Baikov Institute of Metallurgy and Materials Science, Russian academy of Sciences
Activity on Phase Diagrams in 2020

1. Investigations into the ternary phase diagrams of magnesium with two rare-earth metals belonging to different (yttrium and cerium) groups are surveyed. The main attention is paid to near-Mg corner regions. It is shown that, for such systems, trends in changing the phase diagram constitution are found to be a function of the atomic number added rare-earth metals. (L.L. Rokhlin, The regularities in constitution of the ternary phase diagrams of magnesium alloys with two rare-earth metals belonging to different groups (yttrium group and cerium group), *Journal of Phase Equilibria and Diffusion*. 2020, **41**, p. 532-537).

2. The phase equilibria in the copper-magnesium system with the participation of gaseous phase were analyzed. Variants of phase quilibria, projections of maximum solubility on the temperature-composition plane, isobar and isothermal sections of the *p-T-x* phase diagram are reported. (Yu.V. Levinskii, M. I. Alymov, L.L. Rokhlin, “The *p-T-x* phase diagram of the Cu-Mg system”, *Advanced Materials and Technologies*, 2020, No. 1(17), p. 3-7).

3. The most complete graphical representation of equilibria in the Mg-Ni system is given by three-dimension phase diagram: pressure-temperature-composition (*p-T-x*), projection of three-phase equilibrium om pressure-temperature plane (*p-T-state diagram),* isobaric and isothermal sections, and p_{Mg}-*T* diagram. (Yu.V. Levinskii, M. I. Alymov, L.L. Rokhlin, “The *p-T-x* phase diagram of the Mg-Ni system”, *Advanced Materials and Technologies*, 2020, No. 3(19), p. 3-7).

4. Based on quantitative relationships of the main structural components (1:5, 2:17, and 2:7 phases) for the (R,Zr)(Co,Cu,Fe)Z alloys with R = Gd or Sm, sketches of quasi-ternary sections of the (Co,Cu,Fe)-R-Zr phase diagrams at temperatures of 1160–1190°C and isopleths for the 2:17–2:7 phase composition range of the (Co,Cu,Fe)–Sm–Zr system were constructed. (A. G. Dormidontov , N. B. Kolchugina, N. A. Dormidontov, Yu. V. Milov, “Structure of Alloys for (Sm,Zr)$(Co,Cu,Fe)_Z$ Permanent Magnets: First Level of Heterogeneity”, *Materials* **2020**, 13, 3893; doi:10.3390/ma13173893.

5. The phase composition of the Fe-N-O films, in accordance with the chemical composition, is various combinations of nanocrystalline phases, such as the supersaturated bcc interstitial αFe(N) solid solutions, α’ nitrous martensite with the bct crystal lattice, fcc Fe_3O_4 oxide. Some phenomena inherent for the non-equilibrium state of the films were found: the formation of supersaturated interstitial αFe-based solid solution and precipitation of α’ nitrous martensite with the bct crystal lattice. (Sheftel E.N., Tedzhetov V.A., Harin E.V., Usmanova G.Sh., “Phase Composition and Magnetic Structure in Nanocrystalline Ferromagnetic Fe-N-O Films”, *Current Applied Physics*, 20 (2020) 1429–1434.

6. Fe-Ti-B films were prepared by dc magnetron sputtering of the Fe + 15% TiB_2 and Fe + 30% TiB_2 targets. The Fe81.5Ti13.1B3.9O1.5 films prepared by sputtering of the Fe + 15% TiB_2 target are characterized by two-phase (bcc αFe(Ti) + hcp TiB_2) nanocrystalline structure with a volume phase ratio of 93:7. The vacuum annealing at a temperature of 500°C led to an increase in the TiB_2 fraction up to 31%. The Fe70.4Ti8.8B20.2O0.6 films prepared by sputtering of the Fe + 30% TiB_2 target are characterized by a single-phase αFe-based XRD-amorphous structure. (E.N. Sheftel, E.V. Harin, V.A. Tedzhetov, G.Sh. Usmanova, S.Y. Bobrovskii, K. N.Rozanov, P.A. Zezyulina and Ph.V. Kiryukhantsev-Korneev, “Study of high-frequency magnetic properties of Fe-Ti-B films obtained by magnetron sputtering”, IOP *Conf. Series: Materials Science and Engineering* 848 (2020) 012082 doi:10.1088/1757-899X/848/1/012082).

7. DC magnetron sputtering was used to prepare Fe–Ti–B nanocrystalline films containing 0–14.3 at % Ti and 0–28.9 at % B. According to the phase composition, all films are divided in to three groups: (i) single-phase (supersaturated Ti solid solution in α-Fe); (ii) two-phase (α-Fe(Ti)/ α-Ti, α-Fe(Ti)/TiB_2, α-Fe(Ti)/FeTi or α-Fe(Ti)/Fe_2B); (iii) X-ray amorphous. XRA films were shown to possess a mixed structure consisting of the solid solution α-Fe(Ti)

with a grain size from 0.7 to 2.0 nm and the amorphous phase. A suggestion was made and substantiated that the amorphous phase is enriched in boron. As the total content of Ti and B in the films increases, the grain size of the α-Fe(Ti) phase decreases in the range from12 to 46 nm in single-phase and from 4 to 26 nm in two-phase films. It was shown that solid-solution and precipitation strengthening define the grain size of the α-Fe(Ti) phase, which is formed upon deposition. (E. N. Sheftel, V. A. Tedzhetov, , Ph. V. Kiryukhantsev-Korneevb, E. V. Harin, G. Sh. Usmanova, and O. M. Zhigalina, “Investigation of the Processes of the Formation of a Nonequilibrium Phase-Structural State in FeTiB Films Obtained by Magnetron Sputtering”, *Journal of Non-Ferrous Metals*, 2020, Vol. 61, No. 6, pp. 753–761.

8. The structure of the as-sputtered Fe, $Fe_{(1-x)}N_x$, $Fe_{(1-y)}Zr_y$, and $Fe_{(90-z)}Zr_{10}N_z$ films is various combinations of the following phases: nanocrystalline, mixed (nanocrystalline + amorphous) or amorphous (in terms of X-ray diffraction) phases. The composition of the nanocrystalline phases is the supersaturated interstitial bcc Fe(N) and/or substitutional bcc Fe(Zr) solid solutions and fccFe_3O_4 oxide. In the films containing high N (~10 at.%) and/or Zr (~10–15 at.%) with nanocrystalline or mixed (nanocrystalline + amorphous) structure only some portions of Zr and N elements are used for the formation of substitutional and interstitial solid solutions meanwhile the residual part of these elements should be localized within intergranular areas and amorphous phase. (E.N. Sheftel, V.A. Tedzhetov, E.V. Harin, G.Sh. Usmanova, A.L. Dyachkov, “FeZrN films: Role of dc magnetron sputtering conditions in the formation of their elemental and phase compositions”, *Thin Solid Films*, 698 (2020) 137876).

Conferences:

XVIth International Conference on Thermal Analysis & Calorimetry, 2020, Moscow, Russia

L.L. Rokhlin, T.V. Dobatkina, E.A. Luk’yanova, I.E. Tarytina, “Peculiarities of the ternary phase diagrams of magnesium with two rare-earth metals of different groups (cerium and yttrium ones)”.

Critical assessments of ternary and binary diagrams

B-Ce-Fe and Al-Co-Tb were performed as part of an international program on critical assess and creating reference books on phase diagrams of metallic systems and collaboration with Materials Science International Team (MSIT).

Phase diagrams in progress: B-Fe-La and B-Fe-Tb.

Member roster: Academician O.A. Bannykh, Prof. E.N. Sheftel, Prof. L.L. Rokhlin, Dr. N.R. Bochvar, Dr. T.V. Dobatkina, Dr. N.B. Kolchugina.