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Disorder-Induced Enhancement of Avalanche Multiplication in a Silicon Nanodot Array

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In semiconductor devices, atomic disorder should exist near interfaces, which affects the device characteristics, especially in nano-scale devices because of a larger surface-to-volume ratio. The atomic disorder usually degrades the device performances because it is considered to be a kind of defects [1]. Here we theoretically show that the atomic disorder will improve the device performance in the case of avalanche photodiodes consisting of nanometer-size Si nanodots.

Extremely high photocurrent gain has been observed in a metal-semiconductor diode consisting of SiNDs in SiO_2 (see Fig. 1). The quantum efficiency of a 72-nm-thick SiND layer reaches 2,400 % at 77 K under an electric field of 0.9 MV/cm [2]. However, the detailed mechanism of this high carrier multiplication has not been fully understood and explained. In the previous study [3], we calculated impact ionization rate and performed Monte Carlo simulation of electron dynamics in a SiND array, and found that the relaxation of the momentum conservation and the poor inter-carrier screening in a nanodot system lead to high impact ionization rate and large carrier multiplication factor M. The calculated M was, however, smaller than the experimental M. In Ref. [3], we considered a uniform SiND without atomic disorder. However, it should exist near the Si/SiO_2 interfaces in actual SiNDs, which will affect the electronic states and the impact ionization rate. In this study, we theoretically investigate the impacts of atomic disorder existing near the Si/SiO_2 interfaces on the avalanche multiplication in a SiND array.

Atomic structure models for disordered SiNDs were constructed by performing a molecular-dynamics (MD) calculation with an empirical interatomic potential function designed for Si and O mixed systems [4]. The energy levels, E_i, were then calculated by an empirical tight-binding method with the $sp^3d^5s^*$ parameter set given in Ref. [5]. From the energy levels E_i, the impact ionization rate W_c of an electron in a conduction band state c is calculated [3, 6]. Using W_c and inter-dot tunneling time, we performed Monte Carlo simulation of electron motion in a one-dimensional SiND array [7] and obtained the carrier multiplication factor.

We constructed a SiND model from a spherical Si with 3,265 atoms, corresponding to ~ 5 nm diameter (Fig. 2(a)). The oxidation processes were simulated by the MD method to obtain a disordered SiND with ~ 3 nm diameter (Fig. 2(b)). The average bond-length of the SiND is found to be ~ 0.5 % longer than that of

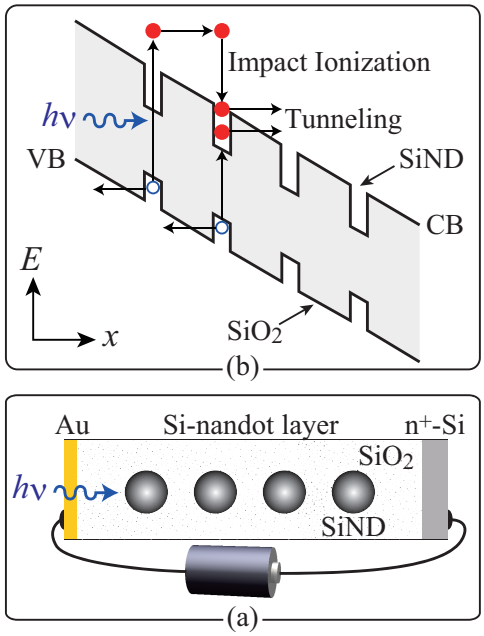

Figure 1: (a) Schematic illustration of a metal-semiconductor diode consisting of nanocrystalline SiNDs embedded in SiO_2. (b) Schematic of the band edges under the reverse bias condition.

the bulk Si. This is primarily due to expansion of a thin SiO_2 shell to outer space. As shown in Fig. 3, the disordered SiND has smaller band-gap compared to an ideal SiND without strain and disorder. This is marked contrast to a uniform tensile strain case, where the band-gap becomes larger by tensile strain [3]. Figure 4 shows the impact ionization rate, W_c, as a function of electron energy. Compared to the ideal SiND, W_c of the disordered SiND becomes higher near the threshold energy, and approaches that of the ideal SiND for higher energy region. Figure 5 shows carrier multiplication factor, M, as a function of the device thickens under a constant electric field $F = 0.9\,\mathrm{MV/cm}$ at $T = 77\,\mathrm{K}$. We find that M is enhanced by the atomic disorder by a factor ~ 2. This enhancement can be attributed to the fact that the impact ionization processes are more likely to occur in lower energy region near the threshold, where W_c is higher for the disordered SiND system.

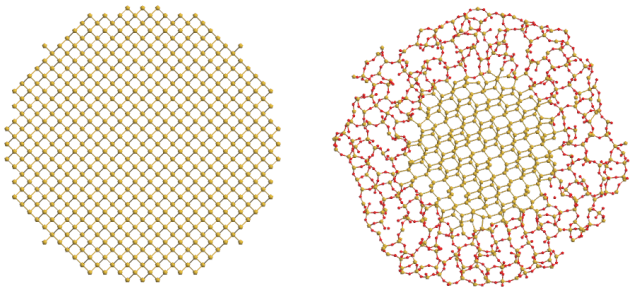

Figure 2: (a) An initial Si before the MD oxidation. (b) A disordered SiND model with ~ 3 nm diameter.

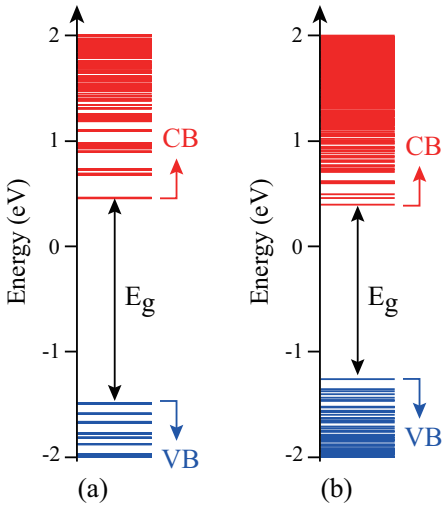

Figure 3: Energy levels of (a) an ideal SiND without strain and disorder and (b) the disordered SiND.

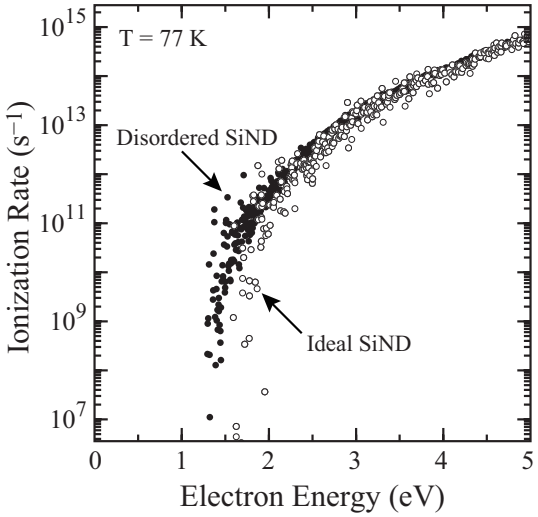

Figure 4: Impact ionization rate W_c as a function of the initial electron energy E at $T = 77\,\mathrm{K}$.

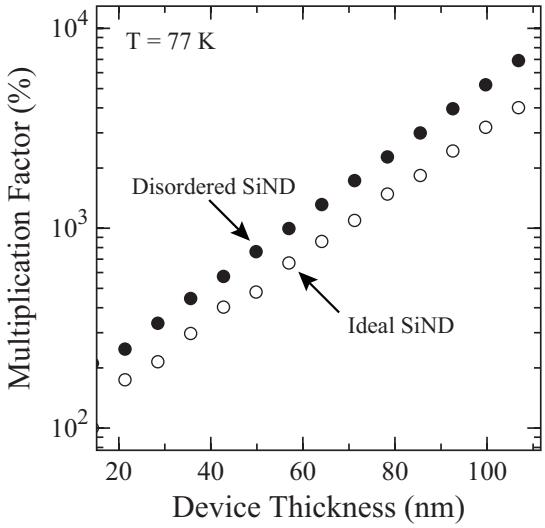

Figure 5: Carrier multiplication factor as a function of the device thickens under a constant electric field $F = 0.9\,\mathrm{MV/cm}$ at $T = 77\,\mathrm{K}$.

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