Highlight #4: NANOSTRUCTURES and METHODOLOGIES

Reversible diffusion of aluminium and silicon atoms in a nanowire

Diffusion is a phenomenon whereby matter is transported from a region with high concentration to a region with lower concentration. We all know its effect: If I open the window on a cold day, the inside and outside temperatures will slowly converge since fast and hot gas molecules from inside mingle with the slower and colder gas molecules from outside. We also know that we cannot reverse this effect and "unmix" the hot and cold molecules, we cannot command the hot molecules to come back inside! But in a specific solid-state system, we can do exactly this.

This reversible diffusion phenomenon was an accidental observation during research on making electrical contacts on semiconductor nanowires. A nanowire is a thin, wire-like structure, of diameter several nanometres to tens of nanometres. Nanowires fabricated from semiconducting materials can be used in devices such as field-effect transistors, light-emitting diodes and solar cells. Nanowires incorporate insertions of different materials but, in devices, they require high-quality electrical contacts.

With colleagues at the Institute for Interdisciplinary Research of Grenoble we have been fabricating aluminium contacts onto Silicon-Germanium (Si-Ge) alloy nanowires. For an electron microscopy study of this process, Al contact-pads were fabricated on a $Si_{0.67}Ge_{0.33}$ nanowire positioned on a thin SiN membrane transparent to the very fast electrons of a scanning Transmission Electron Microscope (TEM). These structures were then heated inside the TEM, to image the solid-state reactions with nanometre resolution.

At 580°C, a solid-state reaction is started where the aluminium from the metal contact pad diffuses progressively into the nanowire, replacing germanium and silicon atoms. The Ge and Si atoms diffuse in the opposite direction, along the nanowire surface, exit the nanowire, and incorporate at surfaces and grain boundaries in the aluminium pad. Thus, a near perfect monocrystalline aluminium nanowire section is formed, with a perfectly abrupt interface to the SiGe nanowire, and making excellent electrical contact with it, see Fig. 1 (top).

Surprisingly, if the heating temperature is lowered very slowly, the Al contacts can no longer contain all the silicon atoms they had stored. The Si atoms (and also, but much less, the heavier Ge atoms) diffuse back along the nanowire and nucleate at the Al/SiGe interface, progressively forming a region of almost pure Si, with a low Ge content. This region grows in the reverse direction as the Al atoms return to the metal pad (Fig. 1, bottom).

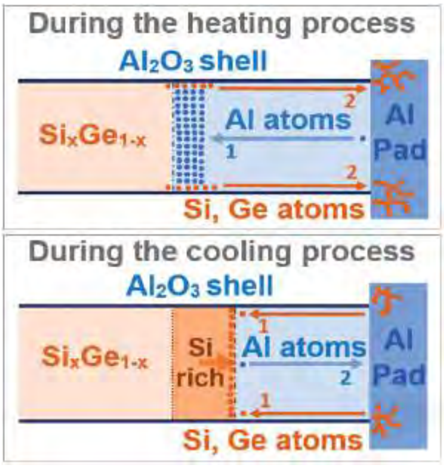

Fig. 1: *At top: Diffusion of aluminium into the $Si_{0.67}Ge_{0.33}$ alloy nanowire, and diffusion of silicon and germanium out into the Al contact pad.*
Below: The reverse diffusion process for Al and Si; the lesser reversibility for Ge diffusion produces a Si-rich region.

We found that the aluminium could move in and out repeatedly. To our knowledge, this work demonstrates a reversible diffusion mechanism for the first time, and absolutely unambiguously, thanks to the in-situ Electron Microscopy experiments. The reversible diffusion arises due to the nanowire geometry and crystallinity.

This concept may be extended to other material systems. In our own work, the different diffusion properties of Si and Ge have allowed us to fabricate and contact complex and abrupt Al metal/Si-rich/SiGe alloy heterostructures with sharp interfaces in a single processing step, all compatible with current Si/Ge technology, see Fig. 2.

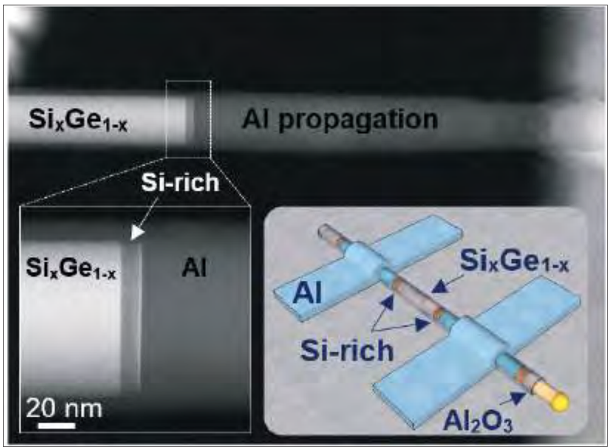

Fig. 2: *At top: Scanning Transmission Electron Microscopy image of a nanowire heterostructure encapsulated in an Al_20_3 shell.*
Below left: A zoom onto the SiGe alloy/Si-rich alloy/ Al metal contact.
At bottom right: a nanowire double-heterojunction structure.

Collaboration

IRIG

Reference

M.-A.Luong, E. Robin, N. Pauc, P. Gentile, T. Baron, B. Salem, M. Sistani, A. Lugstein, M. Spies, B. Fernandez & M. den Hertog, "Reversible Al Propagation in Si_xGe_{1-x} Nanowires: Implications for Electrical Contact Formation", *ACS Appl. Nano Mater.* **3**, 10, 10427 (2020).