Throwing light on the undercooling puzzle

Deep undercooling gives rise to a peculiar state of matter in which a liquid does not solidify even far below the normal freezing point. A good example of this phenomenon is found every day in meteorology: clouds in high altitude are an accumulation of undercooled droplets of water below their freezing points due to the high purity of the atmosphere at these altitudes.

Undercooling was discovered in 1724 by Fahrenheit while observing that water droplets stay liquid below 0°C. However numerous questions about the underlying mechanisms remain nowadays still open. In the 1950's, theoricians postulated the structure at the atomic level to be incompatible with crystallization. This led to the speculation that the atoms in the liquid could locally arrange in icoahedra characterized by a five-fold symmetry. Fifty years after, *ab initio* molecular dynamics simulations revealed for the first time five-fold coordinated clusters (pentagons) in pure liquid metals as well as liquid alloys, some of them being known to form quasicrystalline phases upon rapid solidification [1, 2].

Using *ab initio* molecular dynamics simulations, a new remarkable undercooling phenomenon has been explained [3], namely an undercooling as deep as 350°C for Gold-Silicon eutectic alloy in contact with a specially decorated silicon (111) surface where the outermost layer of the solid featured pentagonal atomic arrangements. Such a five-fold coordinated surface influences the short-range order and the metastability of the liquid, favoring the existence of pentagons in this phase. This result has wide implications not only for fundamental studies of freezing, but also for practical control of the phase transition. For instance it should lead to important technological applications in the field of nanowire growth for which the eutectic alloy act as a catalyst. It is also speculated that the containerless techniques required today to obtain undercooling could be in the future be replaced by icosahedrally coated solid containers.

[1] *N. Jakse and A. Pasturel, Phys. Rev. Lett. 91, 2003, 205702.*

[2] *N. Jakse, O. LeBacq and A. Pasturel, Phys. Rev. Lett. 93, 2004, 207801.*

[3] *T.U. Schulli, R. Daudin, G. Renaud, A. Vaysset, O. Geaymond and A. Pasturel, Nature 464, 2010, 1174.*

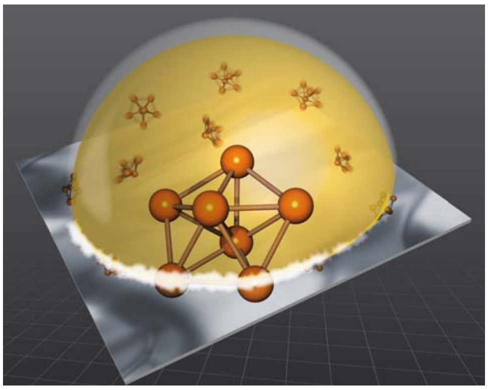

Figure 1: Pentagonal arrangements in the gold-silicon eutectic droplets are stabilized by a decorated silicon (111) surface.

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