

05.1-16 IN-SITU OBSERVATION OF PHASE TRANSFORMATION IN 9R POLYTYPE OF SiC AT 2000°C. By Zenzaburo INOUE and Nobuo SETAKA, National Institute for Research in Inorganic Materials, Namiki 1-1, Sakura-mura, Niihari-gun, Ibaragi 305, Japan

One of the authors (Z.I.) has recently built a high-temperature X-ray diffraction apparatus using a YAG laser beam as a heating source. With this apparatus we have succeeded in observing directly the phase transformation of the 9R polytype at 2000°C. Single crystals of 9R grow together with the 2H type on a Mo substrate through chemical vapor deposit from a mixture of SiCl₄, CCl₄ and H₂ gases at 1400°C. 9R is really a rare polytype. Fortunately, a few specimens of 9R were found in the majority of 2H. Each of the 9R crystals was sealed in an Ar gas atmosphere in a thin glass capsule to prevent the crystals from decomposing. With samples thus prepared, structural changes of 9R were determined while heated in a high temperature X-ray camera. No change of the X-ray diffraction pattern appeared before the temperature reached 2000°C. Upon heating to 2000°C, the diffraction spots corresponding to the 3C type began to appear slightly on the X-ray film, mixing with those of 9R. The 3C spots became clear after 2 hours of heating. This result proves Inoue's principle to be valid, that is, SiC stacking sequence of "1" in Zhdanov symbol will not be stable at temperatures over 2000°C (J. Material Sci. (1982) 17 3189), because the layer stacking sequence of 9R can be represented as (21)₃ by Zhdanov's notation.

05.1-17 PHASE TRANSITIONS IN CUBIC CRYSTALS SPACE SUBGROUPS OF Fm3m(O_h⁵). By Mlik Y. and Ben Ghazlen M.H., Faculté^h des Sciences et Techniques Sfax-Tunisie.

According to Landau theory, second order or nearly first order phase transitions in crystals involve the onset of an order parameter which transforms according to one irreducible representation of the high symmetry space group. In this investigation the irreducible representations of Fm3m are examined at Γ , X, L and W high symmetry points of the cubic face centered Brillouin zone. The order parameters relevant to all the arms of a given star are considered and all the space subgroups of Fm3m are obtained. Some of these results are summarized and compared to the available experimental data relative to Fm3m subgroups.

05.1-18 FINE STRUCTURES OF VALENCE OF ELEMENTS IN PERIODIC TABLE FROM GROUP AI... GROUP B... GROUP AIII, La SERIES RE AND A SEMI-QUANTITATIVE ELECTRON THEORY OF METALLIC PHASE FORMATIONS AND ISOTOPIC PHASE TRANSITIONS. By S.H. Yü, Department of Physics, Jilin University, China. The empirical electron theory of solids and molecules used in an article numbered 08-2-49 of XIIth IUCr Congress and another one at an associated Symposium of Neutron Scattering in 1981 is here applied for the elements just mentioned in the title to determine their fine structures of valence of elements, and on the basis of the valence electron structures to analyse the factors controlling the metallic phase formations and phase transitions. For simplicity, illustration is made in details for the 8 crystal structures of elements Li, W, Fe, Co, and Cu. Firstly, the electronic structures of the hybridization of h and t atomic states of Li, W, β -Co are given. Based on these hybridizations, the distributions of the number of covalent bond electron pairs n_α ($\alpha=A, B, \dots$) as well as the number n_l of lattice electrons are determined directly from the concerned crystal structures. The corresponding hybridizations of states of α -Fe, γ -Fe, δ -Fe, ϵ -Co and Cu as well as the valence electron distributions as already published, (the above mentioned two papers; S.H. Yü, Science Reports of Solid-Molecular State Physics and Chemistry of Jinan Univ. No.1 (1981) 7-25) are presented together with the theoretical magnetic moments of 3d (m_{3d}^{ord}), spin-orbit (m_{ord}), 4s (m_{4s}^{ord}) for α -Fe and ϵ -Co and total atomic magnetic moment (m^{t}) of γ -Fe. The general empirical equation for all group B elements are given for the calculation of cohesive energies E_c of W, α -Fe, ϵ -Co and the related general equation for the melting points T_m are also given to calculate T_m of W, δ -Fe, β -Co and Cu. The agreement between the theoretical and experimental values of the covalent bond lengths $D(n_\alpha)$, magnetic moments, E_c and T_m appear all satisfactory to the first order of approximation. The formula for the calculation of the electrical and thermal conductivities σ and K_{el} all due to lattice electrons are given to calculate their values of Cu, α -Fe, W. The theoretically calculated values are somewhat below the accuracy of $D(n_\alpha)$, E_c , and T_m . Through these agreements it seems to be justified to say that the electronic structures of the hybridization of states including all the concerned parameters, the covalent bond electronic distributions as well as the actual existence of the newly proposed "lattice electrons" for the concerned structures are correct to certain degree. Then we turn to the analysis of the factors controlling the metallic phase formations and transitions semi-quantitatively in terms of simplified form of wave functions. Five factors are observed: that is, the structures of hybridization of states, no. of covalent electron of the atoms, temperature, nuclear field filtered through the core electronic screening, ordered atomic magnetic field. The transitions α -Fe \rightarrow γ -Fe \rightarrow δ -Fe, ϵ -Co \rightarrow β -Co, Li (A2) \rightarrow Li (A3), Li (A1), while K, Rb, Cs, V, Nb, Ta, Cr, Mo, W all continue to be A2; Cu, Ag, Au, Ni, Pd, Pt, Rh, Ir to be A1 and Ru, Os, Tc, Re to be A3 type structures are understood very clearly. Similar phase problems for other elements mentioned in the title can be understood as well by the five factors. They are also discussed to certain extent in the text.