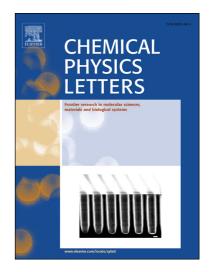
## Accepted Manuscript

Unsaturated coordination and surface stresses in metal nanoparticles

Francesco Delogu

PII:S0009-2614(14)00257-7DOI:http://dx.doi.org/10.1016/j.cplett.2014.03.090Reference:CPLETT 32081To appear in:Chemical Physics LettersReceived Date:6 January 2014Accepted 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

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

## ACCEPTED MANUSCRIPT

1

## 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

Download English Version:

https://daneshyari.com/en/article/5380953

Download Persian Version:

https://daneshyari.com/article/5380953

Daneshyari.com