4-16 wt. pct. transforms to a stable close packed phase under pressure without the occurrence of reversion. The addition of manganese to iron also decreases the transition pressure from 133 kbar for pure Fe to less than 70 kbar for Fe-14Mn. X-ray diffraction, electron-probe microanalysis, electron microscopy, and density results indicate that for the Fe-4Mn and Fe-7Mn alloys, the FCC phase has been stabilized after shock deformation, while the ϵ -phase has been stabilized for the Fe-14Mn alloy. Saturation magnetization studies have detected a residual

reduction in magnetization due to the retainment of the high pressure phase. The results have shown that manganese has modified the temperature-pressure diagram of iron by increasing the field of stability of the FCC and HCP phase. In addition, the reversion to a BCC structure has been prevented by two sets of dislocations interacting to form an extremely high dislocation density,

*Work supported by NWL, Dahlgren; and ARPA

WEDNESDAY AFTERNOON, 31 MARCH 1971

EMBASSY ROOM-PICK-CARTER AT 2:00 P.M.

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(L. F. MATTHEISS presiding)

Energy Bands in Metals (Alloys, Compounds)

Invited Paper

FH 1. Photoemission Studies of Solids and Surfaces. DEAN E. EASTMAN, IBM Yorktown. (30 min)

Windowless photoemission spectroscopy measurements of the energy levels of solids and surfaces using photon energies from 10 to 41 eV will be described. Examples include measurements of d-band structure and optical excitations in crystalline and liquids Au, as well as energy level measurements of metal hydrides (Pd/H) and magnetic semiconductors (EuS). Measurements of chemisorbed gasses and surface oxides will also be described (H $_2$, N $_2$, CO, CO $_2$ and O $_2$ on Ti metal).

*Supported by the Air Force Office of Scientific Research.

Contributed Papers

Electron States of Ordered Copper-Nickel Alloys.* A. C. SWITENDICK, Sandia Laboratories -- APW band calculations have been performed for a cubic structure A3B where A or B = Cu or Ni or Z (a zero potential region). B is at the cube corners and the A's are in the face centers. For Cu3Cu the fcc Brillouin zone is just mapped back onto the cubic zone four times $\Gamma \to \Gamma$, $X \to \Gamma$, $L \to R$, $W \to X$, etc. For A₃B, B \neq A the cubic zone becomes appropriate and certain of the original states having charge density at the B site are modified. For Cu3Ni the modified states are elevated in energy and a set of dbands which are associated with the nickel site are above the original copper d-bands. For NigCu the modified states are more uniformly distributed throughout the nickel d-band energy range. These results are in qualitative agreement with the photoemission results of Seib and Spicerl for nickel-copper alloys which they interpreted in terms of an Anderson-like model.

* Work supported by the U. S. Atomic Energy Commission. 1 D. H. Seib and W. B. Spicer, Phys. Rev. B 2, 1676, 1694 (1970).

FH 3 Calculation of Electronic Properties of Noble Metal Alloys in the Rigid-band Model,* J.M.TRACY and R.H.CAMPBELL, Univ. of Washington--The density of states, optical mass and the intraband conductivity tensor elements have been calculated for the constant energy surfaces of noble metals using the Fermi surface expansion parameters given by Halse¹. Different constant energy surfaces simulate the Fermi surfaces for alloys of different electron-per-atom ratios in the strict rigid-band model. The calculations are useful to compare qualitative expectations with experimental results for weak-scattering alloys. The behavior around the expected second set of Fermi surface necks is of particular interest. A comparison of the calculations with the measured Polar Reflection Faraday Effect in α -phase silver-cadmium alloys will be given.

*Research supported by the Air Force Office of Scientific Research and the National Science Foundation.

M.R. Halse, Phil. Trans. Roy. Soc. 265, 1167 (1969).

FH 4 Application of Coherent Potential Theory of Off-Diagonal Randomness to Disordered Binary Alloy.* S.M.BOSE, Drexel Univ.--The recently developed two-site coherent potential approximation has been used to describe the electronic structure of a one-dimensional disordered binary alloy. A sixth degree equation is obtained for the appropriate Green's function whose imaginary part gives a measure of the density of states. Explicit calculation of the total density of states indicates a broadening and a shift in position of the impurity band.

*Partially supported by NASA under Grant No. NGR+09-005-072.

¹T. Tanaka, K. Moorjani and S. M. Bose, Bull. Am. Phys. Soc. <u>16</u>, 102 (1971).

FH 5 Notes on the Electronic Spectrum of a One-Dimensional Randam Alloy.* J.E. Gubernatis and P.L. Taylor, Case Western Reserve Univ.--The electronic spectrum for a simple model of a one-dimensional, random, binary alloy was calculated numerically by self-consistently solving a functional equation due to Agacy and Borland. The behavior of the density of states near a band-edge was examined and found to display the type of essential singularity suggested by Lifschitz. Within the band the density of states was observed to vanish at the points predicted by Wada. Focusing on one of these points, we found that the density of states near this point exhibits the same type of essential singularity as at the band-edge. A characteristic of the spectrum is the presence of peaks. We were able to determine that these peaks

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