

Superheating Nanoparticles

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“For quite a long time people have been measuring the melting points of small particles,” Shaun Hendy tells *PhysOrg.com*. “They’ve found that the melting point decreases and this decrease is in inverse proportion to the radius of the particle.” He pauses before continuing. “We have found in this case it doesn’t happen. It’s counterintuitive.”

Hendy, a scientist with Industrial Research Ltd. in Lower Hutt, New Zealand and Dmitri Schebarchov, a student at Victoria University of Wellington have developed a model that shows how the melting point can be higher in free nanoparticles, as well as illustrating how the liquid phase can coexist with the solid phase. Their findings, as well as an explanation of their model, can be found in an article published by *Physical Review Letters*. The Letter is titled “Superheating and Solid-Liquid Phase Coexistence in Nanoparticles with Nonmelting Surfaces,” and it was published June 26th.

“We’ve investigated a case that has been neglected, where the molten part of a nanoparticle doesn’t want to wet the solid” says Hendy. He points out that partially melted nanoparticles are typically modeled as spherically symmetric. These models have their flaws, as they do not accurately describe all cases. A possible solution to the problem exists in using an overlapping-sphere model, but with two parameters that can be complicated. Hendy and Schebarchov suggest a simpler model with only one parameter which allows them to solve the equations that result from the model. However, he says, “We expect to find the same sort of features in more complicated models.”

Hendy and Schebarchov's model shows that the melting temperature of a nanoparticle can exceed what would normally be the melting point of the bulk material. Additionally, there is also a point during the melting process when the liquid phase of the particle (the molten part) coexists with the part that is still solid.

Normally, in some materials Hendy explains, "the liquid part tries to avoid the solid part. We have found in these cases it would wet the solid part." This happens due to a phenomenon Hendy explained in a previous paper. "We found that the solid part rearranged itself. Basically it melts and re-crystallizes, becoming more favorable for wetting."

The current model, however, goes beyond describing a mix of solid and liquid phases. It also shows that superheated nanoparticles are stable. While on a substrate, superheating of particles has been observed but if you wait long enough they will melt. Get them away from the substrate, Hendy believes, and they are, in fact, stable. "For instance," Hendy explains, "you can take aluminum particles above the melting temperature and they are only metastable when on a substrate...but taking them away from thermal contact with the environment changes the thermodynamics in a subtle, but important, way."

Hendy goes on to explain that when a nanoparticle is in contact with a substrate, it can draw on the latent heat and melt completely. But when that nanoparticle is "free, not in thermal contact with the environment, then it would be stable. There is a higher melting point if the particle is not in equilibrium with the environment."

While the idea has just been shown by a model to this point, Hendy believes that experiments to test this are possible. It wouldn't be easy, though: "You'd have to do it by observing free particles, or by doing it in a trap." But, he points out, "there are a number of experimental groups with the capability to test this."

Right now, Hendy concedes, there aren't any particular applications for this knowledge. "It's more of an interesting curiosity," he says. But it is a curiosity with the potential for future application, as it can shed further light on the nature of nanoparticles. "Our model will certainly help with the understanding of melting and the properties of nanoparticles," insists Hendy. "Besides, this is a very nice illustration of how when you apply thermodynamics to nanoscale systems that sometimes your intuition is going to be wrong. It's a reminder that things are a lot different down at the nanoscale."

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