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

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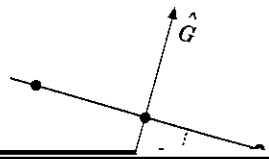
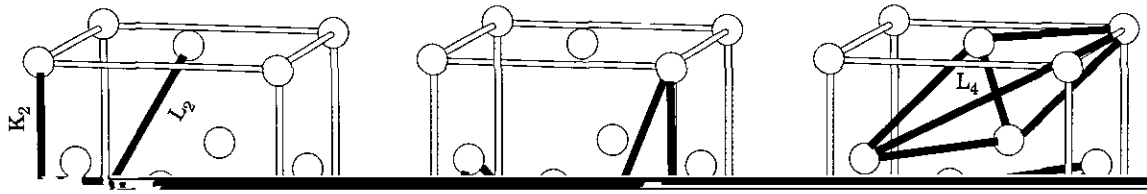
We show how the formation energies of $A_pB_q$ superlattices with arbitrary periods $p$ and $q$ and


$\hat{G}$

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

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

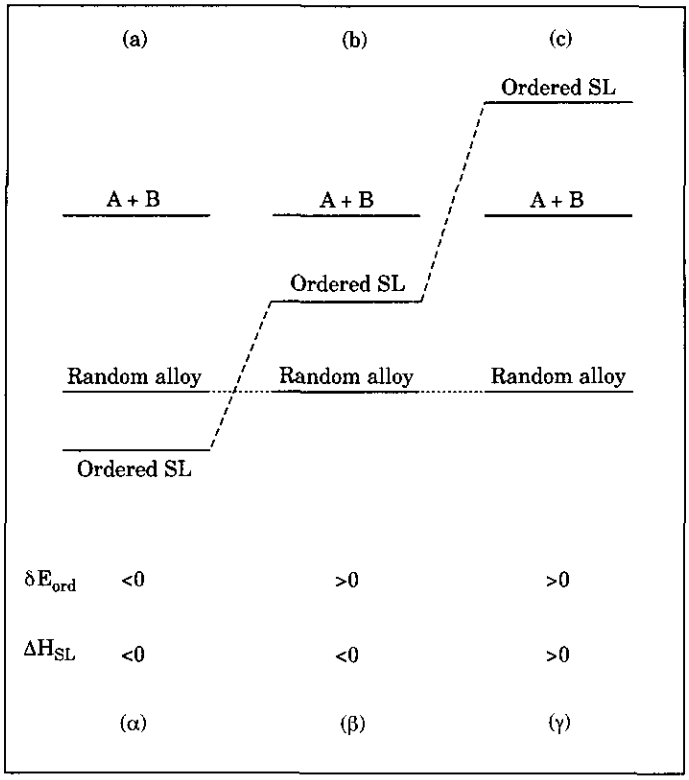
Laks *et al.* [10] introduced, at this point, two modifications:

**Table 3:** Directly calculated relaxed LDA excess energies $\Delta E_{\text{direct}}(\sigma)$ (error $\pm 2$ 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] |
|---|---|---|---|---|---|
| $AB$ | $L1_0$* | $L1_0$* | $L1_0$* | $L1_1$* | $L1_1$* |
| $\Delta E_{\text{direct}}$ | −59.7 | −59.7 | −59.7 | −43.0 | −43.0 |
| $\Delta E_{\text{CE}}$ | −58.7 | −58.7 | −58.7 | −43.5 | −43.5 |
| $A_2B$ | $\beta 1$* | $MoPt_2$ | $MoPt_2$ | $\alpha 1$* | $MoPt_2$ |
| $\Delta E_{\text{direct}}$ | −40.8 | −49.7 | −49.7 | −30.2 | −49.7 |
| $\Delta E_{\text{CE}}$ | −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
$\delta E_{ord}$ <0 >0 >0
$\Delta H_{SL}$ <0 <0 >0
(α) (β) (γ)

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## References