Can metals remember their shape at nanoscale, too?

November 8 2011

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

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