05.1-04 CRYSTAL STRUCTURE OF β-O_2 AT 298 K AND 68 KBAR. By H. d'Amour, W. B. Holzapfel, Universität-GH Paderborn, 4790 Paderborn, Fed. Rep. Germ. and M. Nicol, Department of Chemistry, University of California, Los Angeles

Recent Raman studies on O_2 at 298 K showed three solid phases in the pressure range between 1 bar and 150 kbar. Phase I(β): 59 - 96 kbar, Phase II (α?): 96 - 99 kbar, Phase III (ε): > 99 kbar.
A single crystal of β-O_2 at 68 kbar was grown from the liquid phase by annealing the diamond-anvil cell at 50° C. The intensities were measured with a four-circle diffractometer resulting in a set of 124 symmetry-independent reflections. The crystal structure could be refined to a R-factor of 12.5 %.
The crystal data are:
298 K, 59 kbar: a = 2.849(1)Å, c = 10.232(2)Å
298 K, 68 kbar: a = 2.8078(5)Å, c = 10.218(3)Å
The compression is anisotropic with $\Delta a/a > \Delta c/c$. The structure can be viewed as a cubic close packed arrangement of the O_2-molecules, with the molecular axes parallel to the c-axis. The stacking of the (001) planes is considerably disordered and requires in the evaluation of the data a symmetry reduction from space group $R\bar{3}m$ (β-O_2 at 1 bar, ~35 K) to P321 with site occupation factors smaller than 1/3 for the double occupied 2(d) site. The third molecule in the unit cell occupies the 2(c) site.
(H. d'Amour, W. B. Holzapfel, M. Nicol, J. Phys. Chem. in press)

05.1-05 DISORDER AND PHASE TRANSITION IN COBALT. By F. Frey and H. Boysen, Institut für Kristallographie und Mineralogie, Universität München, Theresienstr.41, W-Germany.

Disorder in both allotropic phases of pure single-crystalline cobalt was studied by elastic neutron scattering in order to separate bulk from surface effects and to remove diffuse inelastic contributions. The intensity variation along (10.l), measured at different temperatures, was analysed in terms of Jagodzinski's disorder theory (Acta Cryst. (1949) 2, 201). The values found for the degree of disorder in the hcp-phase were lower than those reported before for powder samples and remain nearly unaffected when approaching the transition temperature. The fcc-phase is always (below and above the transition) well ordered. However, the temperature behaviour of the fcc- and hcp- precursor regimes in the hcp- and the fcc- modifications, respectively, is different.

The origin of the hcp$\rightarrow$fcc transition is restricted to a few nuclei only, which are preformed below T_m. The transition corresponds to a nucleus growth process. These nuclei are well ordered packets of at least 100 layers with ABC sequence. The transition mechanism is triggered by an elastic shear wave which shows an anomalous temperature behaviour in the critical region (Frey et al., J.Phys.F (1979) 9, 603). The back transformation fcc$\rightarrow$hcp is due to a different mechanism, as no true preformed hexagonal nuclei exist above T_m. In a model proposed by Seeger(Z.Metallk. (1953) 44,247) a special defect configuration corresponds to a "nucleus" for the hcp-phase, running half-dislocations provide the martensitic transition.

05.1-06 THE KINETICS OF PRESSURE INDUCED TRANSFORMATION IN TITANIUM. By A.K.Singh, Murali Mohan and C.Divakar, Materials Science Division, National Aeronautical Laboratory, Bangalore-560017, India.

The α -phase (hcp) of titanium undergoes a transformation to ω -phase (hexagonal) at high pressures (J.C.Jamieson, Science 140, 72 (1963). The α - and the transformed ω - phase exhibit a definite orientation relation (M.P.Usikov and V.A.Zilbershtein, Physica Status Solidi, 19a, 53 (1973). Under moderately high ($\sim$ 6.0 GPa) static pressures the transformation is isobaric. This transformation occurs also under shock loading (A.Kutsar, V.N.German and G.I.Nosova, Dokl. Akad. Nauk, SSSR, 213, 81 (1973). This requires that the transformation be abaric.

A detailed study of the kinetics of $\alpha \rightarrow \omega$ transformation between 5 and 9 GPa shows that the ζ - t data (ζ denotes the fraction of ω -phase and t denotes time) fit Avrami's equation. Further, the kinetics of the transformation becomes faster as the pressure is increased. The pressure dependence of the kinetics predicts that the transformation proceeds with the velocity of sound in solid at pressures around 20 GPa. This value is in reasonable agreement with the transformation pressure under shock loading conditions.

05.1-07 STRUCTURE RELATIONSHIPS IN AMERICIUM METAL. By R. B. Roof, Los Alamos National Laboratory, Los Alamos, New Mexico, U.S.A.

As a function of applied pressure americium metal exhibits four phases in the pressure region of 0 to 20 GPa. Phase I has the double-hexagonal close packed structure (McWhan, et al., J. Inorg. Nucl. Chem. (1962) 24, 1025) and occurs from 0 to 4-6 GPa. The lattice constants at 5.2 GPa are a = 3.43(1), c = 10.91(5) Å. Phase II is face-centered cubic and exists from 4-6 GPa to 10 GPa. The lattice constant at 6.5 GPa is a = 4.684 Å (Akella, et al., J. Less-Common Met. (1979) 68, 95). Phase III is an exotic double body-centered monoclinic material and occurs between 10 and 15 GPa (Roof, J. Appl. Cryst. (1981) submitted for publication). The lattice constants at 12.5 GPa are a = 3.025(5), b = 11.887(19), c = 2.830(5) Å with β = 106.11(14)°. Phase IV displays the α-U structure type from 15 to 20 GPa. The lattice constants at 17.7 GPa are a = 3.046(4), b = 5.957(9) and c = 5.148(7) Å (Roof, et al., Science (1980) 207, 1353). The change in crystal structure that occurs between each of the phases is shown to result from simple shifts in layer stacking sequences with minor adjustments in lattice constants.