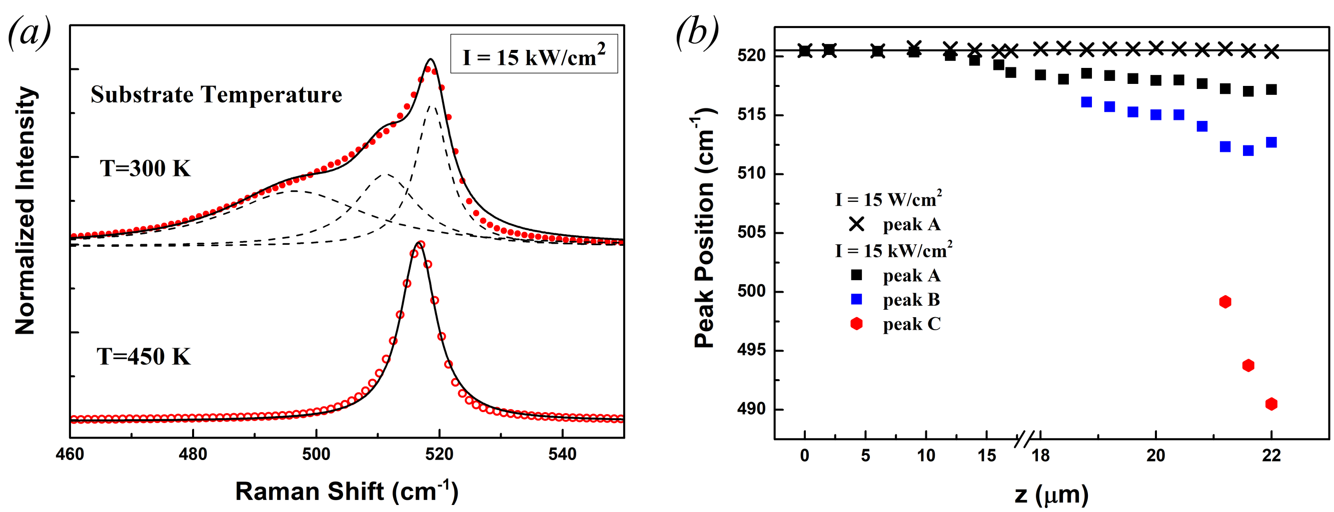

Fig. 2 (a) Raman spectra at the high laser intensity of 15 kW/cm^2 for SiNWs samples with the c-Si substrate at room temperature (upper spectrum) and heated to 450 K (bottom spectrum). (b) Dependence of the spectral position of the Raman peaks of SiNWs as a function of a distance between the c-Si substrate and the heated part of SiNWs. The dependence was measured both at low (15 W/cm^2, black crosses) and high (15 kW/cm^2) laser intensity.

Fig. 2 illustrates the role of the inhomogeneous heating-induced mechanical stresses in the formation of the hex-Si phase in SiNWs under photoexcitation. The destruction of the temperature gradient in SiNWs by thermal heating of the underneath Si substrate or the decrease of the distance between the heated part and the substrate (by scanning the laser beam along nanowires) leads to a disappearance of the Raman peak C, corresponding to the hex-Si phase, as well as to a disappearance of the LO-TO phonon spectral splitting.

3 Analysis of the relative integrated intensities of the Raman peaks of SiNWs

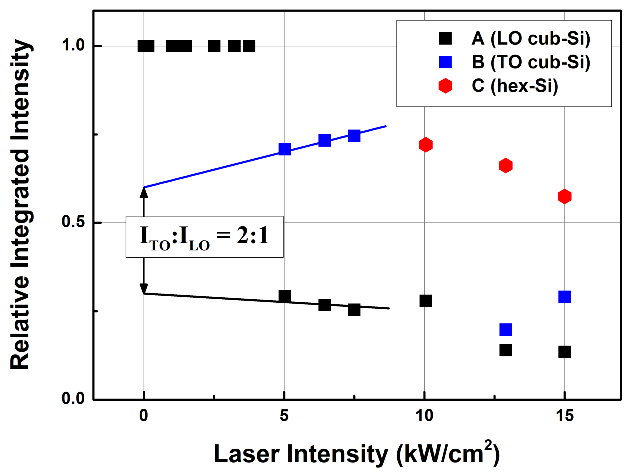

Fig. 3 Relative integrated intensity of the Raman peaks of SiNWs as a function of the laser intensity.

Fig. 3 shows the relative integrated intensity of the Raman peaks of SiNWs as a function of the laser intensity. The change in the relative intensity between LO and TO Raman peaks of c-Si with the laser intensity for $I < 10$ kW/cm^2 can be related to the increase in spectral distance between the peaks which leads to a change in the ratio of the number of phonons for LO and TO modes. The linear extrapolation exhibits the 2:1 ratio between LO and TO phonon intensities at $I = 0$, where no phonon splitting occurs, that corresponds to the two-fold degenerate TO mode in Si. The decrease in the relative contribution of peak C at $I > 10$ kW/cm^2 can be related to the redistribution of the light in SiNWs array due to the thermal heating of SiNWs under high photoexcitation.