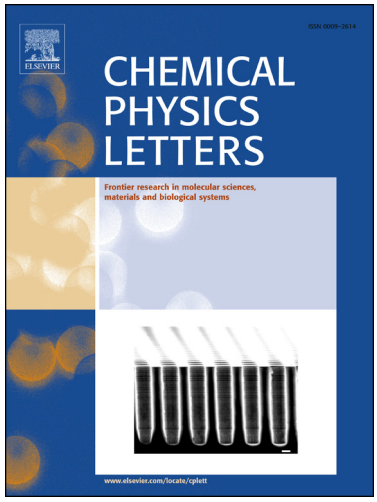

Unsaturated coordination and surface stresses in metal nanoparticles

Francesco Delogu

PII: S0009-2614(14)00257-7
DOI: http://dx.doi.org/10.1016/j.cplett.2014.03.090
Reference: CPLETT 32081

To appear in: *Chemical Physics Letters*

Received Date: 6 January 2014
Accepted Date: 31 March 2014

Please cite this article as: F. Delogu, Unsaturated coordination and surface stresses in metal nanoparticles, *Chemical Physics Letters* (2014), doi: http://dx.doi.org/10.1016/j.cplett.2014.03.090

Unsaturated coordination and surface stresses in metal nanoparticles

Francesco Delogu

Dipartimento di Ingegneria Meccanica, Chimica, e dei Materiali, Università degli Studi di Cagliari, via Marengo 2, 09123 Cagliari, Italy

Abstract

This work focuses on the relationship between structure and thermodynamic properties in metal nanoparticles. It is shown that the many-body character of interactions results in a dependence of interatomic distances on coordination numbers. At the particle surface, interatomic distances contract due to the unsaturation of atomic coordination shells, giving rise to relatively intense surface stresses. These, and the excess surface energy, induce a depression of the vacancy concentration respect to the bulk phase, and the emergence of pre-melting phenomena at the particle surface.

Keywords: Nanocrystalline metals; Surface; Melting; Internal stresses; Modeling.

e-mail: francesco.delogu@unica.it