Dopant activation mechanism of Bi wire-δ-doping into Si crystal, investigated with wavelength dispersive fluorescence X-ray absorption fine structure and density functional theory

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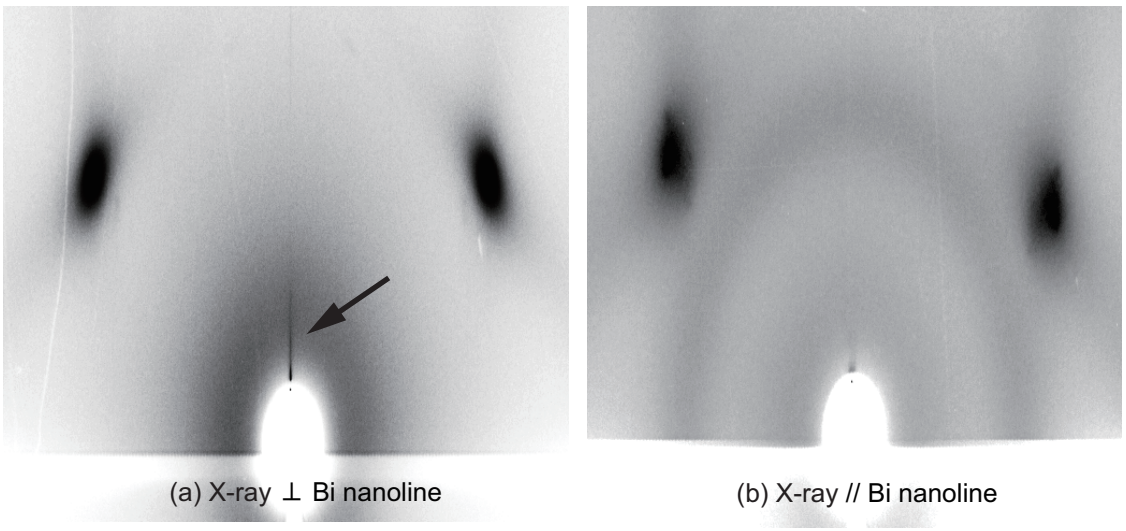

FIG. 1. X-ray diffraction patterns for Bi nanolines with an amorphous Si cap. Patterns are magnified around the direct-beam positions. Incident X-rays were (a) perpendicular and (b) parallel. A long specular spot is only observed in (b), indicating that the one dimensional nature remains.

A. XRD pattern of buried Bi nanoline in amorphous Si

X-ray diffraction patterns for Bi nanolines with an epitaxial Si cap have been reported in the literature [1]. In this case, streaking patterns of $k = 0, \pm 0.5$ are observed, meaning that double periodicity remains. This is in contrast to the XRD patterns for Bi nanolines with an amorphous Si cap, as shown in Fig. 1. A long specular spot is only observed for an incident X-ray perpendicular to the Bi nanoline, indicating a one dimensional feature without double periodicity. Since Bi nanolines on Si(001) have a double periodicity, this supports the idea that the Bi nanolines with an amorphous Si cap are not fully relaxed.

B. Estimation of activation energy of breaking Bi dimer structure

The activation energy for breaking a Bi dimer structure was estimated as follows

$$p_2/p_1 = \nu \Delta t \exp\left\{\frac{E_a}{kT}\right\} \tag{1}$$

where p_2 is the number of relaxed Bi nanolines, p_1 is the initial number of nanolines, ν is the Debye-frequency, Δt is the growth rate (impinging rate) of Si, k is the Boltzmann constant

and T is the substrate temperature. By assuming $p_2/p_1 \simeq 1$ and plugging $T = 400$ ° C, $\nu = 5 \times 10^{12}$ s^{-1} and $\Delta t = 33$ s into the above, we arrive at $E_a = 1.9$ eV.

C. XANES spectra of Bi implanted Si

As reference samples, two Si(001) wafers implanted with (a) 2.31×10^{14} cm^{-2} and (b) 2.31×10^{13} cm^{-2} Bi^+ ions (Si:Bi) were prepared by annealing at 600 °C for 30 minutes in N_2. The top 40 nm of Si was then removed by dry-etching. In the XANES spectra, increasing the Bi ion dose shifted the absorption edge to a lower energy. It is possible that applying the same post-annealing to both samples might not be enough to remove all of the residue of damage. As a result, one possible reason for the lower shift is a high density of Si vacancies or Bi clustering in the Si crystal. Unfortunately, the low concentration of Bi atoms made detailed analysis of the EXAFS spectrum of sample (b) difficult.

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[1] O. Sakata, W. Yashiro, D. R. Bowler, K. Sakamoto, and K. Miki, Phys. Rev. B **72**, 121407 (2005).