

Can metals remember their shape at nanoscale, too?

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University of Constance physicists Daniel Mutter and Peter Nielaba have visualized changes in shape memory materials down to the nanometric scale in an article about to be published in the *European Physical Journal B*.

Metallic alloys can be stretched or compressed in such a way that they stay deformed once the strain on the material has been released. Only [shape memory alloys](#), however, can return to their original shape after being heated above a specific temperature.

For the first time, the authors determine the absolute values of temperatures at which shape memory nanospheres start changing back to their memorised shape – undergoing so-called structural phase transition, which depends on the size of particles studied. To achieve this result, they performed a computer simulation using nanoparticles with diameters between 4 and 17 nm made of an alloy of equal proportions of nickel and titanium.

To date, research efforts to establish structural phase transition temperature have mainly been experimental. Thanks to a computerised method known as molecular dynamics simulation, the authors were able to visualise the transformation process of the material during the transition. As the [temperature](#) increased, they showed that the material's atomic-scale crystal structure shifted from a lower to a higher level of symmetry. They found that the strong influence of the energy difference between the low- and high-symmetry structure at the surface of the

nanoparticle, which differed from that in its interior, could explain the transition.

Most of the prior work on [shape memory materials](#) was in macroscopic scale systems and used for applications such as dental braces, stents or oil temperature-regulating devices for bullet trains. Potential new applications include the creation of nanoswitches, where laser irradiation could heat up such [shape memory](#) material, triggering a change in its length that would, in turn, function as a switch.

More information: Mutter D, Nielaba P (2011). Simulation of the thermally induced austenitic phase transition in NiTi nanoparticles. *European Physical Journal B* (EPJ B) [DOI 10.1140/epjb/e2011-20661-4](https://doi.org/10.1140/epjb/e2011-20661-4)

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