

06.5-1 THE THIRD ORDER STRAIN WAVE IN ANTIFERRO-MAGNETIC CHROMIUM. By J. Ihringer*, K. Knorr*, W. Kugler*, J. Maichle*, A.H. Millhouse**, A. Petcov**, W. Prandl*, J. Reinhardt*, Institut für Kristallographie, Universität Tübingen; ** Institut für Kristallographie, Universität Saarbrücken, Germany, Fed. Rep.

The magnetic structure of Chromium is an antiferromagnetic spin density wave (SDW) with wave vector $q_M = (2\pi/\lambda_M) \cdot (100)$ with $\lambda_M \approx 10.26 \cdot a_0$ at $T < 50$ K. This basic wave is accompanied by a weaker third order SDW having $q_{3M} = 3q_M$. The spatial inhomogeneity of the spin-/magnetization density creates, via magnetostriction, strain waves (SW). The magnitude of the magnetostriction depends on the magnetic energy density. Therefore the basic SW is expected to have a wave vector $2q_M$. It has been observed for the first time by Tsunoda et al. (Sol. State Commun. (1974) 14, 287) and was studied in some detail by Kugler (Dissertation, Tübingen, 1983) recently, in both cases by X-ray methods. Kugler proved, in particular, that the X-ray observations are due to a periodic displacement of the metal ion cores. We have investigated the possibility of higher order SW's with synchrotron radiation at HASYLAB/DESY/Hamburg using the two axis diffractometer (U. Bonse, K. Fischer, Nucl. Instr. Methods (1981) 190, 593). Due to the wavelength $\lambda = 0.53 \text{ \AA}$ used high momentum transfer measurements were possible. Most measurements were done close to the reflection $Q_0 = 2\pi H_0 = (2\pi/a) (10,0,0)$. We found a strong signal at $Q_0 + 2q_M$, no intensity at $Q_0 + 4q_M$, and a weak reflection at $Q_0 + 6q_M$. The latter observation indicates a third order harmonic SW superimposed on the basic SW. Using an absolute intensity calibration for the satellite with $2q_M$ the amplitude of the third order SW is estimated to be $(5 \pm 1.25) \times 10^{-4} \text{ \AA}$ at 10 K with a smooth decrease by about 10 % between 10 and 70 K.

06.7-1 THE BAND STRUCTURE OF SILICON BASED ON X-RAY DIFFRACTION DATA. P. Sommer-Larsen and John S. Avery. Department of Physical Chemistry, University of Copenhagen, Universitetsparken 5, 2100 O, Denmark.

The Fourier coefficients of the electron density in a crystal can be used to construct a one electron Hamiltonian. This can be used to calculate the bandstructure (J.S. Avery, P. Sommer-Larsen, M. Grodzicki - Local Density Appr. in Quant. Chem. and Solid State Phys., p. 733, Ed. Dahl and Avery, Plenum 1984).

From the high quality Pendellosung data of Aldred and Hart on Silicon (Proc. R. Soc. London, 1973, A332, p. 223), it is possible to derive an accurate static electron density for Silicon. Using the measured electron density avoids any need for self consistency. The calculated bandstructure is of high quality, and it agrees well with observed quantities.

The linear muffin tin orbital method (O.K. Andersen, Phys. Rev. 1975, B12, p.3060) and the LMTO program (H.L. Skriver, "The LMTO Method", Springer Series in Solid St. Science, 1984, vol.41, Springer). has been used in the calculation. There may be other systems than Silicon on which a band structure can be done based on their diffraction data. One candidate is Beryllium, where the data properly is of sufficient accuracy.

06.7-2 MULTIPOLE ANALYSIS OF CHARGE DENSITY AND PHYSICAL PROPERTIES : THE ALKALINE-EARTH OXIDES. By Geneviève Vidal-Valat and Jean-Pierre Vidal Groupe de Dynamique des Phases Condensées (UA CNRS 233) Université des Sciences et Techniques du Languedoc 34060 Montpellier Cedex - France and Kaarle Kurki-Suonio and Riitta Kurki-Suonio Department of Physics, University of Helsinki SF-00170 Helsinki, Finland.

The multipole analyses of the charge densities of the alkaline-earth oxides based on accurate X-Ray diffraction measurements are reviewed in a search for systematic features through the whole series from BeO to BaO (Vidal-Valat, Vidal & Kurki-Suonio, 1978, Acta Cryst., A 34, 594-602; Vidal-Valat, Vidal, Kurki-Suonio & Kurki-Suonio, 1987, Acta Cryst. A, in press).

The method of analysis leads to a semi-quantitative breakdown of the experimental information into components which are related to different physical properties of the individual ions.

A comparison with the systematics found in a tabular review of measured physical and chemical properties of the same materials leads therefore to understanding of the relations between the effective charge density and the macroscopic properties and gives some indication of the underlying mechanisms of these properties in an atomic scale.

06.7-3 PROMOTED STATES IN THE BINDING OF TRANSITION METALS. By M.G. Trefry, Department of Physics, University of Western Australia, Nedlands, Western Australia, 6009.

The role of the classical electrostatic overlap energy between atoms in their chemical binding has recently come under scrutiny (M.A. Spackman and E.N. Maslen, J. Phys. Chem., 1986, 90, 2020-27). Viewing the cohesive energy of a solid as a perturbation series in terms of distortions of the free atomic groundstate electron densities, the classical overlap term is the first term of the convergent energy series (C.L. Davis, E.N. Maslen and J.N. Varghese, Proc. R. Soc. Lond. A, 1982, 384, 57-88). Its importance in a wide range of solids has been established (M.G. Trefry, E.N. Maslen and M.A. Spackman, J. Phys. C, 1987, 20, 19-28). The one major discrepancy is gross overestimation of the cohesive energy for the 3d transition metal series. This may be understood in terms of the near-degenerate behaviour of the $(3d^n 4s^2)$ transition metal atomic groundstates. The 3d metals have low-lying atomic states closely spaced in energy but distinct in radial behaviour, giving rise to markedly different classical overlap energies. The energies of states corresponding to single electron promotion to the 3d shell ($3d^{n+1} 4s^1$) are typically one electron volt above the groundstate energy, whereas the classical overlap energies for those states may differ by between 3eV (scandium) and 8eV (vanadium). The groundstates have larger overlap energies, except for the exchange-affected metals chromium and copper. The classical overlap energy is reduced using the first promoted electronic states. This trend continues a fortiori for the doubly promoted ($3d^{n+2} 4s^0$) states. The singly-promoted states give the best first approximations to the cohesive energies and to the electron densities. This conclusion is supported experimentally, notably by positron annihilation data (O. Johnson, Phys. Stat. Sol. B, 1980, 99, 745-54).