



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

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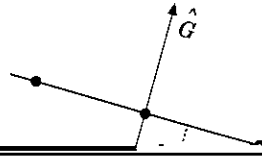
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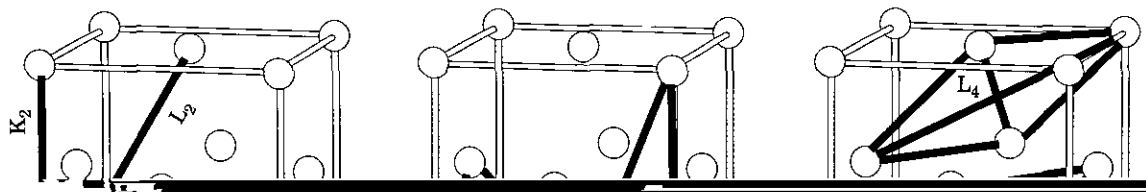
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We show how the formation energies of A_pB_q superlattices with arbitrary periods p and q and



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

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



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

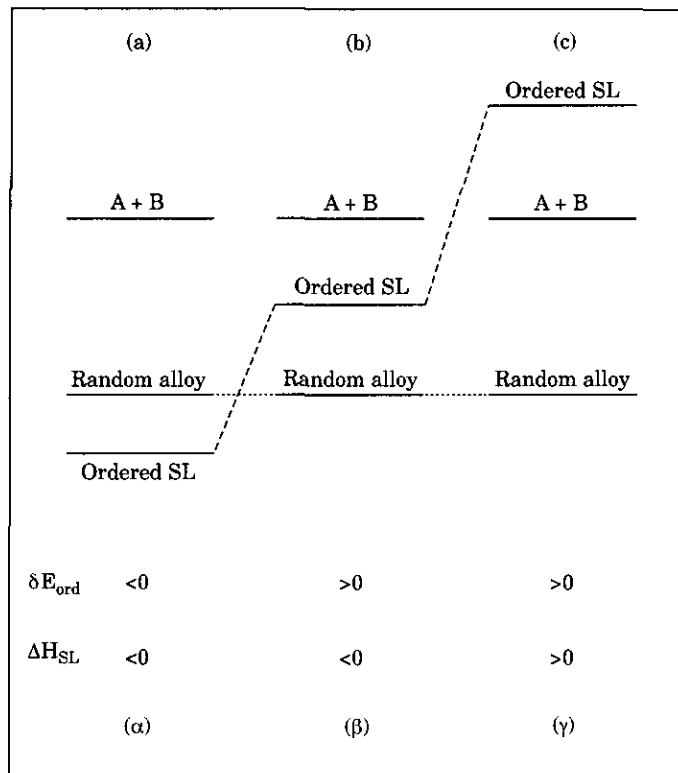
Lake *et al.* [10] introduced, at this point, two modifications:

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] |
|----------------------------|-------------------------------|------------------------|------------------------|--------------------------------|------------------------|
| <i>AB</i> | <i>L1₀*</i> | <i>L1₀*</i> | <i>L1₀*</i> | <i>L1₁*</i> | <i>L1₁*</i> |
| ΔE_{direct} | -59.7 | -59.7 | -59.7 | -43.0 | -43.0 |
| ΔE_{CE} | -58.7 | -58.7 | -58.7 | -43.5 | -43.5 |
| <i>A₂B</i> | <i>$\beta 1^*$</i> | MoPt ₂ | MoPt ₂ | <i>$\alpha 1^*$</i> | 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 |
| <i>AB₂</i> | <i>$\beta 2$</i> | MoPt ₃ | MoPt ₃ | <i>$\alpha 2^*$</i> | MoPt ₃ |

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

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



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