

## Simulation of aluminothermic smelting of the carbon-containing ligature for titanium alloys

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### Abstract

The article reports the results of thermodynamic simulation of the Al-V-Ti-C (AVTU), Al-Mo-Ti-C (AMVTU) and Al-Mo-Nb-Ti-C (AMNTU) ligature alloys smelting from aluminothermic charges containing an appropriate set of oxides ( $V_2O_5$ ,  $MoO_3$ ,  $Nb_2O_5$ ), elemental titanium and carbon. Modeling was performed with the help of the HSC-6.1 Chemistry software package. Melting temperatures, equilibrium phase and elemental compositions of alloys and slags as well as a distribution of carbon to carbide phases were defined according to the material and the thermal balances (subject to “zero” heat loss). According to the simulation results thermic properties of finance charge allow to reach temperatures of up to 3100 °C, thus providing an autogenous process and the possibility of ligatures smelting by the off-furnace method.

In the AVTU alloy titanium has to be mainly in the form of carbide TiC and vanadium – in the form of aluminides  $VA_3$ ,  $V_3Al_2$ . Vanadium in the AMVTU ligature is represented by aluminides, carbides VC,  $V_2C$  and elemental vanadium. The main titanium-containing phases of the AMVTU ligature – carbide TiC and aluminides TiAl,  $TiAl_3$ . In the AMNTU ligature aluminides  $Mo_3Al$ ,  $NbAl_3$  and TiAl are dominating species, and carbide phase consists of TiC and  $Nb_2C$ .

There are predominantly  $Al_2O_3$  (more than 70 wt.%) and calcium aluminates  $CaO \cdot 2Al_2O_3$ ,  $CaO \cdot Al_2O_3$  in the slag of alloy smelting. In the slags of AVTU and AMVTU smelting vanadium and titanium are in the form of oxides TiO and VO. Besides it is probable a formation of oxides  $TiO$ ,  $Ti_2O_3$ ,  $TiO_2$ , as well as titanates  $CaO \cdot TiO_2$  and  $Al_2O_3 \cdot TiO_2$ . Titanium transition to the slag of AMNTU smelting is not more than 2.0% of its amount in the charge.

The article shows the ligatures compositions, designed by the thermodynamic model and obtained experimentally by melting under industrial environments. It is noted a good agreement between the calculated and experimental compositions of ligature alloys. We concluded about the possibility of applying the method of thermodynamic modeling to forecast estimation of aluminothermic smelting of carbonized ligature alloys based on the rare refractory metals.

### References

- [1] A.A. Ilyin, B.A. Kolachev, N.S. Polkin. Titanium alloys. The composition, structure and properties. Handbook. M.: VILS - MATI. 2009. 520p. (russian)
- [2] A.S. Oryshenko, A.S. Kudryavtsev, V.I. Mikhailov, V.P. Leonov. Titanium alloys for marine engineering and nuclear energy. *Problems of Materials Science*. 2011. Vol.1 (65). P.60-74. (russian)
- [3] A.S. Oryshenko, V.P. Leonov, I.A. Schastlivaya, T.N. Igolkina. Titanium alloys in nuclear power. *Titanium*. 2014. No.3. P.20-30. (russian)
- [4] A.L. Bereslavskiy, S.A. Emelyanov, V.M. Maksimov, L.A. Machishina. Ligatures production for smelting of shipbuilding titanium alloys doped with carbon. *Titanium*. 1995. No.3-4(7-8). P.15-17. (russian)
- [5] A.V. Zelyansky, N.K. Mel'nikov, N.P. Pazdnikov, I.Yu. Puzakov, A.N. Rilov, V.F. Novikov, A.Y. Dubrovskiy, M.I. Klimov, A.N. Trubin, V.M. Chumarev. Development of technology and organization of modern industrial production of complex alloys of rare refractory metals for the manufacture of titanium alloys. *Proceedings of conference "Problems and prospects of development of*

- SIMULATION OF ALUMINOTHERMIC SMELTING OF THE CARBON-CONTAINING LIGATURE FOR... 50-56 metallurgy and mechanical engineering using completed basic researches". Yekaterinburg. 2011. Vol.1. P.299-306. (russian)*
- [6] N.P. Liakishev, Y.L. Pliner, G.F. Ignatenko, S.I. Lappo. Aluminothermy. *M.* **1978**. 424p. (russian)
- [7] Y.L. Pliner, G.F. Ignatenko. Reduction of metal oxides by aluminium. *M.: Metallurgy*. 1967. 248p. (russian)
- [8] N.A. Vatolin, G.K. Moiseev, B.G. Trusov. Thermodynamic modeling in high-temperature inorganic systems. *M.: Metallurgy*. **1994**. 353p. (russian)
- [9] G.K. Moiseev, G.P. Vyatkin. Thermodynamic modeling in inorganic systems. Schoolbook. *Chelyabinsk: SUrSU*. **1999**. 256p. (russian)
- [10] G.G. Mikhailov, B.I. Leonovich, Yu.S. Kuznetsov. Thermodynamics of metallurgical processes and systems. *M.: MISIS*. **2009**. 520p. (russian)
- [11] Roine. HSC 6.0 Chemicty. Chemical reactions and Equilibrium software with extensive thermochemical database and flowsheet simulation. *Pori: Outokumpu Research OY*. **2006**. 448p.
- [12] E.M. Zhilina, S.A. Krasikov, S.N. Agafonov, L.B. Vedmid, S.V. Zhidovinova. Thermodynamic and kinetic peculiarities of joint aluminothermic reduction of titanium and zirconium from oxides. *Butlerov Communications*. **2016**. Vol.45. No.1. P.130-135. ROI: jbc-02/16-45-1-130
- [13] A.V. Larionov, L.Y. Udoeva, V.M. Chumarev, A.N. Mansurova. Thermodynamic simulation of phase formation in the Mo-Si alloys doped with yttrium. *Butlerov Communications*. **2015**. Vol.43. No.9. P.84-88. ROI: jbc-02/15-43-9-84
- [14] A.V. Larionov, L.Y. Udoeva, V.M. Chumarev. Thermodynamic simulation of phase formation in the Mo-Si, alloys doped with scandium or neodymium. *Butlerov Communications*. **2015**. Vol.43. No.9. P.89-96. ROI: jbc-02/15-43-9-84
- [15] A.G. Upolovnikova, A.A. Babenco. Thermodynamic modeling of boron recovery from boron-containing slag. *Butlerov Communications*. **2016**. Vol.48. No.10. P.114-118. ROI: jbc-02/16-48-10-114
- [16] S.N. Tyushnyakov, E.N. Selivanov. Thermodynamic simulation of phase formation during cooling of zinc-containing cooper-smelting slag. *Butlerov Communications*. **2015**. Vol.43. No.9. P.102-107. ROI: jbc-02/15-43-9-102
- [17] S.N. Tyushnyakov, E.N. Selivanov. Thermodynamic simulation of zinc reduction from cooper-smelting slag. *Butlerov Communications*. **2015**. Vol.43. No.9. P.108-115. ROI: jbc-02/15-43-9-108
- [18] A.G. Upolovnikova, V.M. Chumarev, L.Y. Udoeva. Thermodynamic modeling of phase formation during the oxidation of niobium aluminide. *Butlerov Communications*. **2015**. Vol.44. No.12. P.146-149. ROI: jbc-02/15-44-12-146
- [19] L.Yu. Udoeva, V.M. Chumarev, A.V. Larionov, A.N. Rylov, M.V. Trubachev. Simulation of the Aluminothermic Smelting of Mo-Ti-Al and Mo-Ti-V-Cr-Al Alloys. *Russian Metallurgy (Metally)*. Vol.2013. No.8. P.564-569.
- [20] O. Kubaschewski, C.B. Alcock. Metallurgical thermochemistry. *Oxford: Pergamon press*. **1982**. 383p.
- [21] The diagrams of binary metallic systems: a handbook. Vol.1. Comm. edit. by N.P. Lyakishev. *M.: Mechanical Engineering*. **1996**. 992p. (russian)
- [22] L.E. Toth. Transition metals carbides and nitrides. *New-York& London: Academic press*. **1971**. 294p.
- [23] N.S. Kulikov. Thermodynamics of carbides and nitrides. Handbook. *Chelyabinsk: Metallurgy*. **1988**. 320p. (russian)
- [24] G.A. Meyerson, A.N. Zelikman. Metallurgy of Rare Metals. *M.: Metallurgy*. **1955**. 608p. (russian)