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STRUCTUAL MODIFICATIONS OF ZrO_2

E. Iarotskaia E. Polianski V. Iarotski
All Russian Institute of Synthesis of Mineral Raw Materials Institutskaya Street, 1 ALEXANDROV, VLADIM OBLAST 601650 RUSSIA

ZrO_2 has some structural modifications. Baddeleyite has monoclinic structure, the facets are (001), (102), (011), (111). Length of the crystals is 10 mm. Baddeleyite may be obtained by firing amorphous ZrO_2 with the mineralizer under 1900ºC in air. Baddeleyite is transformed in tetragonal ZrO_2 under temperature of the 1100-1200ºC. Cubic modification is obtained under temperature over 1900ºC with addition of the dopants (MgO, CaO, Y_2O_3). It has melting temperature is 3000ºC. Opal-like ZrO_2 was synthesized from melt with carbon. It has microbloc texture.

Keywords: ZRO2 MODIFICATIONS BADDELEYITE

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THE TWINNED CRYSTAL STRUCTURE OF $V(NEt_2)_4$

A Dawson S Parsons C.R Pulham
University of Edinburgh Room 85, Chemistry Department, Kings Buildings West Mains Road EDINBURGH EH9 3JJ UK

As part of a wider investigation into the structures of simple amino and alkoxy derivatives of early transition metals, the structure of tetrakis (diethylamino)vanadium was determined. Under ambient conditions $V(NEt_2)_4$ is a dark green liquid. Using low temperature crystal growth techniques, a crystal was grown at 243K, crystallising in the space group P-1. The compound is monomeric, with two independent molecules in the asymmetric unit. The structure has an orthorhombic supercell , and coset decomposition implies that four twin domains corresponding to two fold rotations about the direct [100], [010] and [114] directions are possible. Refinement of the twin scale factors showed that only the first two of these twin laws were significant, however.

Keywords: TWINNING LOW TEMPERATURE CRYSTAL GROWTH

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ORDER-DISORDER TRANSFORMATIONS IN Al-Ni-Co DECAGONAL QUASICRYSTALS

H. Abe[1] H. Saitoh[2] Y. Matsuo[3] H. Nakao[4] K. Ohshima[2]
[1]National Defense Academy Materials Science and Engineering 1-10-20, Hashirimizu YOKOSUKA 239-8686 JAPAN [2]Univ. of Tsukuba [3]Nara Women's University [4]Tohoku University

The diffuse scattering from atomic short-range order (SRO) associated with order-disorder transformations was observed in single decagonal quasicrystals of $Al_{70}Ni_{15}Co_{15}$ (S1) [1] and $Al_{72}Ni_{20}Co_8$ (bNi) [2]. In S1, the anisotropic diffuse scattering derived from phason strains was seen around Bragg reflections. Theoretically, the anisotropic distributions of diffuse scattering are realized if the coupling between phonon and phason are not ignored. In fact, ANC has dependence of full width at half maximum (FWHM) of Bragg reflections. By anomalous-X-ray scattering experiments, ANC has only one kind of a pair correlation function, Ni-Co. Hence, there is long-range order (LRO) between Al and transition metals. In contrast, the isotropic diffuse scattering in bNi was distributed around Bragg and the superstructure reflections. bNi has no G perp dependence of FWHM of Bragg reflections at room temperature. The correlation length of the diffuse scattering was estimated to be 2.8 nm at room temperature and developed into more than 11.0 nm on the superstructure phase at high temperature. At high temperature, peak broadening in bNi appeared both on para and perp. This means both ponon and phason anomalies occurred. However, distributions of diffuse scattering were still isotropic. Therefore we concluded both anomolies appeared independently, that is, no coupling between phonon and phason contribute to order-disorder transformations in BNi

Keywords: DIFFUSE SCATTERING, PHASON, QUASICRYSTALS

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RIETVELD ANALYSIS OF PHASES IN HEAT-RESISTANT STEELS

J.L. Garin R.L. Mannheim
Universidad De Santiago De Chile Ingenieria Metalurgica Casilla 10233 SANTIAGO 2 CHILE

Heat-resistant steels have received much attention because of their interesting mechanical properties and high-temperature applications in the mining industry. Parts in service at temperatures in the range from 600 to 900°C can yield precipitation of intermediate complex phases such as sigma, chi and carbides, which strongly affect the mechanical properties of the material. Therefore in order to compare the behavior of the material with its microstructural features, a complete characterization of the alloys must include the determination of the relative amounts of all components. Owing to the usually complex diffraction patterns of the samples, which disclose many overlapping reflections, Rietveld analyses were conveniently carried out on several HC-type iron alloys (26 wt % Cr, 4 wt % Ni, 0.3 wt % C) prepared by annealing at temperatures from 650 to 900°C for treatment periods of 10 to 200 hrs. The room temperature data collection for each specimen was carried out over the range of 20 to 120° (2θ) with 4500 step intensities, step size 0.02° and measurement time 10 s, using Bragg-Brentano geometry (θ-θ scan) and Cu K-α radiation with graphite monochromator. The X-ray analyses were performed assuming pseudo-Voigt profiles for all reflections; the refinement cycles were based upon the variations of isotropic thermal parameters, scale factors, preferred orientation coefficients, surface roughness, background polynomial coefficients, sample transparency and displacement and so on. This procedure permitted an accurate quantification of phases such as austenite, ferrite, ternary solid solutions, carbides $(Fe,Cr)_7C_3$ and sigma (Cr_6Fe_7).

Keywords: RIETVELD, STEELS, INTERMEDIATE PHASES