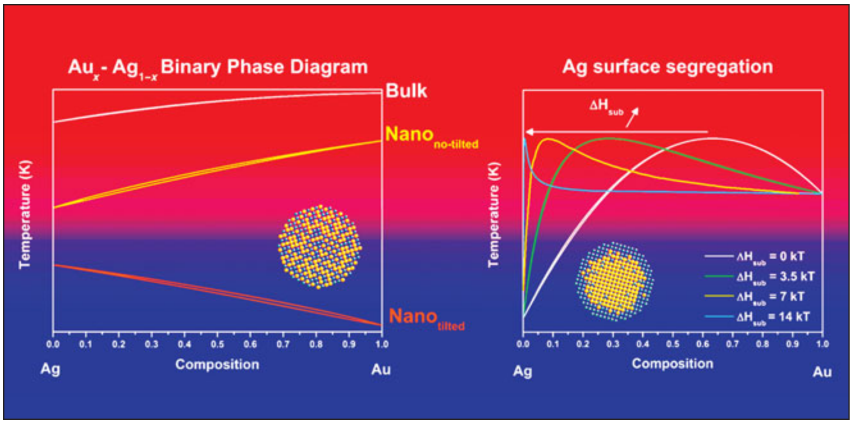
Nano Focus

Nanothermodynamics modeling characterizes electrum at the nanoscale

Electrum is one of the oldest alloys known to humankind. Homer mentions the silver-gold alloy in the *Illiad*, and coins made of electrum were minted by the Lydians in seventh century BC. Despite the long history with the alloy, its structure at the nanoscale is still not well characterized. A study recently published in *ACS Nano* (DOI: 10.1021/acsnano.5b05755) utilizes theoretical modeling to show the way electrum reacts under various conditions, yielding surprising results not only for this alloy but also for similar bimetallic alloys.



Nanothermodynamics modeling studies of Electrum (Ag-Au alloy) points to two rules for segregation for bimetallic materials. Credit: *ACS Nano.*

A phase diagram is one of the first steps in trying to understand the characteristics of the material, says Grégory Guisbiers, a materials scientist at The University of Texas at San Antonio. And while bulk phase diagrams have been developed for electrum, nothing similar has been achieved on the nanoscale due to technical limitations that do not allow for precise calorimetry. Instead, Guisbiers and his team turned to modeling using nanothermodynamics, the thermodynamics of small systems. Building off previous attempts published by others,

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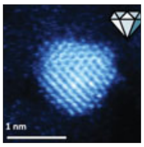

Nanodiamonds, or pure diamonds with a length scale less than a micrometer, are a materials scientist's best friend in areas such as imaging, spintronics, and quantum computing. But synthesizing particles of reliable size distribution, with the desired surface structure and chemistry, has long been a challenge. Now, a team of researchers based in the Czech Republic have developed a straightforward way of producing extremely small, stable, and pure nanodiamonds from commercially available diamond powders.

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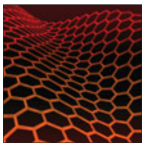

You'd think twice about snapping a selfie if the camera flash was bright enough to burn your skin off. Biologists face a similar problem when studying proteins under the microscope, as modern imaging techniques can destroy the molecules. Now graphene—the ultrathin form of carbon—has come to the rescue, and delivered the very first pictures of a single protein.

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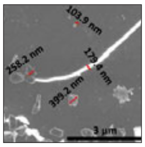

Q-carbon is the latest candidate in the family of carbon allotropes. This harder-than-diamond material not only shows novel chemical and physical properties like ferromagnetism at and above ambient temperature, it can also turn to diamond in ambient temperature and pressure.

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they hoped to better understand how size, shape, and segregation effects might alter the nanophase diagram of electrum nanoparticles.

Though size and shape had some impact during changes in phase, the modeling showed a particularly unexpected effect in segregation.

"No matter what the temperature was, silver was always on the surface," Guisbiers says. This was strange, he says, because typically it's expected that whichever element has the highest melting point would be the most stable and therefore would be segregated to the surface. In the case of electrum, gold should therefore be on the surface because its melting temperature of 1063°C is about 100 degrees higher than silver.

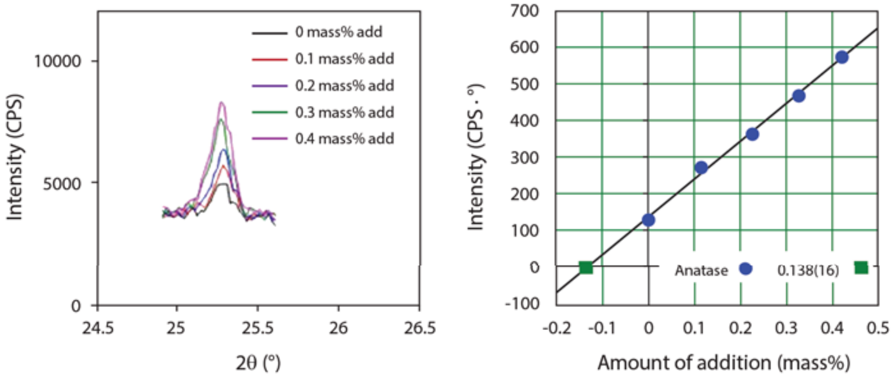
However, says Guisbiers, the fact that the melting temperature did not seem to play a major role had them rethink the mechanism behind segregation. They developed two rules for segregation for bimetallic materials. First, temperature is still the primary driving factor. If two elements have melting temperatures that are fairly far apart, the one with the highest melting temperature will be on the top. However, if their melting temperatures are close together, a different mechanism takes over. The second rule is driven by surface energy. The element with the smaller surface energy will segregate to the surface.

"These rules can apply to other bimetallic alloys," Guisbiers says. Using this thermodynamic modeling, "we can speed up the fabrication process. We don't need to make the alloy first and do experiments. We can predict it," Guisbiers says.

"Thermodynamics is a powerful tool to predict the phase stability even [at the] nanoscale," says Joonho Lee, a materials scientist at Korea University in Seoul who is unaffiliated with the current research. "This paper is one example [of] how we can predict the phase stability of nanoparticles by considering various factors … although we still need to [continue improving] the thermodynamic model for this type of nanomaterial, [this] model would be a useful guidance."

Guisbiers agrees that additional studies are needed to more fully flesh out the thermodynamic modeling of nanoalloys. One particular aspect he would like to further investigate is optical properties. The initial modeling with electrum suggests that the optical properties are not affected much by varying particle size and shape. Instead, it appears that the solvent used to fabricate the alloy plays a bigger role. He plans to look at gold-palladium next, an important catalyst used in many applications. In addition, he aims to look at alloys that are used in biomedical applications.

Meg Marquardt



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