

Complex structures in the Au – Cd alloys: electron origin of diffusion ordering

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In the Au–Cd alloy system there is a large number of the intermediate phases. This is due to the substantial increase in effects of ordering and the contribution of the band structure energy of valence electrons. The classical example of the diagram with the Hume-Rothery phases is the Cu – Zn diagram and related diagrams. Few and relatively simple phases in Cu–Zn change to structurally complex compounds in Au–Cd. The structures of Au–Cd compounds can be combined into groups according to their relation to the high-symmetry structures: Au_3Cd -*tI16* is related to *fcc*; phases $AuCd$ -*mP6*, *oP4* and *hP18* are related to *bcc*. Au_5Cd_8 -*cI52* and $AuCd_3$ -*hP24* can be considered as structures derived from *bcc* with superlattices and vacancies. Several compounds have separate phase regions and are defined by the formation of the tetrahedral, icosahedral and trigonal-prismatic clusters such as in Au_3Cd_5 -*tI32*, $AuCd_2$ -*mC72* and $AuCd_4$ -*hP273*. The latter phase provides an example of a complex structure forming an almost completely spherical Brillouin zone (BZ) polyhedron accommodating the Fermi sphere (FS).

By constructing the BZ-FS configurations [1] for the Au–Cd compounds we can see the complex polyhedra with the BZ planes touching the FS that demonstrates significance of the band structure energy of valence electrons for the phase stability [2]. The driving force to form a variety of diffusion ordering superlattices in the Au–Cd alloys can be understood as an advantage of the band structure energy over the electrostatic energy. Additional BZ planes that arise due to formation of the ordered supercells lead to formation of many-faced polyhedra that accommodate well the free-electron Fermi sphere.



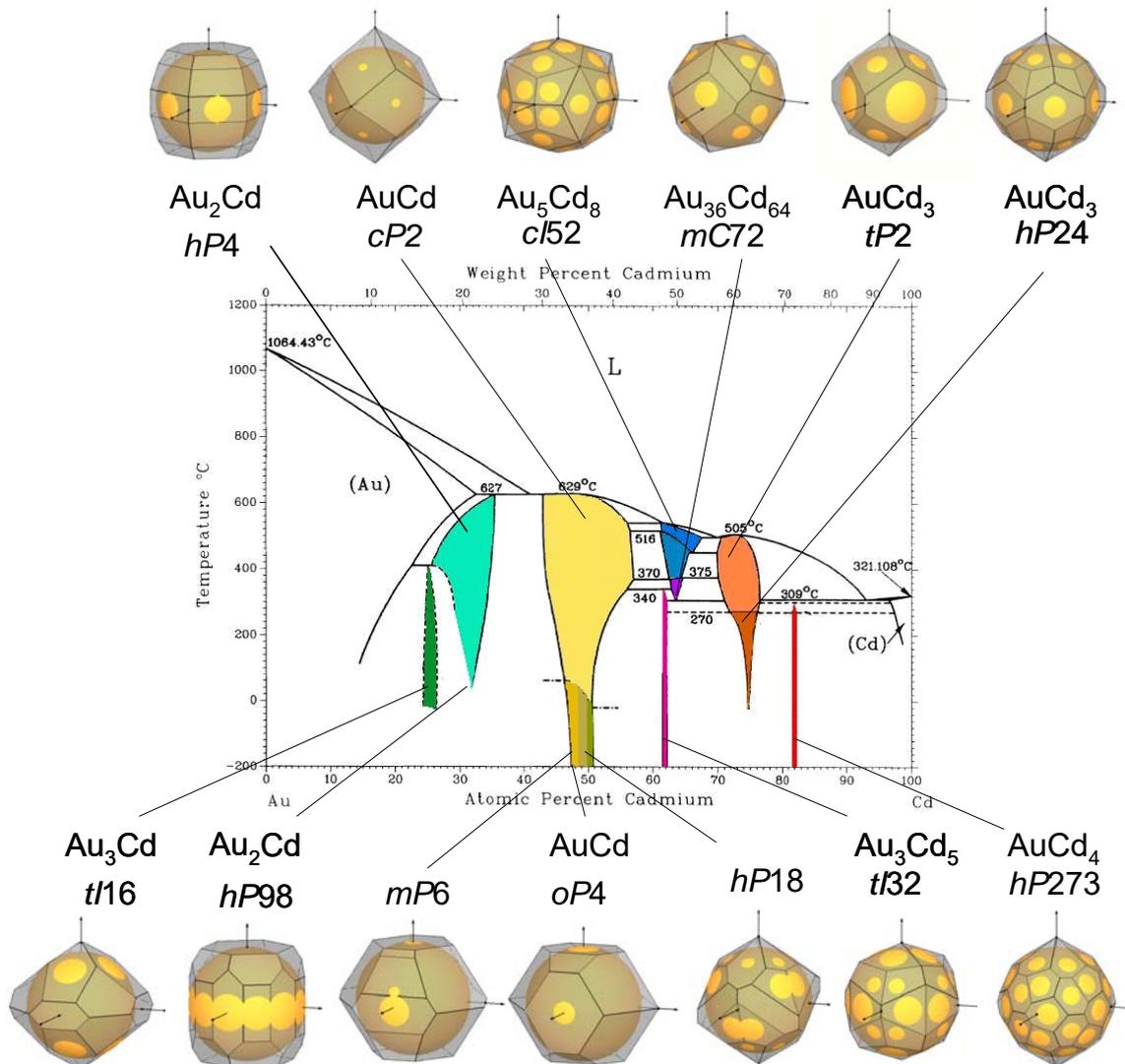


Figure 17: Au – Cd phase diagram. Constructions of FS-BZ configurations are shown for the intermediate compounds with indicated compositions and structure types.

References

- [1] V.F. Degtyareva, I.S. Smirnova: *BRIZ: A visualization program for Brillouin zone–Fermi sphere configuration*. *Z. Kristallogr.* **222**, 718–721 (2007).
- [2] V.F. Degtyareva, N.S.Afonikova: *Complex structures in the Au-Cd alloy system: Hume-Rothery mechanism as origin*. *Solid State Sci.* **49**, 61-67 (2015).