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paramagnetic and ferromagnetic phases of nickel by the tight binding method. The crystal potential was constructed from a superposition of free atom charge densities, and an exchange potential was included according to the Xα method. The basis set contained atomic wavefunctions consisting of linear combinations of Gaussian-type orbitals[1] for 1s, 2s, 3s, 4s, 2p, 3p, and 4p states. Individual Gaussian orbitals were used for the 3d state. The appropriate integrals were obtained by extending the work of Chaney, Tung, Lin, and Lafon.[2] Sums were carried to convergence. The resulting energy bands are very similar to other band calculations for nickel by other techniques.[1] A self consistent calculation is now under way.

*Supported by Air Force Office of Scientific Research.
[1]A.J.H. Wachters, J. Chem. Phys. 52, 1033 (1970).
[2]R.C. Chaney, T.K. Tung, C.C. Lin, E.E. Lafon, J. Chem. Phys. 52, 361 (1970).

AH 7 Phase-Shift Analysis of Copper.* JERRY C. SHAW, J. B. KETTERSON and LEE R. WINDMILLER, Argonne Nat'l. Lab.--A presentation of the results of a computer study of the Fermi-surface parameterization scheme suggested by Ham and Segall[1] will be given. This study was conducted using the KKR formalism and a special algorithm allowing analytic calculation of band velocities and other derivatives. Quality-of-fit was quantitatively determined in the least-squares sense using the functional $\langle \Delta E^2(E_F,\eta_\ell)\rangle = (1/N)\sum_i^N (E_i-E_F)^2$, where E_i are the KKR energies corresponding to a set of N k-vectors derived from the Fourier series inversion of dHvA data, and where the Fermi energy, E_F, and the phase shifts, η_ℓ, are parameters. A discussion of uniqueness as well as comparison with the results of Cooke, et al.[2] and Lee[3] will be given. In addition, results using a least-squares-fit to the Fermi radii will be presented.
*Work performed under the auspices of the USAEC.
[1]B. Segall and F. S. Ham, Methods in Computational Physics 8, 251 (1968).
[2]J. F. Cooke, H. L. Davis and R. F. Wood, Phys. Rev. Letters 25, 28 (1970).
[3]M. J. G. Lee, Phys. Rev. 187, 901 (1969).

AH 8 **Strain-induced Deformations of the Fermi Surface of Copper.*** PETER GOESSING and J.R. CHRISTMAN, Tufts Univ.--**Changes in the Fermi energy and surface of copper due to uniaxial elongations are calculated by means of the APW method to first order in the strain parameter. Potentials for both strained and unstrained crystals are constructed by superposing atomic potentials and adding full Slater exchange. For the unstrained crystal the Fermi energy and surface obtained agree with those of Faulkner, Davis, and Joy[1] who used the KKR method. For the strained crystal a perturbation scheme is employed to trace out deformations of several energy surfaces. The volume enclosed by each is computed and the Fermi energy is obtained. Finally, the Fermi surface for the deformed crystal is calculated by fitting the previously obtained deformations to power series in the energy. Results are presented for uniaxial elongations in the [100], [110], and [111] directions.**

***Work supported in part by the National Science Foundation, grant GP 15993.**
[1]J.S. Faulkner, Harold L. Davis, and H.W. Joy. Phys. Rev. 161, 656 (1967)

AH 9 Pressure studies in Copper - A Preliminary Report D. GRAY and A. MARCUS GRAY, Watervliet Arsenal -- Due to the small size of the electronic energy changes produced by strains confined to the elastic region a perturbation approach would appear to be best. A test of our MPW computer program precision for a perturbation calculation is described. A more sophisticated perturbation approach along the lines of Christman's[1] will probably be required. A second series of calculations indicated that energy shifts due to potential effects and to geometric effects are of the same order of magnitude and can be either in the same or opposite direction. Brief comments on comparison with reflectance measurements and on symmetry changes under uniaxial strain will be given.

*Supported in part by U.S. Army Ballistic Research Labs
[1]J.R.Christman (to be published). See also: Bull. Am. Phys. Soc., 15,345 (1970).

AH 10 Pressure Dependence of the Electronic Structure of Palladium.* S.D. Das, Argonne Natl. Lab., D.D. Koelling, Northwestern Univ., and F.M. Mueller, Argonne Natl. Lab.--We have considered the effects of up to 100 kilobars of hydrostatic pressure on two experimental measurements involving the Fermi surface of palladium: dHvA extremal cross-sectional areas and positron annihilation spectra of polycrystalline samples using slit detectors. For latter calculations, the difference in the momentum dependence of the plane wave-like and d-like states has been included. Our calculations show that a decrease of 1% in the lattice constant decreases the density of states at the Fermi energy by 10% in palladium.

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AH 11 Electronic Structure and Local Atomic Environment. V. HEINE*, Bell Labs.--To study bonding, energy of defects, surfaces, etc. in transition metals, a method of calculating the electronic structure is being developed which does not depend on crystal periodicity. Based on a tight binding model, it is an extension of the method pioneered by Cyrot-Lachmann involving closed chains of atoms. With relatively little extra work it is possible to sum a large number of multiply linked chains describing the interaction of an atom with its near neighbors, and to obtain an explicit expression for the density of states instead of fitting moments.

*On leave from Cavendish Lab., Cambridge, England.

AH 12 The Pseudopotential Approach to the Optical Absorption of Simple Metals. M. ASHKIN, Westinghouse Research Labs.--The projected wave-field approach of Bassani et al[1] for incorporating the orthogonalized-plane wave method into the many body problem is used in performing a perturbation calculation, along the lines of Hopfield[2], of the absorption. The unperturbed system is the uniform part of the project wave field Hamiltonian including the electron-electron interaction and the perturbation is the remainder. Included in the calculation are all terms quadratic or bilinear in a pseudopotential and core projection. The formal expression of the model, which is exact in the uniform part of the valence electron-valence electron interaction, reduces to the form of ref. 2 for a local potential, otherwise simple screening does not obtain. Comparison with other pseudopotential methods will be made.

1. F. Bassani, J. Robinson, B. Goodman and J.R. Schrieffer, Phys. Rev. 127, 1969 (1962).
2. J.J. Hopfield, Phys. Rev. 139, A419 (1965).

AH 13 THE IMPORTANCE OF OFTEN-IGNORED CONTRIBUTIONS TO THE ORBITAL SUSCEPTIBILITY OF BLOCH ELECTRONS. WARREN D. GROBMAN, IBM Watson Research Center -- The expression for the low field susceptibility of spinless Bloch electrons in a solid, χ_{orb}, was first given by Hebborn and Sondheimer,[1] but has not yet been evaluated for realistic wave functions. We are calculating χ_{orb}