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Thermodynamic instability of Ag/Au and Cu/Pd metal superlattices

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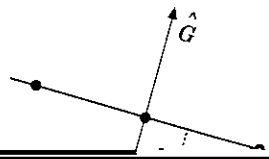
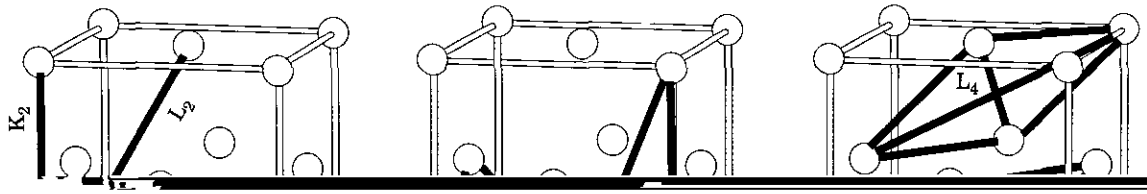
We show how the formation energies of A_pB_q superlattices with arbitrary periods p and q and


$\hat{G}$

$$\Delta E_{CS}(\hat{G}) = \frac{p}{p+q}[E_A(\hat{G},a_s) - E_A(a_A)] + \frac{q}{p+q}[E_B(\hat{G},a_s) - E_B(a_B)]. \quad (5)$$

For lattice matched constituents ($a_A \sim a_B$) we thus expect $\Delta E_{CS} \approx 0$ and $\delta H_{SL} = \Delta H_{SL}$ while in lattice mismatched systems $\Delta E_{CS} > 0$ and $\delta H_{SL} < \Delta H_{SL}$, so *bulk unstable SLs* ($\Delta H_{SL} > 0$) *can become epi-*


K2
L2
L4

that often atoms move off their ideal lattice sites ('relaxation') and that when this happens the

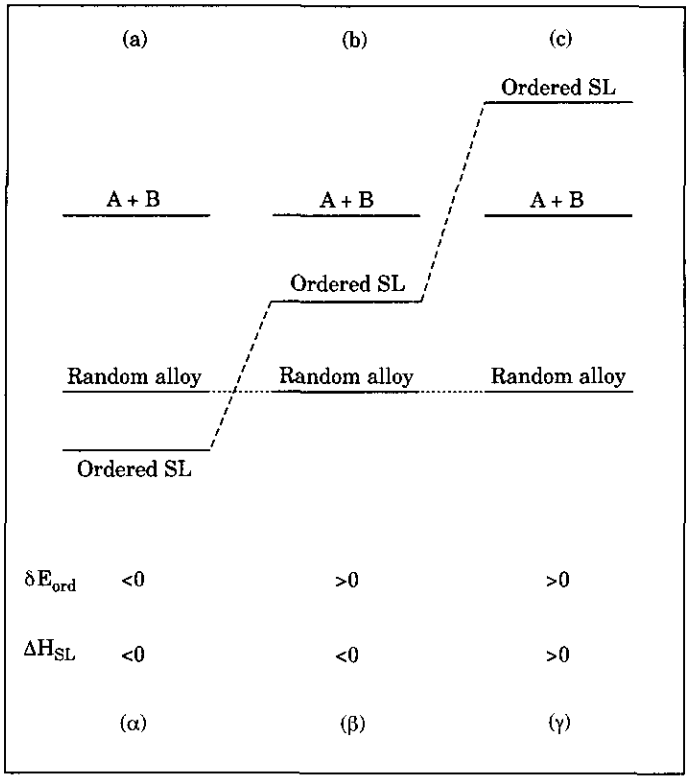
Laks *et al.* [10] introduced, at this point, two modifications:

Table 3: Directly calculated relaxed LDA excess energies $\Delta E_{\text{direct}}(\sigma)$ (error ± 2 meV atom^{-1}) and the corresponding cluster expanded [Eq. (17) and (19)] formation energies $\Delta E_{\text{CE}}(\sigma)$ (in meV atom^{-1}) for Ag-Au. See caption for Table 2 for definition of the structures. The structures labeled here with the symbol * are used in the fit of eqn (19); others are for predictions.

Orientation formula	[001]	[011]	[012]	[111]	[113]
AB	$L1_0$*	$L1_0$*	$L1_0$*	$L1_1$*	$L1_1$*
ΔE_{direct}	−59.7	−59.7	−59.7	−43.0	−43.0
ΔE_{CE}	−58.7	−58.7	−58.7	−43.5	−43.5
A_2B	$\beta 1$*	$MoPt_2$	$MoPt_2$	$\alpha 1$*	$MoPt_2$
ΔE_{direct}	−40.8	−49.7	−49.7	−30.2	−49.7
ΔE_{CE}	−40.4	−47.2	−47.2	−29.0	−47.2
AB_3	$\beta 2$	$MoPt_2$	$MoPt_2$	$\alpha 2$*	$MoPt_2$

tures $\{\sigma'\}$ that are not used to obtain $\{J\}$s. Comparing with directly-calculated LAPW values, we find an average prediction error of $\delta \sim 1.5$ meV atom^{-1}, with a maximum prediction error of 2.5 meV

Table 5: Constituent strain energy $\Delta E^{eq}(\hat{G}, \nu)$ $(x = 1/2)$ and


(a)
(b)
(c)
Ordered SL
A + B
A + B
A + B
Ordered SL
Random alloy
Random alloy
Random alloy
Ordered SL
δE_{ord} <0 >0 >0
ΔH_{SL} <0 <0 >0
(α) (β) (γ)

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