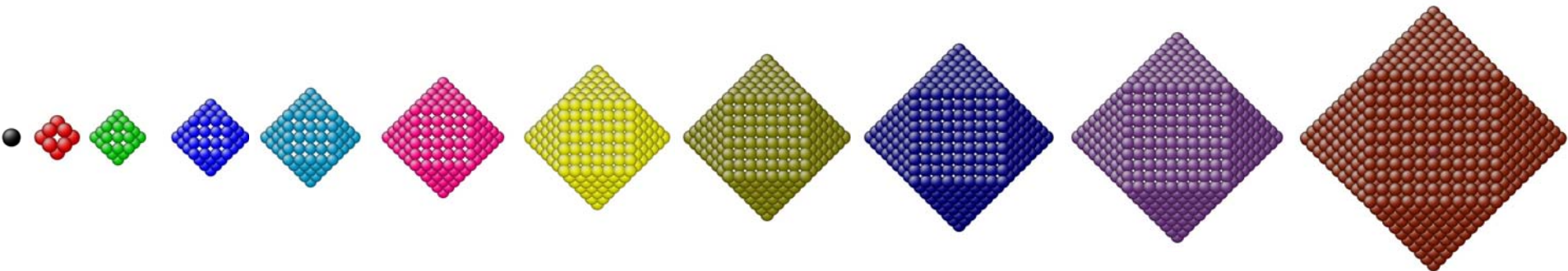


Superficial phase transitions in nanoalloys

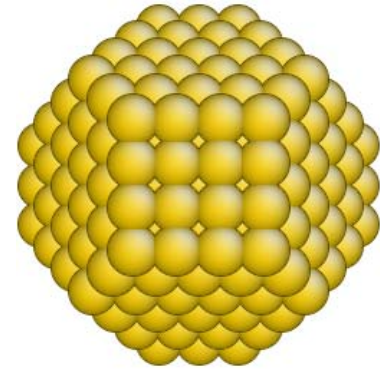
L. Delfour, M. Briki, J. Creuze, F. Berthier, B. Legrand
ICMMO/LEMHE - Orsay, SRMP-CEA Saclay



System and numerical methods

Cu-Ag

- strong tendency to phase separation
- $r_{\text{Ag}} > r_{\text{Cu}}$, $\Delta r / r = 13\%$
- $\gamma_{\text{Ag}} < \gamma_{\text{Cu}}$

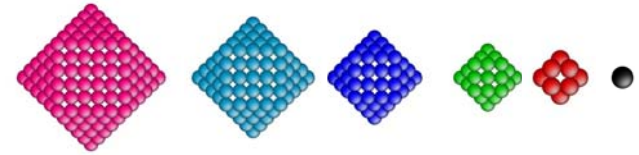
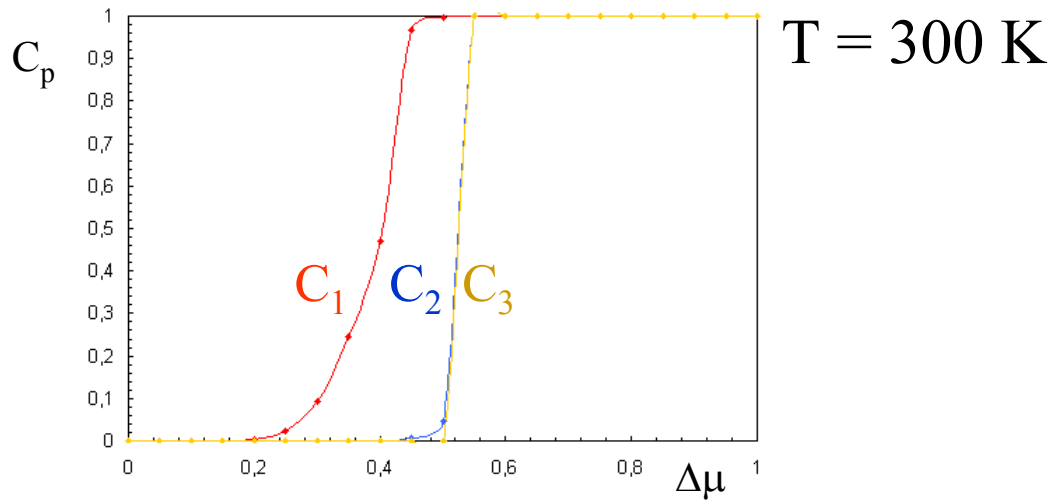


405-atom truncated octahedron

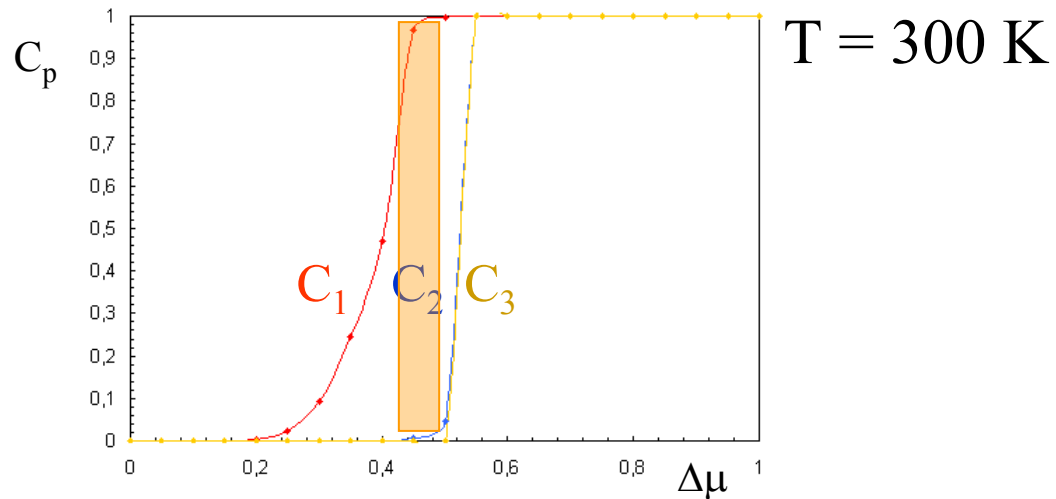
Monte Carlo simulations N -body interatomic potentials

- GC : Pseudo-grand canonical ensemble
- C : Canonical ensemble

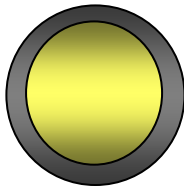
From the outer shell isotherm... to the different sites



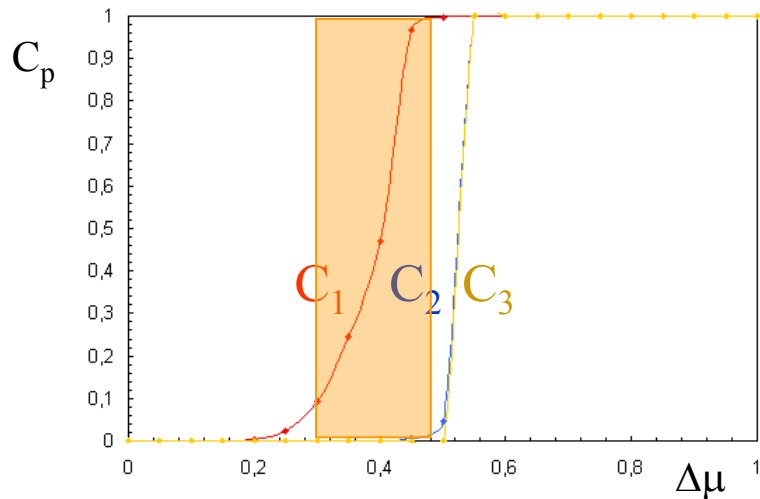
From the outer shell isotherm... to the different sites



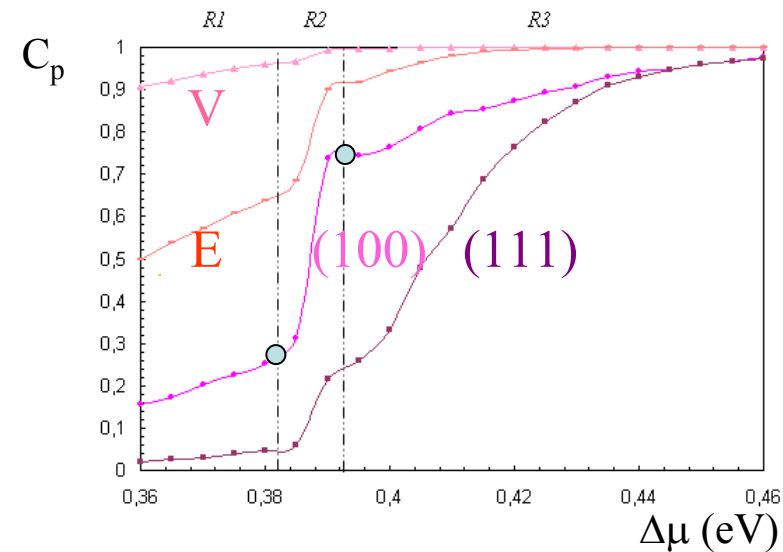
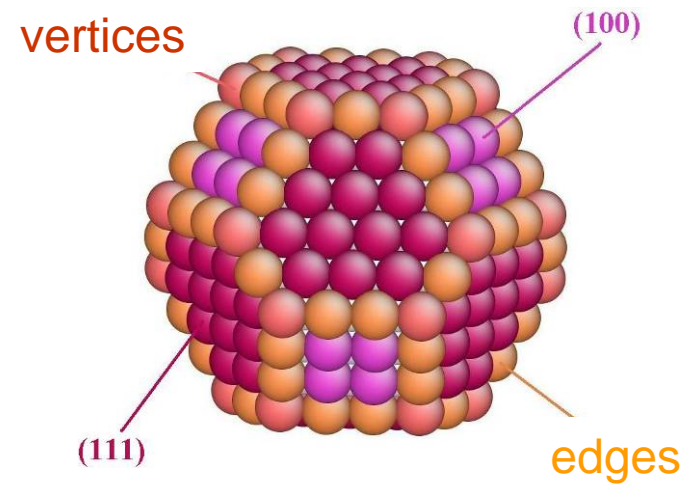
‘core-shell’



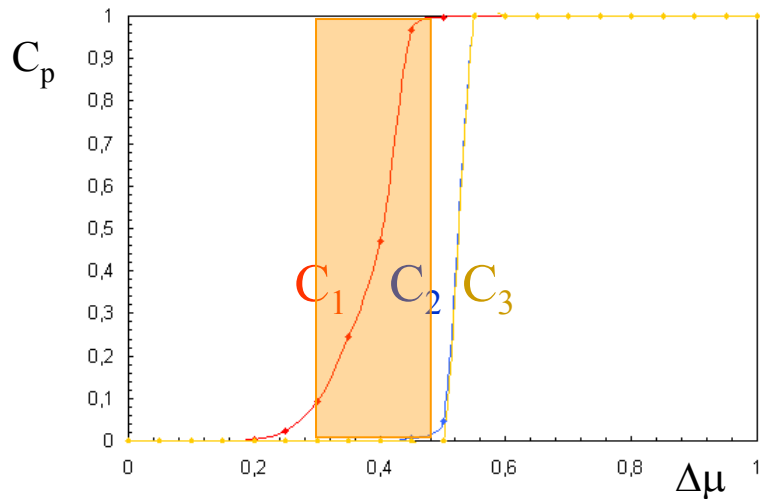
From the outer shell isotherm... to the different sites



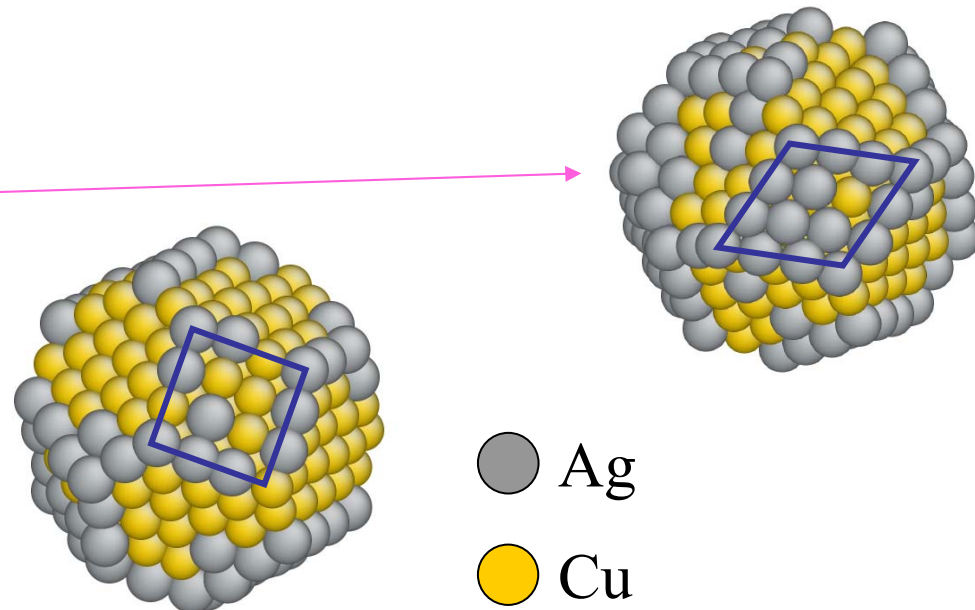
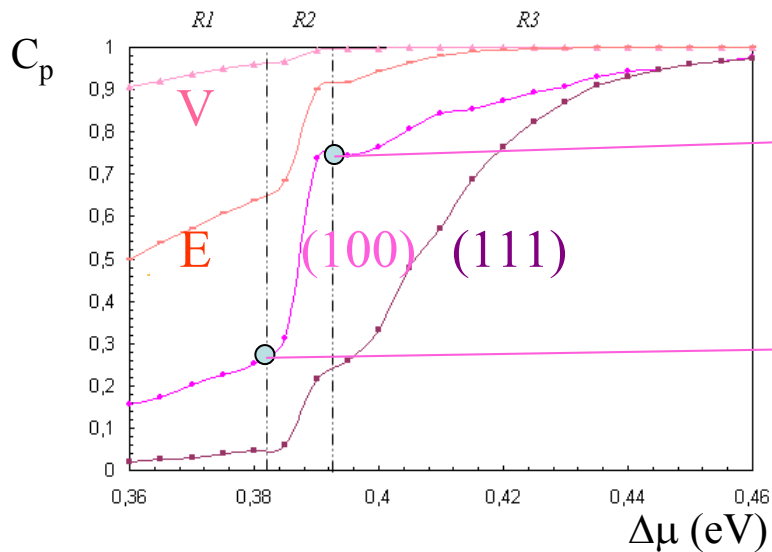
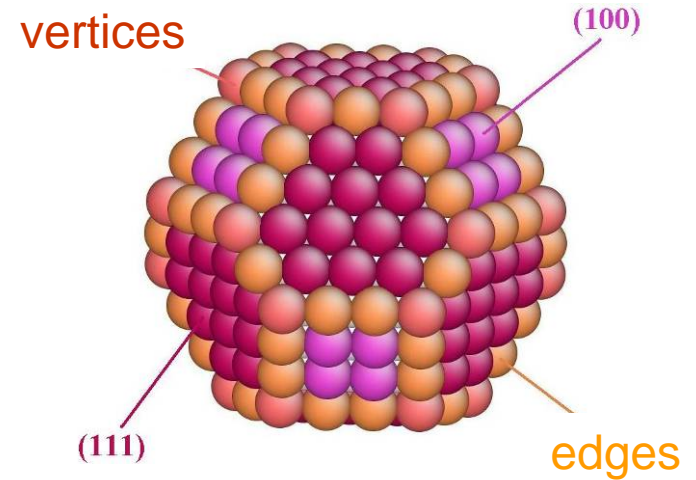
$T = 300$ K

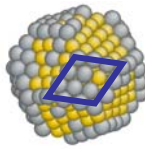
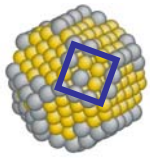


From the outer shell isotherm... to the different sites



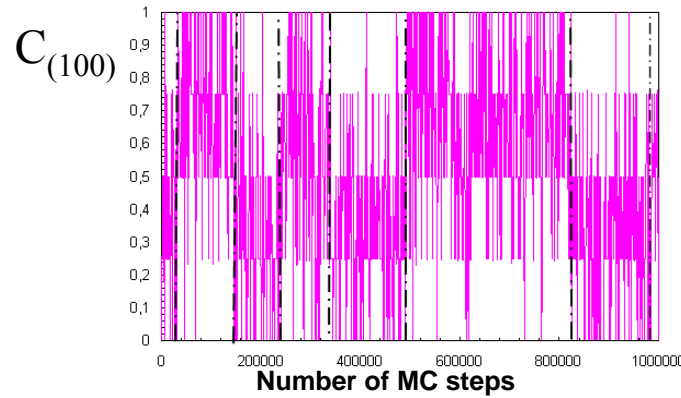
$T = 300$ K





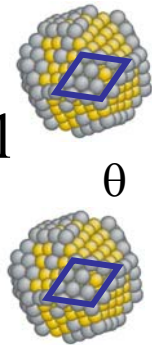
Chemical and structural bi-stability

One (001)
facet

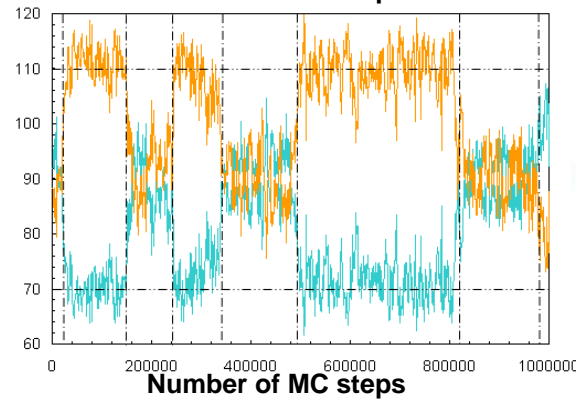


Chemical-

Angles of all
(001) facets

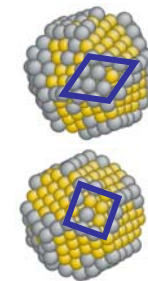
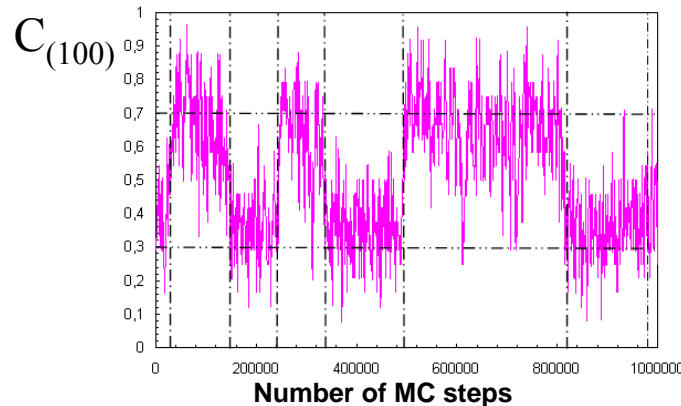


θ



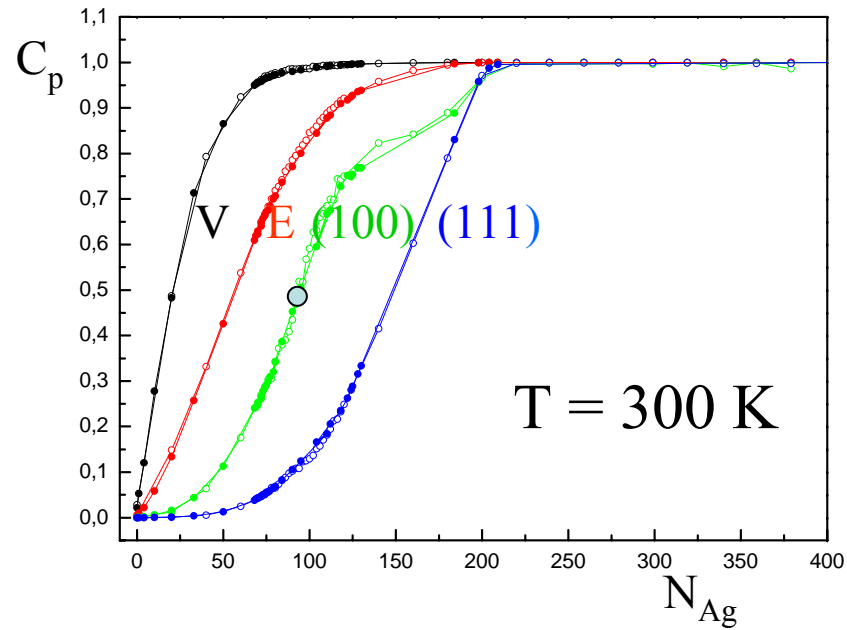
Structural-

All (001)
facets



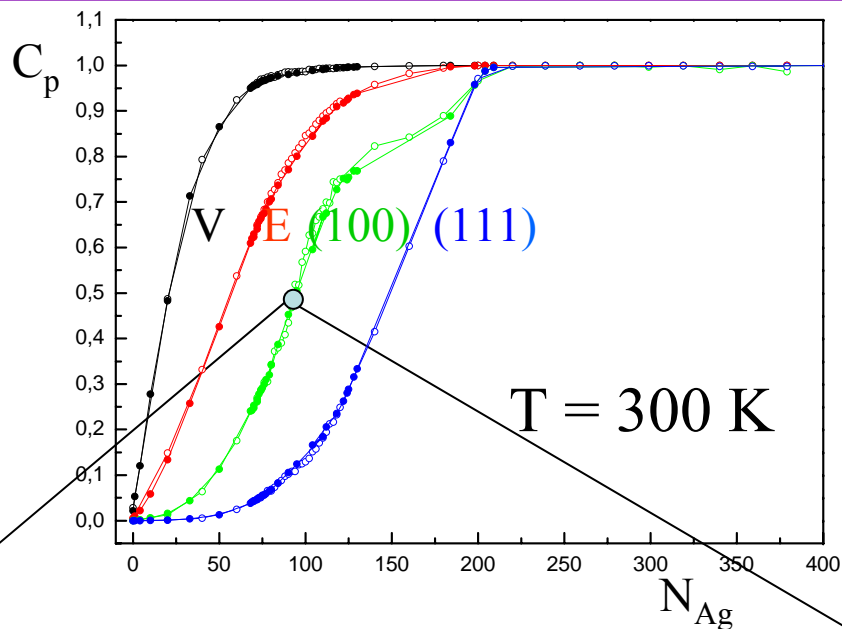
Collective
Bi-stability

From GC... to C...



$C \equiv GC$!!!

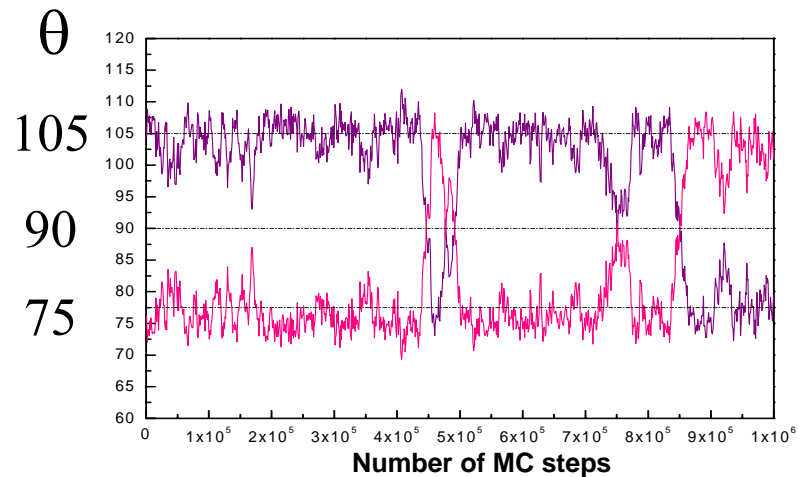
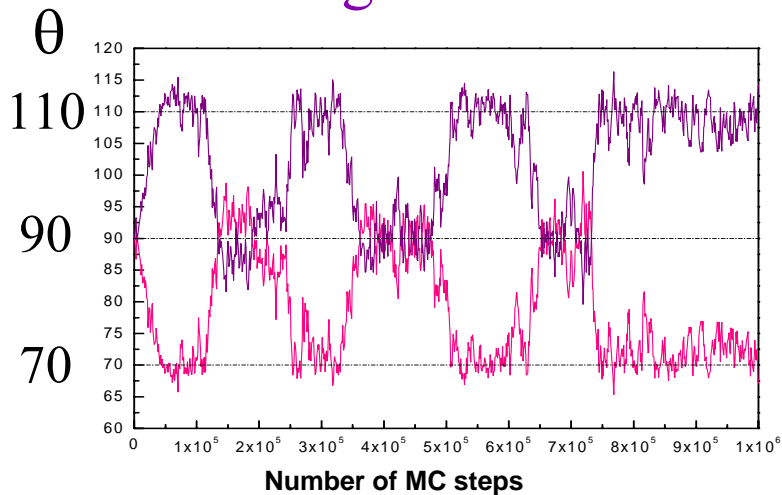
From GC... to C...

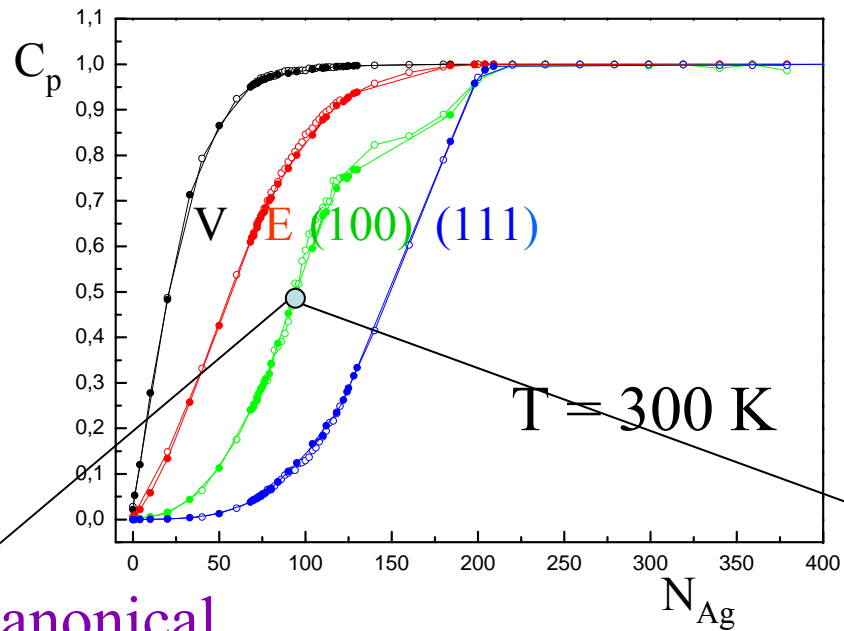


C \equiv GC !!!

Pseudo-grand canonical

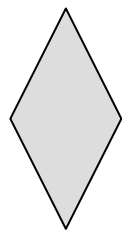
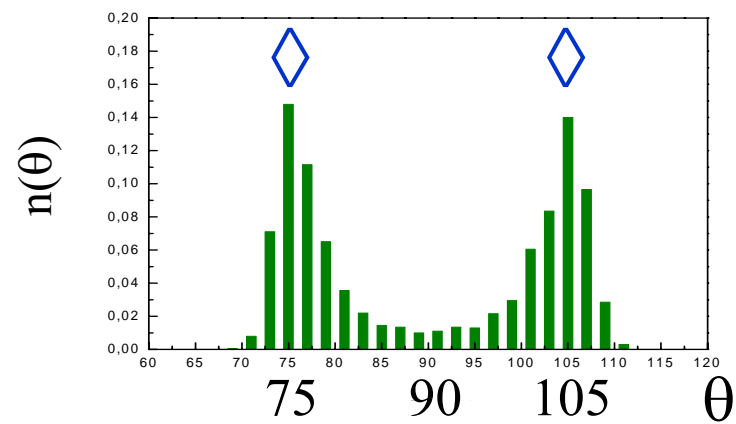
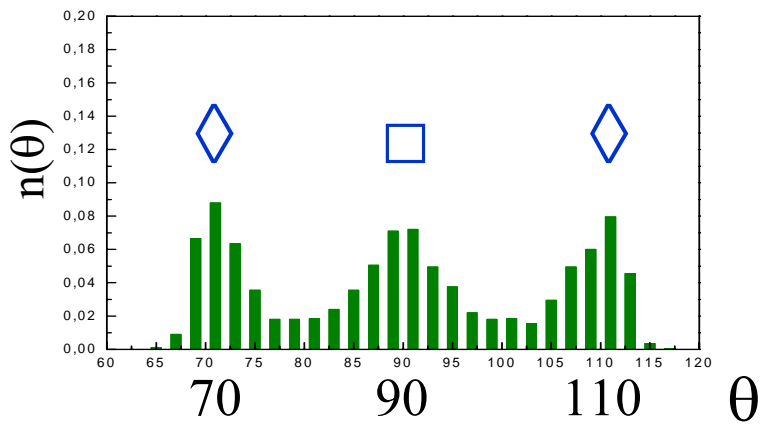
Canonical



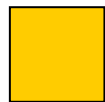


Pseudo-grand canonical

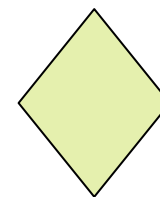
Canonical



+



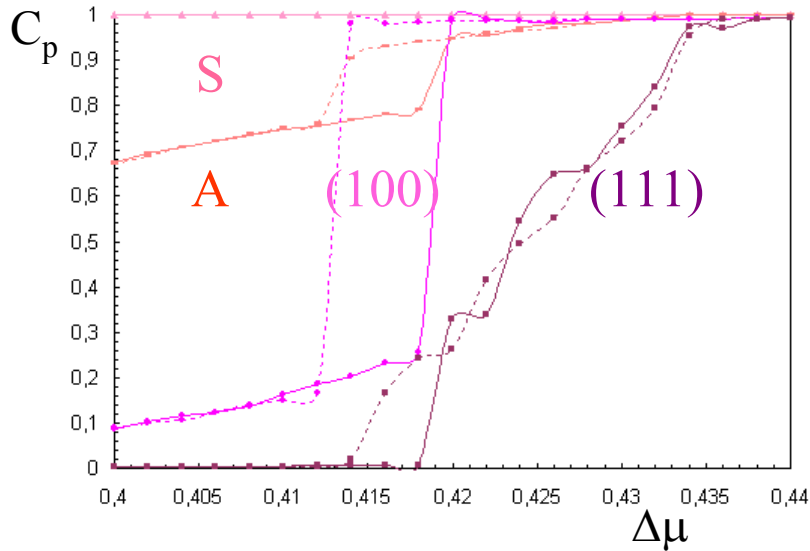
≡



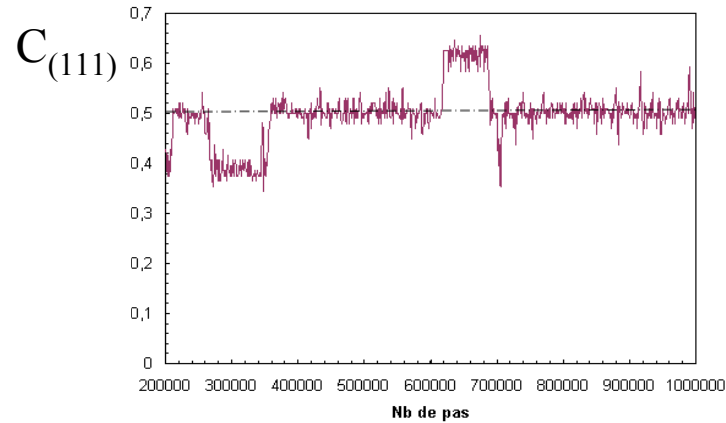
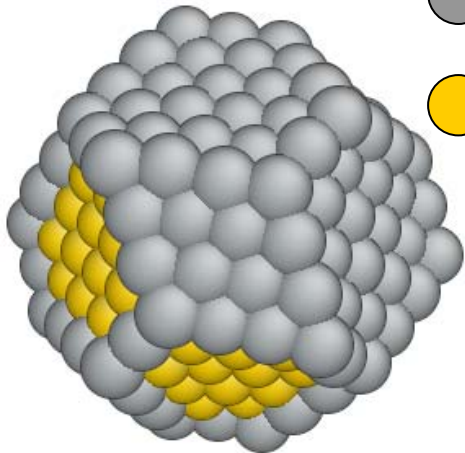
Experimental observations ???

From (001) to (111) facets

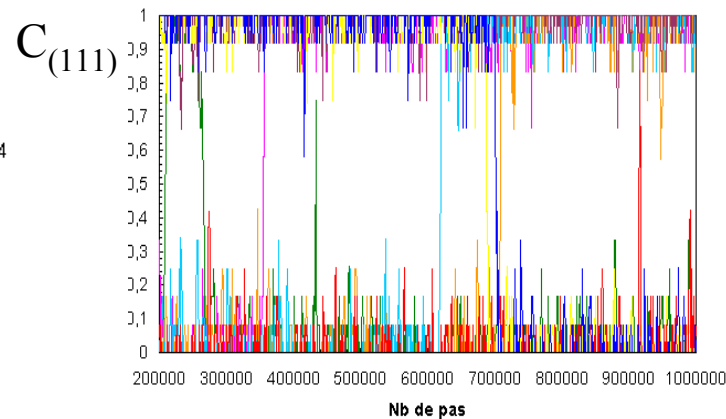
T = 130 K



● Ag
● Cu



All (111) facets



one (111) facet

(111) : individual chemical bi-stability

GC \equiv Canonique multi-objects