PS10.11.15 STACKING FAULTS IN HEXAGONAL C_{70} SINGLE CRYSTALS STUDIED BY DIFFUSE X-RAY SCATTERING.

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Pure C_{70} crystallizes in close-packed crystal structures. Both the hexagonal close packing (*hcp*) and the cubic close packing (*ccp*) are known to exist. Most crystals at our disposition (Hoechst Chemical Company) were hexagonal prismatic. Their X-ray diffraction photographs show Bragg-like peaks, primarily in places expected for the *hcp* ordered material, but also in places expected for the *ccp* ordered material. The peaks are connected by diffuse rods of intensity which are best observed along the 101 *l*, 202 *l* and 213 *l* lines of the reciprocal lattice. Qualitatively, this indicates the presence of domains of both stacking types [1,2]. The intensities along these three diffuse rods were measured on a single-crystal diffractometer of the Swiss-Norwegian Beam Line at ESRF, Grenoble. The diffuse squared structure amplitude is the product of the squared structure amplitude of a single molecule and an interference function typical of the stacking sequence. The former was calculated assuming a librating spinning top [3]. The latter was calculated as a function of two probabilities, α that during crystal growth a layer is deposited in a *c*-position on a *c*-stack (*e.g.* ...ABC continues with A), and β that a layer is deposited in a *c*-position on an *h*-stack (*e.g.* ...ABA continues with C). The corresponding Markov chain was solved explicitely. Quantitative agreement with the observations was obtained with $\alpha = 0.77(2)$ and $\beta = 0.17(1)$. We conclude that an *h*-stack continues to grow preferentially as an *hcp* domain, while a *c*-stack prefers to grow as a *ccp* domain. In addition, *ccp* domains are on average smaller. This work has been accepted for publication in *Europhysics Letters.*

[1] van Tendeloo G. *et al.* (1993). *Europhys. Lett.*, **21**, 329 - 334.
[2] Muto S. *et al.* (1993). *Philos. Mag.*, **B67**, 443 - 463.
[3] Blanc, E. *et al.* (1994). *Europhys. Lett.*, **27**, 359 - 364.

Materials XII
Local Order and Defect Scattering In Crystals

MS10.12.01 PHASE DIAGRAM OF THE PLATINIUM-VANADIUM SYSTEM AS DEDUCED FROM DIFFUSE SCATTERING OF NEUTRONS.

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The order-disorder behavior of alloys, and particularly their phase diagrams, is governed by the interaction energies between atoms, which can be extracted from diffuse scattering data in the *disordered* state. In situ elastic diffuse scattering of neutrons was performed on the $Pt_{(1-c)}V$ system at two concentrations c = 1/4 and 1/9. For this system, the distribution of the diffuse intensity in the reciprocal space is very sensitive to the concentration and the temperature. Through inverse Monte-Carlo simulations, sets of effective pair interactions (EPI) were deduced within the Ising Model for the two different concentrations. Surprisingly, despite quite different SRO patterns, the EPI are almost concentration and temperature independent. Hence, the two very different diffuse intensity maps, at c = 1/4 and 1/9 are well reproduced with a unique set of interactions. That set allowed us to describe also properties of the ordered states: in particular, the degeneracy effects between long periods at c = 1/4 and the transition temperatures T_c are well reproduced. Such sa situation, where the interactions are independent of the concetrtation and the temperatire, The predicted phase diagram is discussed. It is in a good agreement with the known transition temperature for the ordered states at c = 1/4 and 1/9. Furthermore, we predict the existence, at very low temperature, of a new phase of composition c = 1/6 which has never been observed until now.

MS10.12.02 THE MODELLING OF THE REAL STRUCTURE OF SINGLE CRYSTALS WITH CHEMICAL INHOMOGENEITY.

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We have studied the possibilities of the analysis of basal peak profiles based on the theory of X-ray diffraction by disordered lamellar structures (V. Drits, C. Tchoubar, 1990) in revealing and describing with statistical parameters some structural peculiarities of single crystals consisting of layered modules with different composition, which are invisible for commonly used X-ray structural analysis.

The approach has been succesfully applied to the study of various perovskite like HTSC single crystals with layered structure. Their structural inhomogeneity along [001] has been described in terms of two-component irregular interstratified structures with different nature of admixture layers, their proportion and character of distribution within the crystal. It has been shown that the statistical parameters of these structures, varying from one crystal to another, determined the scale of inhomogeneity and were connected with the formation conditions of crystals and their SC-properties.

The use of the approach for the study of real structure of single crystal of edenite, a representative of natural calcium amfiboles from Khibins, helped revealing the irregular alternation of layers with different composition along two directions [010] and [001]. Thus, the crystal contains two sets of lamellae with essentially different thickness.

The data obtained proved the advantages of the approach in studying a real structure of single crystals with chemical inhomogeneity. The restrictions of the modelling originate from the use of method of trials and errors. In this connection it is expedient to combine it with other techniques such as high-resolution electron microscopy, detailed electron probe microanalysis and electron diffraction.

MS10.12.03 STRUCTURAL FLUCTUATIONS AND THE KINETICS OF THE MARTENSITIC PHASE TRANSITION.

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The nonequilibrium kinetics of the nucleation and growth in martensitic phase tarnsition have recently been drawing attention. In particular, athermal and isothermal martensitic phase transitions have been investigated from the thermodynamical point of view on nucleation. The amount of athermal martensite has been considered to be a function of temperature only. The isothermal martensite phase transition has been considered not to take place until the temperature is brought down below Ms, the martensitic transition start temperature, which is always below the thermodynamical equilibrium temperature, T0, between the parent and lowtemperature phases. On the other hand, the amount of isothermal martensite has been thought to be dependent on both temperature and time, where a waiting time (or an incubation time) is needed until the martensite phase transition starts while the temperature is kept constant. We have already found a characteristic waiting time at fixed temperature above Ms in three different kinds of materials (metallic sodium, In-Tl and Au-Cd alloys) with the use of X-ray and neutron scattering experiments. Strong diffuse scatterings were also observed on the diffractin patterns for the specimens after phase transition. The relationship between the structural fluctuations and the kinetics of martensitic phase transition is presented using the new concept of first order phase transition proposed by Roitburd (Mater. Sci. Eng., A127, 229, 1990).