Atomistic understanding of melting mechanisms in core-shell nanoparticles

Roberto Tabacco[1*], Jean Furstoss[2] and Julien Lam[1]

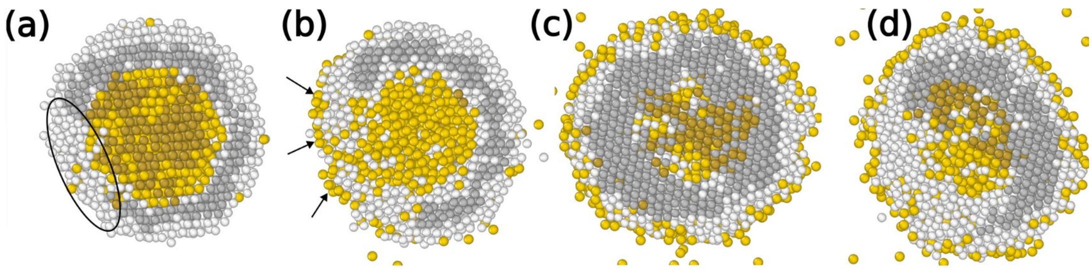
[1]Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France
[2]Institut P' , CNRS UPR 3346, Université de Poitiers, SP2MI, Boulevard Marie et Pierre Curie, TSA 41123, 86073 Poitiers Cedex 9, France

**roberto.tabacco@univ-lille.fr*

ABSTRACT

While melting mechanisms have been largely explored in mono-atomic nanoparticles, core@shell nanoparticles raise an additional layer of complexity due to the crucial role played by the interface. We use molecular dynamics simulations to provide a comprehensive picture of the melting mechanisms occurring in core@shell nanoparticles. In particular, we focus on the case where the core material has a lower melting temperature than the shell which corresponds to many metallic pairs like Au@Pt, Pb@Al, Al@Cu and Cu@Pt. In order to thoroughly explore the influence of the lattice mismatch and the chemical composition, we use molecular dynamics simulations and employ a simple model made of Lennard-Jones (LJ) particles.

To begin, we demonstrate that beside its apparent simplicity the LJ model is still able to retrieve most of the characteristics found both in experiments and in simulations with more complex models. For instance, when comparing our model with the EAM potential for Au@Pt, we retrieve in both cases the superheating mechanism and similar melting temperatures over several core sizes. Then, we generalize our results towards different lattice mismatches. We observe that the melting mechanism of the core depend on the sign and magnitude of the lattice mismatch. A negative lattice mismatch leads to interdiffusion between core and shell atoms, which disrupts the crystalline structure and fosters the nucleation of the liquid. A positive lattice mismatch is related to a high stress in the core, which escapes from the shell during melting. Our findings clarify the effects of the lattice mismatch on the melting mechanism of core@shell nanoparticles and the role of the interface in determining the melting temperature of the core.



Evolution during heating of a nanoparticle with core atoms larger than shell atoms, that involves the core escape and the shell recrystallization afterwards