structures, appearing at compositions $x = 0$, 0.25, 0.5, 0.75, and 1. However, in 1973, Anderson [9] noted experimentally the existence of a group of crystalline materials where, ''within certain composition limits, every possible composition can attain a unique, fully ordered structure without defects.'' Furthermore, such ''infinitely adaptive structures'' had a multiplicity of discrete higher energy, fully ordered structures which were separated energetically by only a small amount, for any one composition. An example of the then recognized [9] infinitely

D_f stands for the number of equivalent clusters per lattice

Cu_2Au_3, $CuAu_2$, $NiPt_7$ as 412, 516, 575, 587, 597, and 371 K, respectively.

A[illegible].—Figure 1 shows that in the heavy metal rich compositions there is a (quasi)continuum [21] of ordered structures, separated at each composition by only a vanishingly small energy difference from the next excited configurations. Examining the crystal structures at those compositions, we find that they are all made from (001) stacking of two simple fcc lattice planes, denoted in

the (001) direction is particularly soft [Fig. 3(b)], thus offering a clear structural selectivity. On the other hand, the chemical energy is less selective here: The calculated Cu-Au bond strength of 179 kJ/mol (cohesive energy per bond obtained by adding the theoretical compound heat of formation to the experimental heat of atomization of the elemental solids [24]) is rather similar to the Cu-Cu or Au-Au bond strength (168 kJ/mol and 184 kJ/mol for Cu-Cu and Au-Au, respectively). Therefore, there is no large chemical penalty for forming planes of pure Cu-Cu or pure Au-Au bonds without cross Cu-Au bonds, yet there is a substantial gain in strain energy [particularly for (001) stacking] in doing so. Thus, the ground state structures are based on (001) stacking of type-I planes (Fig. 2), consisting of pure Cu and pure Au. The reason that the stable repeat unit consists of a subunit of $(\mathrm{I_{Cu}})_1(\mathrm{I_{Au}})_1 \equiv L1_0$ layered with n monolayers of Au is that this particular structural motif offers exceptionally low (001) strain: the $L1_0$ structure of CuAu has tetragonal symmetry, permitting its (001) tetragonal c/a ratio to deviate from 1. Our calculations show that $c/a = 0.915$. This (001) shrinkage is accompanied (via the volume conservation principle) by a significant expansion of the in-plane lattice constant, beyond the 50%-50% (Vegard) value. This in-plane expansion gives $a_{\text{in-plane}}$ that is nearly (within 3.2%) lattice matched with pure fcc Au. Thus, (001) stacking of Au on $L1_0$ CuAu costs only little strain energy. This suggests that the Au-rich alloy will have particularly low interfacial energies, with potential implications on microstructural morphology.

In the NiPt system one can draw a similar conclusion about the stacking of the planes along the (001) direction, since the strain energy of NiPt is very similar to that in CuAu; i.e., strain energy along the (001) direction at the Pt-rich region is much softer with respect to the other high symmetric directions. Therefore, as in the CuAu system one expects to see adaptive structures with (001) orientation at the Pt-rich region. However, contrary to the CuAu system, the Ni-Pt bond strength (calculated at 252 kJ/mol) is stronger than the Ni-Ni bond (214 kJ/mol [24]), which means the pure Ni atomic planes are unfavorable. But the pure Pt atomic planes are energetically favorable because of the strong Pt-Pt bonds (282 kJ/mol [24]). Consequently, adaptive structures at the Pt-rich side prefer to have mixed Ni-Pt (001) planes layered with pure Pt planes, but without pure Ni planes.

We conclude that fcc adaptive structures of the sort discovered here must contain an fcc element whose bcc energy is not too high above fcc (Cu, Ni), and a larger element (Pt, Au) that acts to expand the smaller element into the regime of its transition to bcc, thus creating asymmetric (001) strain softness. We call for experimental testing of this novel concept of phase ordering.

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