

APEXII single crystal diffractometer, MoK α radiation) and has been solved by direct methods and refined using the SHELX-97 program package [1]: $Fmmm$, $a=4.9484(7)$, $b=8.4367(7)$, $c=29.171(1)$ Å, $R_w=0.0549$, 312 unique reflections, 45 variables. The final atomic parameters for the $Li_{18}Cu_{15}Al_7$ compound are summarized in the following table.

Atom	Wyck	x/a	y/b	z/c	Occupation
Cu1	8e	1/4	1/4	0	1
Cu2	16j	1/4	1/4	0.66754(6)	1
Cu3	4a	0	0	0	1
M4	8i	0	0	0.6801(2)	0.39(4) Cu + 0.61(4) Li
Al5	8i	0	0	0.6337(3)	1
Al6	8i	0	0	0.5397(3)	0.73(7)
Li7	16m	0	0.670(3)	0.5873(9)	1
Li8	8i	0	0	0.772(1)	1
Li9	8f	1/4	1/4	1/4	1

Crystal structure of this compound is a derivative from the $CuAl_2$ binary compound. Forming of the $Li_{18}Cu_{15}Al_7$ compound can be formally presented as additional lithium layers into $CuAl_2$ with an expansion of the c parameter from 6.480 Å to 29.171 Å. Another peculiarity of the crystal structure of this compound is the formation of hexagonal columns which are filled by lithium atoms. Similar columns with lithium atoms in the crystal structures were established for $Li_{12}Cu_{16+x}Al_{26-x}$ and $Li_8Cu_{12+x}Al_{6-x}$ compounds [2,3].

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Keywords: lithium, intermetallic compound, crystal structure

FA2-MS13-P05

Fe-Ni-C alloy crystalline structure of tempered martensite. Viktor Iakovlev, Vitaliy Danilchenko. *G.V. Kurdyumov Institute for Metal Physics, Kyiv, Ukraine.*
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High-carbon crystalline structure of iron-nickel martensitic alloy after direct γ - α - and reverse α - γ - transition was studied using X-ray diffraction in single crystal specimens. The test material was Fe – 9,7 wt.%Ni – 1,54 wt.% austenite alloy. The direct transition occurred when cooling at liquid nitrogen and the reverse transition occurred when heating in salt bath at 700°C. The instability interval of retained austenite was partially overlapped by an interval of the reverse martensitic transition. This led to initiating the direct α - γ transition. The X-ray investigations were realized on single crystal specimens in rotating chamber RKV-86 with cobalt emission.

On three-phase dissolution stage during low-temperature tempering (100-200°C) two α -solid solutions (α_1 - and χ -phases) with reduced content of carbon (1,2 % and 0,25% accordingly) were formed. Occurrence of reflections after tempering of χ - martensite testified about first stage decomposition ending at 300°C. On the second one-phase dissolution stage further martensite depletion led to decreasing

of χ -phase lattice tetragonality up to 1 at 300°C. Heating up to 700°C has resulted in reverse α - γ - martensitic transition. Orientation of the martensitic lattices with respect to initial austenite lattice was equal.

Considering the position of martensitic reflections on the diffraction pattern of the single crystal specimens we can arrive at a conclusion that the orientation of martensitic lattices was similar to the initial austenite lattice. This means that α - α_1 - and α_1 - χ - transitions are associated only with the redistribution of carbon atoms and are not connected with the crystallographic restructuring of the metal lattice atoms.

Keywords: martensitic transformation, X-ray diffraction, single crystals

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Cd-rich Cadmides of the System Na/K/Cd. Viktoria Mihajlov, Caroline Röhr. *Institut für Anorganische und Analytische Chemie, University of Freiburg, Germany.*
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Binary alkali metal (A^I) zinkides [1] and cadmides are only known in the A^I -poor region of the respective phase diagrams. The structure of the sodium cadmide Na_2Cd_{11} , which was known from early film experiments[2] (Mg_2Zn_{11} type, cubic, $Pm\bar{3}$, $a = 958.75(9)$ pm, $Z = 3$; $R1 = 0.042$) was confirmed and refined using single crystal data. The new ternary phase KNa_xCd_{11-x} ($x = 0.87/0.53$), tetragonal, $I4_1/amd$, $a = 1222.98(6)/1215.17(12)$ pm, $c = 766.05(4)/769.05(7)$ pm, $Z = 4$, $R1 = 0.021/0.024$) forms the $BaCd_{11}$ structure type, which was previously unknown for alkali metal compounds. The Ba site of the basic structure type is occupied by K, whereas one Cd site is statistically occupied by Na and Cd. In the structure, the atoms of the two pure Cd positions form channels running along the tetragonal c axis, in which the K and Na/Cd atoms alternate. A similar structural motif is found in the second border compound K_3Cd_{16} , formerly described as $K_{0.37}Cd_2$ [4]. In the Cd channels the K atoms are no longer disordered: A detailed inspection of the diffraction images revealed satellite reflections indicating an almost commensurately modulated superstructure. In the new structural model with a quadrupled c axis (tetragonal, $P4/nnc$, $a = 915.2(6)$, $c = 1159.0(4)$ pm, $Z = 2$) the formerly singular K position splits into two, resulting in three potassium cations per channel. Both the significant structural factors (strongly changing radius of the A^I -cations) and the electronic criteria, which can be assessed from the pseudo band gap calculated using FP-LAPW-DFT methods, are discussed. A structural map that takes the radius ratios $r_M:r_A$ and the v.e.c. into account nicely separates the different structure types of Zn/Cd-rich A^I/A^{II} metallides.

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