Negative pressure in free standing particles and the resulting enhancement of properties

Nava Setter
Ceramics Laboratory, EPFL – Swiss Federal Institute of Technology, 1015 Lausanne, Switzerland

Strain engineering has been often utilized in thin films to enhance properties. For example, biaxially strained silicon layers, obtained due to crystalline lattice mismatch with the underlying substrate exhibit high electron mobility, which is useful in CMOS technology. Strain engineering in free-standing elements has been rarely obtained and (to the best of our knowledge) has never been used to modify functional properties.

We demonstrated recently the creation of negative pressure (tension) in free-standing ferroelectric nano-particles. As predicted a decade ago from first principles (ref.1), the material shows enhanced properties.

To obtain the negative pressure we use materials that undergo a solid-solid phase transformation in which the density of the final phase is higher than that of the initial phase, in parallel exploiting conditions during the transformation that prevent the transformed structure from relaxation: We prepared nano wires of lead-titanate in its PX phase (ref.2,3). The low-density PX phase was converted to the high-density ferroelectric perovskite phase by heating in air. This conversion requires catalytic oxygen, which diffuses from the surface into the particle. Because the conversion of the outer shell precedes that of the inner part, the inner part is prevented from relaxing during its conversion and remains stretched. The negative pressure persists for long time. It is manifested by modification of the lattice parameters of the material and by cavitation in form of nanopores. The properties, Curie temperature and spontaneous polarization are enhanced dramatically (ref.4). The piezoelectric activity is enhanced too.

The process may work on a large range of materials to potentially produce a variety of nano- and micro-structures with properties enhanced by negative pressure.

References: 1. Tinte, S., Rabe, K. M. &Vanderbilt, D. Phys. Rev. B. **68,**144105 (2003). 2. J. Wang et al., *Chemistry of Materials*, 23, 2529 (2011). 3. J. Wang et al., J Cryst-Growth 347, 1-6 (2012). 4. J. Wang et al., *Nature Materials*, 14, 985 (2015)