Reply to “Comment on ‘Comment on “Observation of Low-Temperature Elastic Softening due to Vacancy in Crystalline Silicon” ’’”


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In the above comment, Miyake and Matsuura extended our discussion further: Using their equation, eq. (3), they estimated the probability that a specified monovacancy (abbreviated as MV hereafter) collides with another MV in the diffusion process. According to them, the probability is about $1/10^{15}$ when $l_D = 8.6 \times 10^{-2}$ cm. Hence, they claimed that most MVs at high temperatures are still isolated MVs at room temperature.

In the above estimation, they assumed that the capture radius of MV is the nearest neighbor distance of Si crystal. This radius, however, corresponds to the equilibrium distance between two MVs in a divacancy. An MV has an elastic strain field which extends much further than the nearest neighbor distance. If we assume the capture radius to be 0.52 nm, their collision probability becomes about 0.5. This means that most MVs disappear from the isolated state if the capture radius is larger than 0.52 nm since two MVs are lost by one collision. We therefore think that isolated MVs do not exist in the as-grown crystal, in accordance with the result of the second estimation method using chemical reaction equations.

In the second paragraph of our paper, we referred to the case of hydrogen in Si crystals since the behavior of hydrogen has been well clarified experimentally. We can detect hydrogen molecules$^{[3]}$ from the measurement of their optical absorption, in contrast to the difficulty in the detection of divacancies. MVs and hydrogen atoms show similar behavior with respect to temperature change: Both are isolated and uniformly distributed in Si crystals at high temperatures.$^{[2]}$ During quenching to room temperature, they become supersaturated, most forming pairs by themselves$^{[1]}$ but some forming hydrogen–vacancy complexes.$^{[3]}$ The isolated atomic state of hydrogen at high temperatures$^{[2]}$ and molecules$^{[1]}$ at around room temperature after quenching strongly support our conclusion in the second estimation.

Finally, we should repeat the definition of the density in the Table I since there seems to be some confusion. Our density corresponds to the uniformly distributed MV density with the separation of the diffusion distance. In the most “favorable” case in which they diffuse to each other, two MVs form a pair during cooling. Hence, this density corresponds to the minimum MV density, above which MVs can interact with themselves during cooling.

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