On the mechanism of {113} defect formation in Si: a study by in situ HREM irradiation

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Keywords: silicon, {113} defects, *in sutu* HREM irradiation

Type {113} defects in Si are crucially important for device manufacture because they strongly influence the diffusion of dopant atoms at elevated temperatures during the technological process. The equilibrium hexagonal structure of interstitial type {113} defect has already been established [1], however, its initial formation stages are still unclear. There are two main questions: what is the mechanism for interstitial chains formation and why the structure of the defect is so complex? *Ab initio* calculations propose only compact configurations of the initial cluster [2]. Recently, a new four-fold-coordinated point defect (FFCD) corresponding to the close-bonded interstitial-vacancy pair was proposed as a building block for more extended defects [3, 4]. However, this FFCD has not been detected experimentally yet. In fact, we have already shown by using *in situ* HREM irradiation experiments that self-interstitials and vacancies in Si tend to aggregate together at {113} habit planes [5]. In the very initial stages, both <110>-split interstitials and vacancies are arranged within [110] atomic chains located on {113}. Due to the energy barrier (~1.3eV) for recombination of self-interstitials with the aggregates of vacancies, different intermediate defect configurations are formed at {113} and {111} habit planes depending on the local supersaturation of point defects at low temperature [6].

Here we present the experimental evidence of the existence of {113} defects consisting of FFCDs. The *in situ* HREM irradiation experiments were carried out on a JEOL-4000EX at 400 keV at room temperature. Electron irradiation at energies higher than the threshold of 200 keV in Si at room temperature has the advantage of creating only Frenkel pairs and allows a very detailed investigation of point defect clustering even at the strained Si/SiGe interface [7]. TEM specimens were prepared by chemical etching of high pure n-type FZ-(110)Si wafers with 4000 Ωcm resistivity. Thin specimens were then covered with a 5 nm thick Si_3N_4 film to reduce point defect sink to the surface. Structural atomic models were optimized by the MM+ force field. Simulated HREM images of thus optimized models were calculated with the multislice program Musli.

Figure 1a presents the experimental HREM image of the intermediate structure of a {113} defect preceding the final hexagonal structure formation. A schematic model superimposed on the image at Fig. 1(b) shows that the defect consists of eight-fold rings surrounded by five-fold rings. At the right side of the {113} defect an interstitial hexagonal structure starts to appear.

Assuming that self-ordering of point defects takes place along the <110> direction we construct the model (Fig. 1c) of extended defects consisting of paired [110] rows of <110> split interstitials and vacancies located at the neighbouring atomic chains on a {113} plane. A simulated HREM image of this optimized model shown in Fig. 1d corresponds well to the experimental one in Fig. 1a. We show by means of modelling that further insertion of interstitials inside eight-fold rings will lead to the equilibrium hexagonal structure of the interstitial type {113} defect as revealed by S. Takeda [1]. In fact, the real atomic structure of the {113} defect will depend strongly on the correlation between the recombination rate, which depends mainly on the temperature, and the rate of point defect arrival to an extended cluster, which depends mainly on the local point defect supersaturation.

Finally, we conclude that combined clustering of interstitials and vacancies on a {113} plane corresponds to their recombination in extended shape as it was earlier assumed [8]. Key step of {113} defect origination is the formation of four-fold coordinated point defects which provides the complex structure of the {113} defect. Recombination of point defects on {113} planes under interstitial supersaturation ultimately leads to the interstitial {113} defects.

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9. We kindly acknowledge the help of Russian Foundation of basic Research supporting this work, grant № 01-02-17451.

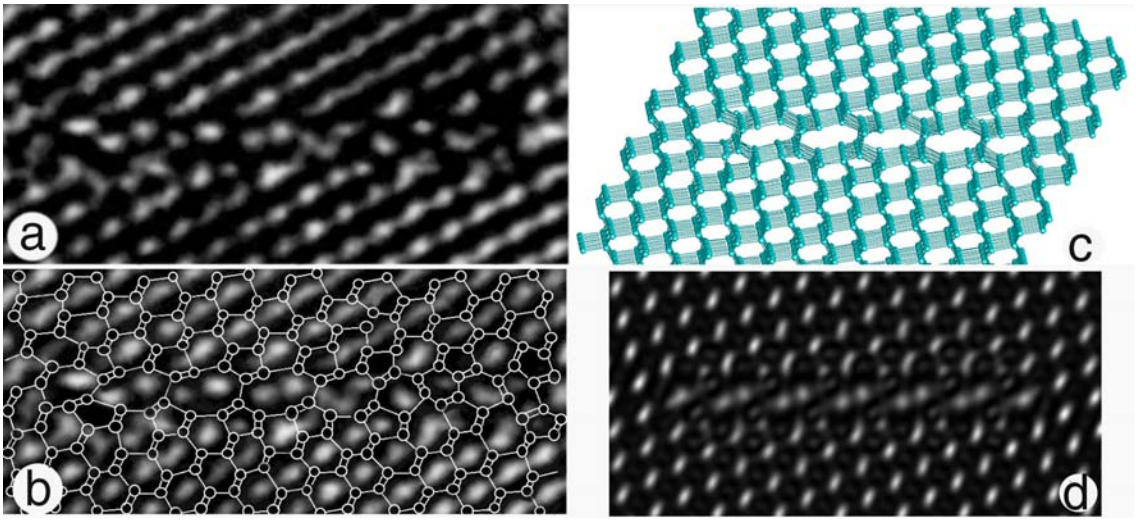

Figure 1. a) [110] HREM image of {113 defect introduced in FZ-Si by *in situ* electron irradiation in the JEOL-4000EX at room temperature. The intensity of irradiation is ~10^{20} electrons/cm^2sec. b) experimental model of {113} defect as superimposed on the experimental HREM image; c)- Part of simulated model of the {113} defect inside 3372 atomic cluster optimized by Mm+ force field; d)- Simulated HREM image of {113} defect based on the optimized model.