SESSION E17: DCMP: ELECTRONIC STRUCTURE: METALS AND ALLOYS
Tuesday morning, 23 March 1993; Room 606 at 8:OO; 0. Johnson, presiding

Invited Paper

8:OO

E17 1 Predicting Stable Structures of Intermetallic Compounds.*

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The voluminous catalogues of phase-diagrams of intermetallic compounds testify to the great structural diversity in these systems. Attempts have previously been made at explaining this type of selectivity by contrasting the self-consistently calculated total energies of a few ordered structures. Such calculations select but a small, O(l0) set of "intuitive structures" out of the 2N possible configurations of two types of atoms on a fixed lattice with N sites, searching for the lowest energy. Clearly, the potential for omitting unsuspected, yet stable structures, is great. We use instead first-principles calculations of the total energies of O(l0) structures to define a multi-spin Ising Hamiltonian, whose ground state structures can be systematically searched using methods of lattice theories. This is illustrated here for the intermetallic compounds AlNi, CuRh, CuPd, CuPt, CuAu, PtAu, PtPd, PtRh, PtNi, and PdRh, [1,2] for which the correct ground states are identified out of N 65,000 configurations. This establishes a direct and systematic link between the electronic structure and phase stability. The analysis reveals intriguing cases such as relativity-induced long-range order (NiPt) and phase separation (PtAu).3 Combined with simulated annealing, such an Ising expansion yields thermodynamic quantities, and short range order parameters which can be compared with experiment.

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'2. W. Lu, S.-H. Wei, A. Zunger, Phys. Rev. Lett. 88, 1973 (1991); ibid 68, 1961 (1992).
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