First-Principles Predictions of Yet-Unobserved Ordered Structures in the Ag-Pd Phase Diagram

Na4 a Re e ab e E e La 0.0L8 44 11 -- 4 1. a dPL 4e .

e a d e 4 a e f 4 e 4e e a4 e,

D 10.110 P Re. Le. 48 .1 0

PACS be 1. .D , 1.4 .B

A 4e e a4 e e ed, a e b b a d e. e 4 a e 4 e a e e a a4e de . E e e 4a 1 4 , A -Pd 4 f 4 a c b e d - de ed d 4 d 4 ~800

ab . e

a d

0.5 0.5 e4a .

50% 50%

e4a . e4a .

1_0 2 1_1

e4a .

$1-x$ x

$x = 0.50$ 3

1_2

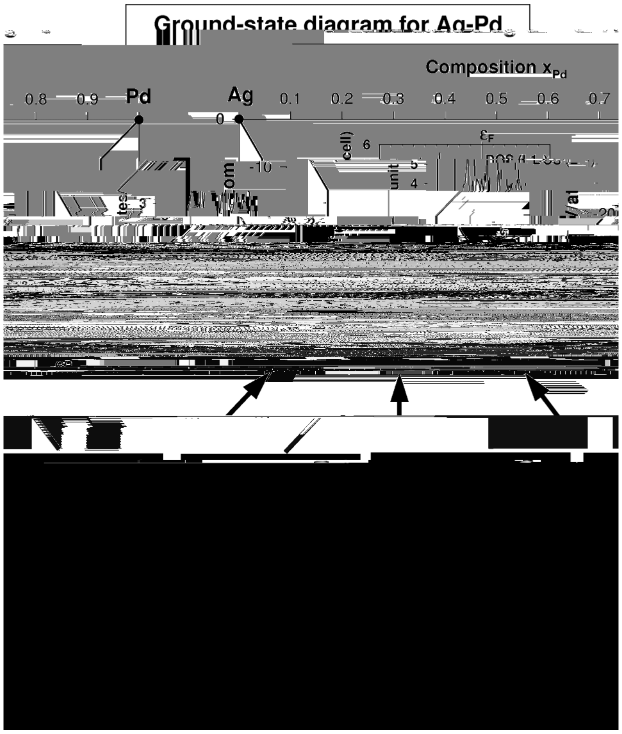
$x = 0.50$

A_{1-x} x

2

A (10)

( ) $= 1, \ldots, 2$



[illegible] $= 0$ [illegible] $x_{\rm Pd} = 0.25$ [illegible] 1_1 [illegible]

[illegible] $= 340$ [illegible] $x =$ 0.25 [illegible] $= 1235$ [illegible] $x \rightarrow 0$ [illegible] $= 1828$ [illegible] $x \rightarrow 1$ [illegible] $= 500$ [illegible] $x = 0.25, 0.50, 075$ [illegible]

e - $4fac4$ $e4a$.

1_1

1_1 1_0

1_1 1_0

1_1

1_0

1_1 1_0

1_1 1