Prediction of alloy precipitate shapes from first principles

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 $1-$ alloy $\frac{1}{2}$ may confidently $\frac{1}{2}$ siste out of homogeneous single-phase regions (such as ordered compounds A \bar{B}_1 , or disordered compounds \bar{A}_1 solid solutions) as well as heterogeneous, phase-coexistence regions (such as phase-separation). First-principles calculations based on the density-functional approach have been very useful approach have been very useful approach \mathcal{A}_c in helping one to understand the stability of simple single-phased materials. This includes calculations of perfectly *ordered compounds* [2] as well as perfectly *random alloys* [3, 4], both requiring for their crystallographic description only small unit cells, containing O(10) atoms. The restriction to simple homogeneous structures leaves unexplored significant portions of the theoretical por phase diagrams of many materials. Perhaps the best-known examples of heterogeneous phase coexistence are phase separation of an allow into its constituents f_1 and A_{1-} B \Rightarrow (1−x A xB \overline{f} , into a constituent plus a compound A_{1-} B \rightleftharpoons A_3B \overline{A} . Such solid-state decomposition reactions create *precipitates* which define an important part of the microstructure of many allows the early stage of the early stage of the formations the formation of the formations o of *coherent precipitates* that adopt the crystallographic lattice of the alloy from which they emerge [5]. Coherent precipitates have practical importance, as they act to impede dislocation motion, and thus lead to "precipitation" in many allows $\frac{m}{\sqrt{5}}$. Despite the im-despite their importance, precipitate microstructures were thus far not amenable to first-principles theories, since the their description requires \mathcal{C} containing 103–105 atoms or more, well beyond beyond beyond beyond beyond \mathcal{C} current capabilities of first-principles methods. Of particular interest are the *shapes* and *sizes* of precipitates which are found to be strongly correlated: For example, Al¹[−] Cu alloys exhibit a transition of coherent precipitates from {100

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 θ , 1 \sim θ \sim θ \sim θ \sim θ \sim θ \sim θ \approx θ $\$ shown. With decreasing temperature, the shape changes from a nearly spherical (large c/a) to a more c \Box **b** (since c/a) form.

Mean precipitate radius r_m [

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