Modeling the thermal stability of core-shell Iron-Gold nanoparticles

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Iron and gold do not easily mix in bulk phases. At the nanoscale, core-shell iron-gold nanoparticles are potentially useful owing to the magnetic properties of iron and the biocompatibility of surrounding gold. In this contribution we explore the stable structures of small iron-gold nanoparticles at finite temperature by means of computational modeling. A many-body empirical potential of the embedded-atom family was designed using ingredients for the individual metals, and fitted to reproduce density-functional theory data for impurities in bulk or clusters materials as well as surface energies and intermetallics.

Core-shell nanoparticles containing a few thousand atoms were modeled assuming a cubic iron core with bcc symmetry surrounded by a gold shell of fcc symmetry, keeping an epitaxial relationship at the (100) contact between the two metals. Using exchange Monte Carlo simulations, the thermal stability of so prepared nanostructures was investigated and the core-shell phase segration found to prevail even beyond the melting range.[1]

In contrast, using the alternative potential previously proposed by Zhou and coworkers[2] we find that the nanoparticles readily transform into randomly mixed cubic structures already at room temperature.

[1] F. Calvo, M. Benoit, N. Combe and J. Morillo, J. Phys. Chem. C **121**, 4680-4891 (2017).
[2] X. W. Zhou, R. A. Johnson, J. N. G. Walley, Phys. Rev. B **69**, 144113 (2004).

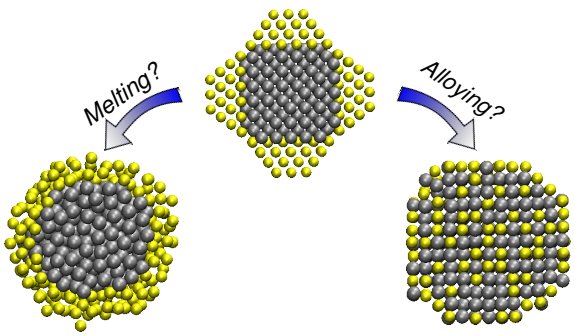

Figure 1: How do core-shell iron-gold nanoparticles melt in the computer?