Researchers show that gold doping increases nickel catalyst activity for carbon nanostructure formation

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(PhysOrg.com) -- Researchers from the CNST and Arizona State University have demonstrated that the overall catalytic activity of nickel particles for the formation of carbon nanostructures is improved by the addition of a small amount of gold (below 0.2 mol fraction).

In a recent Nano Letters article, the researchers evaluate Au/SiO_2, Ni/SiO_2, and $Au\text{-}Ni/SiO_2$ nanoparticles as catalysts for carbon nanotube (CNT) and carbon nanofiber (CNF) formation by measuring the number of particles active during tube formation using in situ dynamic imaging in an environmental scanning transmission electron microscope.

Carbon nanostructures are generally synthesized by catalytic chemical vapor deposition from carbon sources such as acetylene (C_2H_2) and nucleate from catalyst particles, including Ni. However, only some catalyst particles are active in the formation of nanostructures. This limitation affects the ultimate density and placement of the nanostructures, an important factor for nanofabrication applications.

Using high-resolution images and spectroscopy data collected during and after the synthesis, the researchers showed that most of the Au segregates to form an inactive Au-rich cap, with only a small amount of Au present in the active region of the particles.

They also show that the structure of Ni catalyst particles transforms from

fcc metal to orthorhombic nickel carbide (Ni_3C). They believe that carbides form due to the dynamic equilibrium conditions present under these reaction conditions. Density functional theory calculations support the hypothesis that low levels of Au doping (0.06 mol fraction) increases the number of particles active for carbon nanostructure formation by lowering the energy barrier for the diffusion of carbon in doped Ni to 0.07 eV compared to 1.62 eV for pure Ni.

The researchers are extending this technique to evaluate the role of metal carbide formation in the activity of other metal catalysts used for carbon nanotube synthesis, such as Fe and Co.

More information: Evaluation of the role of Au in improving catalytic activity of Ni nanoparticles for the formation of one-dimensional carbon nanostructures, R. Sharma, S. Chee, A. Herzing, R. Miranda, and P. Rez, *Nano Letters* 11, 2464-2471 (2011). pubs.acs.org/doi/abs/10.1021/nl2009026

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