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Enhancement of Ni Diffusion Rate in Disordered Si Nanocrystal Studied by Molecular Dynamics Simulation

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Introduction Electrode formation is an essential technology for electron device fabrication. Silicidation reaction is a very common method for the formation of electrodes in Si devices. Among various silicides, nickel mono-silicide (NiSi) is one of the suitable material owing to its low series resistance and low formation temperature. As the emerging of low-dimensional Si devices such as Si nanowire, the control of Ni silicidation reaction is increasingly important. Unlike the bulk Si, a unique manner of Ni diffusion is observed in Si nanowire (NW). Katsman et al. [1] indicated that the Ni diffusion is enhanced in the vicinity of SiO_2 film covering Si-NWs. We have also reported an enhancement of Ni diffusion rate in NW, and found that it is related to the oxide-induced lattice disorder [2]. In this study, we perform a molecular dynamics (MD) simulation for Si-Ni mixed system to investigate the detailed mechanism of the Ni diffusion in Si, focusing on the effect of the disordered Si lattice on the diffusion rate.

Calculation The interatomic interaction model employed in this work is the extended Stillinger-Weber potential [3]. We newly prepare a set of parameters for Ni-Si interaction to reproduce the interstitial Ni diffusion in Si lattice. Fig. 1 shows the simulation model in which a crystalline Si (c-Si) or amorphous Si (a-Si) block sandwiched by Ni layers. A three-dimensional periodic boundary condition is posed. The Ni diffusion process is simulated by the MD simulation of 500ps. The system is thermostated at 1000K during the MD simulation.

Results and Discussions Fig. 2 compares the Ni diffusion rates in c-Si and a-Si. The vertical axis is the mean square displacement (MSD) of Ni atoms which were located within 2 Å from the Si/Ni interface at the initial time. Fig. 2 shows that the Ni diffusion is significantly enhanced in the a-Si. It is considered that the a-Si includes many stable interstitial sites and they form a percolation path of the diffusion of Ni atoms. The result indicates that Si atomic disorder is an important factor for the Ni silicidation reaction. To control precisely the Ni silicidation reaction in Si nanocrystal, it is effective to make the Si crystallinity uniform over the cross-sectional area of Si-NW.

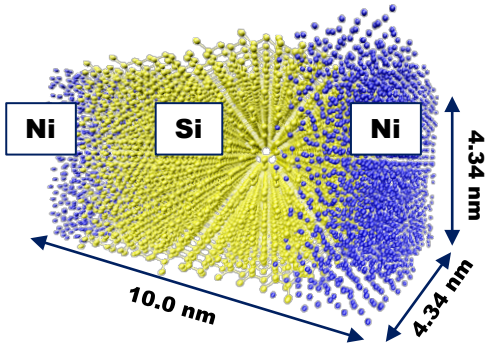

Figure 1 Atomistic model of MD simulation (left: 3D view of Ni/Si/Ni, right: model before/after simulation)

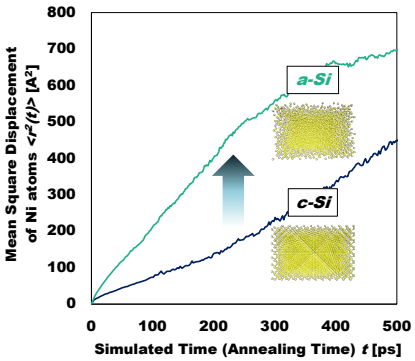

Figure 2 Si crystal structure dependence on Ni diffusion rate.

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Reference [1] A. Katsman et al., J. Elec. Mater., **39.4**, 365-370 (2010). [2] S. Hashimoto et al., 27th International Microprocesses and Nanotechnology Conference (2014). [3] T. Watanabe, et al., ECS Trans., **33.6**, 901-912 (2010).