VOLUME 61, NUMBER 13 PHYSICAL REVIEW LETTERS

Epitaxial Eff'ects on Coherent Phase Diagrams of Alloys

26 SEPTEMBER 1988

D. M. Wood and Alex Zunger
Solar Energy Research Institute, Golden, Colorado 8040I
(Received 7 June 1988)

Using a cluster description of a coherent binary alloy, we predict and contrast bulk and epitaxial composition-temperature phase diagrams. For alloys with stable ordered compounds in bulk, epitaxial growth away from the lattice-matched composition distorts phase boundaries and changes ordering tem-peratures. For alloys insoluble in bulk

VOLUME 61, NUMBER 13 PHYSICAL REVIEW LETTERS 26 SEPTEMBER 1988

or epitaxial conditions by minimization of the alloy free
energy F=E—TS with respect to the [P„]using the
cluster variation method of Kikuchi' within the tetra-
hedron approximation (i.e., including effective nearest-
neighbor interactions through four-body terms). One
can hence evaluate F for each possible state of order (taken as ordered A3B and AB3 in the L12 structure, '
ordered AB in

VOLUME 61, NUMBER 13 PHYSICAL REVIEW LETTERS 26 SEPTEMBER 1988

900

8QO—

(B) a = Cu3Au
T = 6893
x = 0 267

P

= CuAuI
T = 7131
x = Q.499

I I

l

Bulk CuI.

VOLUME 61, NUMBER 13 PHYSICAL REVIEW LETTERS 26 SEPTEMBER 1988

value by a factor & 20, making this a very conservative
estimate.

In conclusion, we have developed a microscopic
cluster-based formalism which makes possible