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Predictions of New Semiconductor of Transition Metal Structures and Their Properties

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I describe how one can use the "Cluster Expansion Method" to predict systematically what are the thermodynamical-
ly stable crystal structures on a given lattice type. The method is used to illustrate how high temperature and low

I will discuss here the prospects of the recently developed "cluster expansion methods"⁶⁾ which allow one to

system.¹³⁾ For example, information about the values of the J 's may be extracted from experimental critical tem-

peratures.¹³⁾ This approach is the simplest, but it provides

atomic configurations and, (ii) obtain the temperature-composition phase diagram in a *first-principles manner*,

little new information about the properties of the alloy. *The second approach* is to determine the J 's by treating

ground state search comparing different structures at the same composition as well as the stability of the

form, Cu, Pd, Pt, and Rh are all fcc metals, their 50%-

homogeneous structure against mixing of two (ordered range of structural symmetries.^{24,25} CuAu has the fcc-

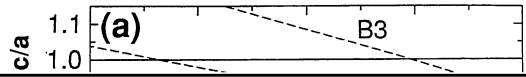
metries established clearly from experiment²⁴⁾ are also layer (AC)₁/(BC)₁ superlattices in the (111) orientation³²⁾
found theoretically, see the end of the article (the "C-D-like structure"). The degree of ordering

ted from the basis set used to extract J_F some of the struc- never perfect; it can however, be maximized in certain
tures which are known to be ground states. Note the growth temperature ranges and substrate misorienta-

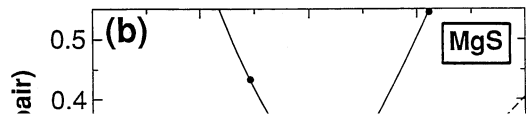
grown on GaAs⁴²⁾ (rather than the alloy). There are now experimental confirmations of this idea.⁴³⁾ (ii) Use of strain to convert the *indirect* gap Si_nGe_n SL grown on Si to a *direct* gap SL when grown on Si_{1-x}Ge_x or on some Ge

The terms in brackets are the nearest-neighbor terms of eq. (3). All odd terms were omitted, assuming that the Hamiltonian is invariant under the A ↔ B interchange. Using the LADW method we have calculated the

[Fig. 6(b)]. The maximum equilibrium solubility of ZnSe in CuInSe₂ with the chalcopyrite structure is 22% (at T = 770 K) while CuInSe₂ becomes completely soluble in



order temperature of CuInSe₂. Our results hence show that, contrary to the other known heterostructural ternary alloy (GaAs)_{1-x}Ge_{2x}, characterized by vanishing solid solubility of (CuInSe₂)_{1-x}(ZnSe)_x, should exhibit substan



2) D. M. Wood and A. Zunger: Phys. Rev B 34 (1986) 4105.

24) P. M. Hansen: *Constitution of Binary Alloys* (McGraw-Hill, New York, 1958).

3) A. E. Carlson, D. M. Wood and A. Zunger: Phys. Rev. B 32