

separated octahedral blocks. This new interpretation is verified by the results of FP-LAPW computational studies.

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Keywords: lanthanum stannides, Rietveld refinement, electronic structure

FA2-MS13-P10

Influence of low temperature aging on the crystalline structure of the carbon martensite Vasily Tarasov, Vitaliy Danilchenko, Viktor Iakovlev. *G. V. Kurdyumov Institute for Metal Physics, Kyiv, Ukraine.*

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Thermal stability of the α -martensite after cyclic γ - α - γ martensitic transitions was investigated using the x-ray method and single crystal specimens of two types of alloys: alloy 1 – Fe - 24,5 wt.% Ni - 0,5 wt. % C, alloy 2 – Fe - 9,7 wt. % Ni - 1,54 wt. % C. Specimens had the austenitic structure at room temperature. The direct γ - α transition occurred when cooling in liquid nitrogen. The reverse α - γ transition was realized by heating in salt bath up to 550 °C (alloy 1) and 700 °C (alloy 2) with the heating rate of 60 °C per second. Under such conditions the reverse α - γ transition was shear and diffusionless. The X-ray investigations were realized in rotating chamber RKV-86 with iron emission. Carbon α -martensite decomposition was observed by the change of the angular position (Bragg angle) of diffraction reflexes (200) _{α} and (002) _{α} and by the martensitic lattice tetragonality rate c/a change.

It was determined that the α -martensite formed in the austenite after γ - α - γ transitions decomposed more intensively. As a result, when heated up to 100 °C, the amount of depleted carbon of α -solid solution (χ -phase) in the alloy 1 raised up to 50 % relatively to its raising up to 20 % in the initial alloy. High carbon martensite of the alloy 2 decomposed with forming the only one carbon-depleted α -solid solution except the two in the initial alloy. The aged martensite of both alloys was depleted of carbon to a value close to its equilibrium concentration in α -Fe. This process ended as early as 80-120 °C.

The intensification of the carbon martensite decomposition after γ - α - γ transitions associated with the influence of crystalline structure defects which appear during direct γ - α and reverse α - γ transitions. The electron microscopic study shows the density of dislocations in reverted austenite is more than three orders bigger than in initial austenite. Moreover, additional subboundaries of disoriented fragments appeared. The martensite received these defects after reverse α - γ transition. As a result, the diffusion of carbon atoms on crystalline structure defects was enhanced. This caused the acceleration of the carbon α -solid solution decomposition.

Keywords: crystalline structure, X-ray crystal structure analysis, electron microscopy analysis

FA2-MS13-P11

A high-pressure study of Realgar. Daniel M. Többens, Raffaella Sagl, Clivia Hejny. *Mineralogy and Petrography, University of Innsbruck, Austria.*

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Realgar, chemical composition As₄S₄, is well known for its use as a red color pigment in painting and art for many centuries. In addition, it is a naturally occurring semiconductor, used in a number of optoelectronic applications. A natural sample from the "Baia Sprie" mine in Rumania was studied in a diamond anvil cell in order to analyze the behavior of Realgar under high-pressure conditions. Single crystal data could be obtained at pressures up to 5.4 GPa, powder data up to 43 GPa (ESRF/U. of Heidelberg, Miletich-Pawliczek R., Pippinger T., Ullrich A.). Electron microprobe analysis gave a composition close to ideal for this sample. For a deeper understanding of the experimental results DFT calculations were done using the software CRYSTAL06 [1], with Gaussian basis sets modeled as pseudo-potentials in DURAND-311G(1) and DURAND-3111G(1) contractions for sulfur and arsenic, respectively, and the generalized gradient approximation Perdew–Wang 92 (PW92). The structure of Realgar is characterized by cage-like molecules, oriented in rods parallel [100] and packed along [010]. The intra-molecular distances do not show a measurable shortening. Compression occurs mainly between the molecules, more precisely between the rods stacked along [010]. The compressibility was fittable by a Birch–Murnaghan equation of state, with resulting bulk modules $K_0 = 11.0(4)$ GPa, $K' = 9.0$ (from single crystal data) and $K_0 = 11.7(2)$ GPa, $K' = 7.8(1)$ (from DFT calculations up to 38 GPa). No phase transition was observed for the entire pressure range in spite of a compression to about 60% of the initial volume. During pressure increase, a continuous color change from yellow through red into black was observed. The color change is reversible on pressure decrease. UV-Vis spectroscopy (U. of Vienna, Wildner M.) showed this to be caused by a shift of the optical absorption edge to higher wavelengths with increasing pressure. It was assumed that this behavior is caused by a reduction of the direct band gap, and thus is a feature of the ideal crystal structure. Band gaps calculated by DFT methods are known to be too narrow generally. To overcome this problem simplified expansions according to the BZW-optimization process [2] were used to calculate the band structure. The values resulting from this were satisfactory, being only 15% smaller than the experimental ones. The calculated pressure dependency of the direct band gap is in full agreement with the experiment. Raman spectroscopy (U. of Vienna, Nasdala L.) revealed a general hardening of those vibrations associated with movements of the molecules as a whole. Vibrations associated with intra-molecular bending and stretching were affected less.

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FA2-MS13-P12

Neutron investigation of martensitic and superelastic shape memory NiTi wire. Michael Tovar. *Helmholtz-Zentrum Berlin (HZB) für Materialien und Energie, Berlin, Germany.*

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