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LAB TALK

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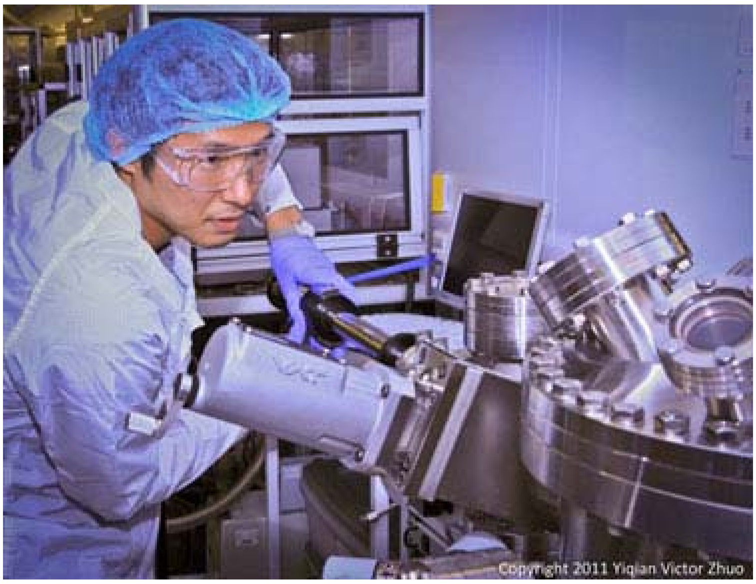
Silicidation kinetics of quantum wires on show

The ever decreasing feature size of both top-down processed and bottom-up assembled materials means that developers are keen to know more about the thermodynamics and kinetics governing synthesis and processing at the nanometre scale. The increased influence of interfacial energies, and other conditions such as stress pile-up, can lead to significant differences between nanoscale systems and bulk/thin-film reactions. This is highlighted by a recent study (http://iopscience.iop.org/0957-4484/22/36/365305) published in the journal *Nanotechnology* on the silicidation of Si nanowires led by the Hofmann group at Cambridge University, UK.



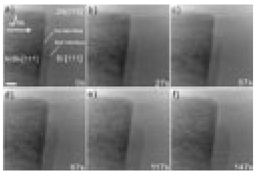
(http://images.iop.org/objects/ntw/journal/10/9/18/image1.jpg)

Sample loading: Ken Ogata prepares the CVD chamber (http://images.iop.org/objects/ntw/journal/10/9/18/image1.jpg)

The team has systematically studied the solid-state reaction of micron-sized Ni contacts with sub-100 nm Si quantum wires. Since Ni is the dominant diffusing species, an axial intrusion of Ni silicides occurs upon annealing. The researchers witnessed the phase formation during annealing through real-time observations using transmission electron microscopy (TEM).

Model system

They used nickel silicide formation in Si nanowires (NW) as a model system to study how nanoscale effects like a high surface to volume ratio, radial stress and volume constraints alter the dynamics of silicidation. In their work, the scientists compared as-grown (with a native oxide layer) to oxidized Si nanowires with different crystallographic orientations and core diameters.

 (http://images.iop.org/objects/ntw/journal/10/9/18/image2.jpg)

TEM sequence (http://images.iop.org/objects/ntw/journal/10/9/18/image2.jpg)

For temperatures in the range 300-440 °C, the total axial silicide intrusion is proportional to the square root of reaction time for both types of NWs. A temporal square root dependence is indicative of a diffusion limited reaction. Therefore, the group concluded that Ni diffusion through the newly formed silicide wire segment limits silicide formation. The experiments showed a clear retardation of Ni silicide formation for oxidised Si NWs. As-oxidized Si NWs have a thick rigid outer coating and the team inferred that the stress induced by the oxide shell lowered the Ni diffusion coefficient, thus slowing down the overall silicide growth rate.

Observing the process

Real-time, lattice resolved TEM movies clearly show the silicidation process. The researchers observed the formation of crystal structures that were not expected based on the equilibrium bulk phase diagram. Specifically, the first silicide phase nucleated is cubic $NiSi_2$ for both the as-grown and oxidised Si nanowires, in contrast to the equilibrium orthorhombic Ni_2Si or NiSi commonly found at the same range of temperatures in the bulk/thin-film reactions.

It is to be noted that $NiSi_2$ is only formed at a higher temperature range (>~700 °C) in the bulk/thin-films. This suggests that interfacial lattice matching at the Si-silicide interface, rather than the bulk Ni-silicide formation energy, plays a key role in the initial phase formation.

The researchers rationalised their results using a simple Ni-diffusion model where Ni atoms preferentially diffuse through the surface of the quantum wires. They found the model to be in good agreement with the extrapolated Ni-diffusion coefficients. It also explains why the observed silicide formation is dependent on NW diameter.

The team believes that this simple diffusion model could be used to explain silicide formation in other metal-silicon systems including Li/Co/Mn/Pt-SiNWs.

More details (http://iopscience.iop.org/0957-4484/22/36/365305) can be found in the journal *Nanotechnology*.

About the author

The work was performed by researchers from Cambridge University, UK, and Brookhaven National Lab, US. Ken Ogata performed the main experiments and is a PhD student in the Department of Engineering at Cambridge University. Xueni Zhu is a PhD student in the same department and Dr Stephan Hofmann leads the team. Dr Eli Sutter is a research scientist at Brookhaven National Lab.