

meanwhile a covalent nature could be observed between Al and O.

[1] Xu C. N., *Encyclopedia of Smart Materials*, 2002, **1**, 190. [2] Liu Y., Xu C. N., *Appl. Phys. Lett.*, 2004, **84**, 5016.

Keywords: Rietveld structure analysis, maximum-entropy method, luminescent compounds

P.10.02.22

Acta Cryst. (2005). A61, C372

RE₆Ni₂In (RE = Gd, Tb, Dy, Ho, Lu) – The New Representatives of Ho₆Co₂Ga Structure Type

Yaroslav Galadzhun^a, Mariya Dzevenko^a, Vasyl' Zaremba^a, Julia Stepień-Damm^b, Yaroslav Kalychak^a, ^a*Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Ukraine.* ^b*W. Trzebiatowski Institute of Low Temperature and Structure Research, Wrocław, Poland.* E-mail: galadzh@mail.lviv.ua

The compound Ho₆Ni₂In was synthesized in an arc-melting furnace under an argon atmosphere and special heat treatment was applied for the growth of single crystals. Intensity data were collected by use of a KM-4 CCD diffractometer with graphite monochromatized MoK α radiation. The structure was refined by direct methods with anisotropic displacement parameters for all atoms using SHELX-86 and SHELXL-97 programs: sp.gr. *Immm*, $a = 9.319(2)$, $b = 9.523(2)$, $c = 9.930(2)$ Å, $Z = 4$; $R1 = 0,0401$, $wR2 = 0,0891$ for 581 reflections with $I > 4\sigma(I)$. The 2(a) site shows mixed occupancy Ni_{0,64(4)}In_{0,36(4)}.

Atom	Site	x	y	z	U _{eq} , Å ²
Ho1	8(n)	0.2912(1)	0.1840(1)	0	0.0140(3)
Ho2	8(m)	0.3032(1)	0	0.3222(1)	0.0107(3)
Ho3	8(l)	0	0.1963(1)	0.2232(1)	0.0200(3)
Ni1	4(j)	1/2	0	0.1226(4)	0.0136(8)
Ni2	4(g)	0	0.3603(5)	0	0.0179(9)
In	2(c)	1/2	1/2	0	0.0103(6)
M	2(a)	0	0	0	0.020(2)

The structure of the Ho₆Ni₂In compound belongs to the Ho₆Co₂Ga structure type [1]. Isostructural compounds were found also with Gd, Tb, Dy, and Lu.

[1] Gladyshevskii R., Grin Yu., Yarmolyuk Ya., *Dop. AN URSSR*, 1983, (2), 70.

Keywords: crystal structures, rare-earth compounds, indium compounds

P.10.04.1

Acta Cryst. (2005). A61, C372

White Phosphorus: The Equation of State and Pressure-Induced Transitions

Joseph M. Zaug^a, Simon M. Clark^b, Martin Kunz^b, Raymond Jeanloz^c, ^a*Lawrence Livermore National Laboratory.* ^b*Lawrence Berkeley National Laboratory.* ^c*University of California at Berkeley.* E-mail: zaug1@llnl.gov

We conducted angle dispersive x-ray powder diffraction measurements of hydrostatically compressed white phosphorus, P₄, to determine the equation of state and pressure dependant thermal expansion coefficients. We discovered a pressure-induced change in the powder pattern at ambient temperature. In addition, we have preliminary data that partially details the melting curve of P₄. Our condensed fluid state diffraction results will be used to deduce radial structure factor information. Our measurements were conducted on the new California high-pressure science observatory BL12.2.2 (<http://xraysweb.lbl.gov/bl1222/HOME.htm>) located at the Advanced Light Source at Lawrence Berkeley National Laboratory. An externally heated and membrane driven diamond anvil cell was employed to confine samples at controlled pressures and temperatures.

Ambient condition white phosphorus exists as a bcc crystalline solid with a I-43m space group. Upon increasing pressure, P₄ transforms at approximately 2.5 GPa to the orthorhombic black allotrope with a Cmca space group. The exact allotropic transition pressure depends most likely on the magnitude of shear forces present within the sample. For example, temperature annealing seems to extend the pressure stability of the bcc phase to nearly 6 GPa. When

heated to modest temperatures, P₄ transforms, upon increased pressure, to what we describe as an amorphous black phase.

Keywords: phosphorus, equations of state, phase transitions

P.10.04.2

Acta Cryst. (2005). A61, C372

X-ray Study of the Iridium-Osmium System

Ilya Korolkov, Sergey Gromilov, Kirill Yusenkov, Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia. E-mail: x-vizor@yandex.ru

Os and Ir metals are of particular attention regarding their characteristics. For example, the osmium has the highest bulk moduli value of 462 GPa [1] among all other materials. Furthermore, Os and Ir possess the high values of density, melting temperature, etc. A phase diagram of Os-Ir system belongs to the peritectic type. Single-phase areas with the face-centered cubic (fcc) and hexagonal close packed (hcp) lattices are separated by a diphasic area.

In some cases, it is possible to obtain a non-equilibrium solid solution that is placed into the diphasic area. To get the single Ir_{0,5}Os_{0,5} phase we have thermolized a precursor complex [Ir(NH₃)₅Cl][OsBr₆] at 700°C in hydrogen atmosphere. Finally, according to X-ray analysis data, a single phase with the hcp lattice was obtained. After further heating up to 800°C for 24 hours in vacuum the sample became diphasic. The lattice parameters of the hcp phase are close to Ir_{0,5}Os_{0,5}. The lattice parameter of the fcc phase is close to the pure iridium.

Besides, we have obtained the Ir_{0,67}Os_{0,33} fcc phase from the [Ir(NH₃)₅Cl]₂[OsCl₆]Cl₂ complex by prolonged heating; another phases Ir_{0,5}Os_{0,5} (hcp, non-equilibrium), Ir_{0,75}Os_{0,25} (fcc) and Ir_{0,25}Os_{0,75} (hcp) were synthesized by thermolysis of salt solid solutions (NH₄)₂[OsCl₆]_(1-x)[IrCl₆]_x (0 ≤ x ≤ 1). For all of the phases we have calculated a “volume per atom” parameter. The calculated values fit a line that connects the values for pure iridium and osmium.

[1] Cynn H., Klepeis J. E., Yoo C. et. al., *J. Phys. Rev. Lett.*, 2002, **88**, 135701.

Keywords: platinum group, thermal study, X-ray analysis

P.10.04.3

Acta Cryst. (2005). A61, C372-C373

Crystal Phases in Glasses

Andrei Lysiuk, Institute of Geology Russian Academy of Sciences, Syktyvkar, Russia. E-mail: andra227@yandex.ru

We investigated crystal phases of fulgurite glasses. Fulgurites is a glassware tubular bodies, which formed after the melting of rocks by the hit of a lightning. The successful case was presented to us to study the structure and composition of two fulgurite fragments of Sonora desert (south of Mexico). Earlier we have studied the fulgurite from area of Nigoziro in Karelia, Russia, which was formed on a carbon-containing aleurolites. Thus an excellent opportunity has appeared to make the comparative analysis of fulgurites, formed on completely various geological breeds.

By data received with the help of X-Ray analysis the basic volume of all investigated fulgurite glasses is the X-Ray amorphous phase. For Mexican fulgurite it is a prevailing phase. Also we expose the heterogeneity of glasses which consists in combined presence of amorphous glassy matrix and crystalline formations with different composition: orthoclase, hematite, chlorite, pyrite.

By the micro-probe analysis we determined that the main mass of glassy fulgurite substance is a thickened Si-Al-Fe fusion. In the main mass of fusion the areas of almost pure glasses are distinguished. The simultaneous appearance of fragments as glassy such as residual quartz in fusion tells that the temperature of fusion in that zone was near the temperature of quartz melting, this is about 1700 C.

In the outlying districts of fulgurite iron contains by the higher portions. Here we find a great amount inclusions, mainly of Fe-Al composition. In the fulgurite glass we also find an inclusions of almost pure alloy which consists from the iron and aluminium with the small admixture of magnesia. That inclusions are characterised by the good crystallographic cutting. The presence of costal growing forms tells about the post-melting formation of this inclusions. Also we often meet inclusions of hematite Fe₂O₃. Its grains have the straight borders.