Phase separation in binary alloys under temperature / pressure action: valence electron energy as origin

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Formation and stability phases in binary alloys are defined by several factors as atomic size differences, electronegativities and Hume-Rothery effects. The classical example of the Hume-Rothery phases is the Cu – Zn diagram and related diagrams where the phase boundary restricted by the number of valence electrons per atoms or electron concentration. The physical basis was given within the model of the Fermi sphere – Brillouin zone (FS-BZ) configuration assuming the gain in the band structure energy by the contact of the Fermi sphere to the Brillouin plains and formation of the energy gaps (see [1, 2] and refs. therein). The FS-BZ approach can be extended for understanding of great variety of phase transitions in binary alloy systems under temperature or pressure action.

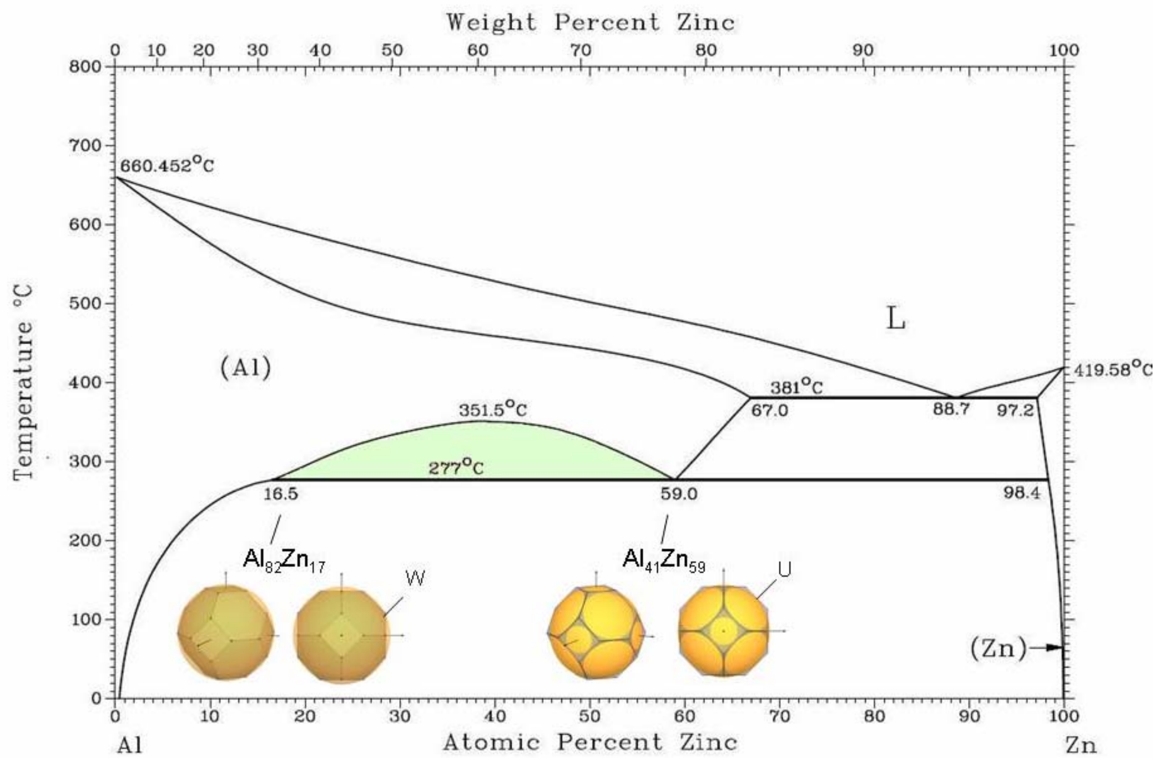

Figure 3: The phase diagram Al – Zn. The Al(Zn) solid solution region with the *fcc* structure contains a miscibility gap with two-phase region (colored). For the boundary phases with ~17 and 59 at% Zn constructions of FS-BZ are given with a common view and a view along a*.

For polyvalent metals the volume of the valence electrons in the FS is large than the volume of the BZ. Therefore the Fermi surface cuts many zone planes and contributions to the crystal energy from regions near the plane intersections may lead to important effects for phase stability. An interesting case of the *fcc* phase decomposition is observed in the Al – Zn alloy system, where Al(Zn) *fcc* solid solution is stable at high temperature and below 352°C there is a miscibility gap of two *fcc* phases with ~17 and 59 at.% Zn. The contacts FS with BZ occur for W-type corners and for the edges of (111) planes in the point U, respectively (Figure 1). In this case the electronic structure factor reveals as driving force for diffusion and phase separation.

Phase separation under pressure was observed for binary compound In_5Bi_3 at 15 GPa and 150°C [3]. Two phases of different compositions were found with tetragonal distortions of the body-centered cubic phase with axial ratios $c/a > 1$ and $c/a < 1$. There is an example of chemically ordered compound decomposition with diffusion into two disordered phases. Structures of high-pressure phases follow the Bain path of tetragonal distortion and defined by minimization of the valence electron energy [3].

References

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[3] O. Degtyareva, V.F. Degtyareva: *Structural transformations in the* In_5Bi_3 *compound under high pressure.* J. Phys.: Condens. Matter **14**, 407-414 (2002).