

DEFORMATION EFFECT ON STRUCTURE AND PROPERTIES OF SURFACE LAYERS IN IRON ALLOYS UNDER NITROGEN AND CARBON ALLOYING

Lesya D. Demchenko

National Technical University of Ukraine 'KPI' Metal Physics Department 37 Peremogy Prospect KYIV 03056 UKRAINE

The aim of this work was to study the effect of plastic deformation (0 - 70%) on the structure, chemical and phase composition, mechanical properties of surface layers formed in iron and iron-based alloys under alloying by nitrogen and carbon in ammonia and propane-butane environment with various ratios gaseous components at 853 K during 0.5-6 hours. Obtained surface layers were studied by means of X-ray diffraction, electron probe analysis, Auger-electron spectroscopy, microhardness and wear resistance tests. It was established that the surface layer after nitrogen and carbon saturation consists of epsilon-phase with the hexagonal closed packed crystal structure or theta-phase with the orthorhombic structure isostructural to cementite lattice and the solid solution of nitrogen and carbon in alpha-phase. The deformation within the range of 25 - 30 % essentially effects on the structure, phase and chemical composition and properties of surface layers. The theta-phase was revealed in the layer after such (25 - 30 %) deformation and saturation in gas mixture of 90 % ammonia and 10 % propane-butane. Obtained in this way layers show maximum microhardness, wear resistance and depth. The epsilon-phase was found in the alloy after deformation out of the 25 - 30 % ranges. The lattice period of the alpha-phase containing nitrogen and carbon decreases non-linearly within the 25 - 40 % degree of plastic deformation. We assume that high mechanical properties of the surface layers results from participation of disperse carbonitrides on such crystal lattice defects as dislocations.

Keywords: SURFACE LAYER, STRUCTURE, DEFORMATION

POLYTYPES AND STRUCTURAL TRANSITION IN CALCIC ALUMINATES HYDRATED $[Ca_2Al(OH)_6]_x \cdot [X, 2H_2O]$ - WITH X = Cl, Br AND I

M. FRANCOIS¹ J.P. RAPIN² G. RENAUDIN³ J.P. RIVERA⁴

Universite Henri Poincare Nancy I Laboratoire De Chimie Du Solide Mineral UMR777 Boulevard Des Aiguillettes BP 239 VANDOEUVRE LES NANCY 54506 FRANCE

¹Laboratoire de Chimie du Solide Mineral UMR 7555 BP 239 F54056 Vandoeuvre-les-Nancy Cedex. ²Laboratoire de Chimie du Solide Mineral UMR 7555 BP 239 F54056 Vandoeuvre-les-Nancy Cedex. ³Laboratoire de Cristallographie - Universite de Geneve, 24 quai Ernest-Ansermet CH-1211 Geneve 4, Switzerland ⁴DCMA, Universite de Geneve, 30 quai E. Ansermet, CH-1211 Geneve 4, Switzerland

The compounds presented in the title were studied as a function of temperature, by X-Ray Diffraction on powder with high resolution (radiation synchrotron), on single crystal, by Differential Scanning Calorimetry (DSC) and by optical polarized light microscopy. These lamellar double hydroxides (LDH) compounds are made up of rigid layers positively charged in which Ca^{2+} and Al^{3+} are ordered. According to the nature of halide X, inserted anion which allow the re-establishment of the electroneutrality, one or two polytypes were identified: X = Cl (polytype 6R (Space Group= $R-3c$); X = I (polytype 3R (SG= $R-3$), X = Br (polytypes 6R and 3R). Structure transformations occur at a temperature T_s which depends on the nature of halide: $T_s(Cl) = 35^\circ C$, $T_s(Br) = -40^\circ C$ and $T_s(I) = -150^\circ C$. These transitions are accompanied by a lowering of symmetry from a high temperature to a low temperature phase according to: from $R-3c$ to $C2/c$ and from $R-3$ to $P-1$. The origin of the transition is due to the ordering of the network of hydrogen bonds $Cl \cdots H$ in the inter lamellar part of the structure. The transition leads to a displacement up to 0.5 Å of the inserted species H_2O and X. The transition is narrowly correlated to the hydration enthalpy of the anions X. The study of the solid solution $[Ca_2Al(OH)_6]_x \cdot [Cl_{1-x}, Br_x, 2H_2O]$, with x varying from 0 to 1, confirms these results.

Keywords: PHASE TRANSITION LAMELLAR DOUBLE HYDROXIDES CRYSTAL STRUCTURE

STRUCTURAL INVESTIGATIONS ALONG THE JOIN $CaTiOGeO_4$ - $SrTiOGeO_4$

R. Ellemann-Olesen T. Malcherek

Institut F. Mineralogie, WWU Muenster Institut F. Mineralogie, WWU Muenster Corrensstr. 24 MUENSTER 48149 GERMANY

The titanite structure type can accommodate a wide range of different chemical compositions. The present study is focusing on the titanyl-compounds $CaTiOGeO_4$ and $SrTiOGeO_4$. In analogy to titanite, $CaTiOSiO_4$, $CaTiOGeO_4$ undergoes a displacive phase transition from the low temperature phase $P2_1/a$ to the high temperature $A2/a$ -phase. The structural phase transition $A2/a - P2_1/a$ in $CaTiOGeO_4$ has been observed using *in situ* heating X-ray powder diffraction methods. The transition occurs at approximately 623 K and is accompanied by a significant expansion of the a-axis. The components of the strain tensor have been determined. Only the e_{11} and e_{13} components contribute significantly to the strain tensor associated with the phase transition. Electron diffraction patterns of $CaTiOGeO_4$ were obtained along a number of zones and showing two families of spots: the sharp and intense spots with $k + l = \text{even}$ reflections and the weak superstructure reflections $k + l = \text{odd}$. The structure of $CaTiOGeO_4$ has been refined using single crystal X-ray diffraction data. Rietveld refinement on X-ray powder diffraction data has been used to characterize a series of compounds along the solid solution $CaTiOGeO_4 - SrTiOGeO_4$. Deviation from linearity of the cell dimensions is observed close to the $CaTiOGeO_4$ end-member in the lattice parameters a and β .

Keywords: TITANYL COMPOUNDS, PHASE TRANSITION, LATTICE PARAMETERS

ATOMIC AND MAGNETIC STRUCTURE OF MnF_3

B. A Hunter¹ T. Vogt² B. J. Kennedy³

¹Neutron Scattering Ansto Building 58 Pmb 1 MENAI NSW 2234 AUSTRALIA ²Brookhaven National Lab, Physics Division, Upton, NY, USA ³Sydney University, Chemistry Department, Sydney, NSW, Australia

The magnetic and atomic structure of MnF_3 has been investigated at low temperatures (4-300 K) using powder neutron diffraction. The structure showed a negative thermal expansion below the Neel temperature (43 K), very similar to other manganates that show colossal magnetoresistance. Unlike these other manganates there can be no charge ordering. The structural results are discussed in relation to the colossal magnetoresistance class of manganates.

Keywords: MAGNETIC STRUCTURES, NEUTRON POWDER DIFFRACTION, COLLOSAL MAGNETORESISTIVITY