# T-x-y Diagrams Verification after Thermodynamic Calculation: Ag-Cu-Ni

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## Abstract

To optimize thermodynamic calculations, specialized databases are created with a limited number of chemical compounds, their parameters and interaction models. However they all can have some drawbacks that can lead to errors. As an additional verification and validation of the obtained data, the authors developed a computer-aided design method used to visualize multicomponent phase diagrams and generalize information about phase equilibria.

## Introduction

For a long time, the issue of creating lead-free solders that would not be inferior in properties to an alloy of lead with tin and would meet the requirements of environmental safety remains relevant. Special reference atlases were published containing information on the phase diagrams of ternary systems without the lead. The Ag-Cu-Ni system is promising for the development of environmentally friendly solders. Therefore, it was decided to build a spatial (3D) computer model T-x-y diagram of the Ag-Cu-Ni system and compare the results with those published in [1-4].

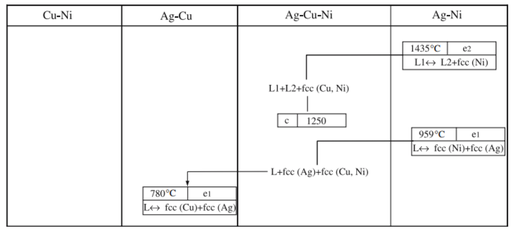


**Figure 1.** Reactions scheme of the Ag-Cu-Ni system (According to this scheme, taken from [3], 3-phase region Ag+Cu+Ni is impossible, but it was imaged on some isopleths in the papers, published later by the same authors)

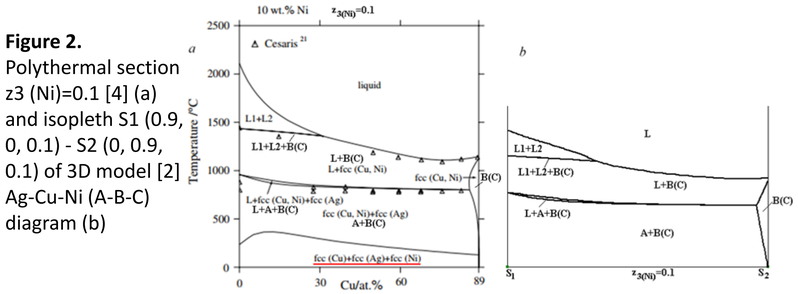


**Figure 2.** Polythermal section z3 (Ni)=0.1 [4] (a) and isopleth S1 (0.9, 0, 0.1) - S2 (0, 0.9, 0.1) of 3D model [2] Ag-Cu-Ni (A-B-C) diagram (b)

## Methods

To generalize information about phase equilibria in boundary systems and create its complete geometric structure as the phase regions are assembled, computer-aided design methods for assembling phase diagrams have been developed. The design of such three-dimensional (3D — for ternary systems) and four-dimensional (4D — for quaternary systems) computer models allow obtaining a complete image of the phase diagram, including all its geometrical elements.

It is possible to carry out on this basis the necessary research:

- to calculate isothermal sections and isopleths;
- to image the crystallization schemes and analyze the microstructures formation.

3D models are not associated with special databases and can use hypothetical information to calculate a prototype of the phase diagram, when the initial information is insufficient, or to simulate only a fragment of the phase diagram. Then the prototype can be supplemented and revised if experimental data are available. The Phase Diagram Designer (PD Designer) software is used to design 3D and 4D computer models of phase diagrams and their 2D and 3D sections.

Discussed approach does not compete with a classical CALPHAD description of the multicomponent systems based on the established binary and ternary boundary systems.

Proposed technique does not use the thermodynamic models for phase diagram optimization but helps to visualize phase equilibria through geometrical construction of phase diagram elements using experimental data.

## Acknowledgements

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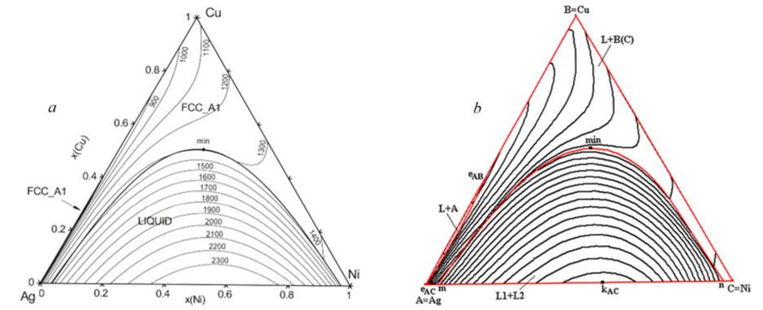


**Figure 3.** Projections of the Atlas liquidus [1] (a) and 3D model (b) (in the Atlas figure the phase region of the primary crystallization of silver should be named as LIQUID + FCC_A1, not as FCC_A1, and the immiscibility area as LIQUID1 + LIQUID2, not as LIQUID)

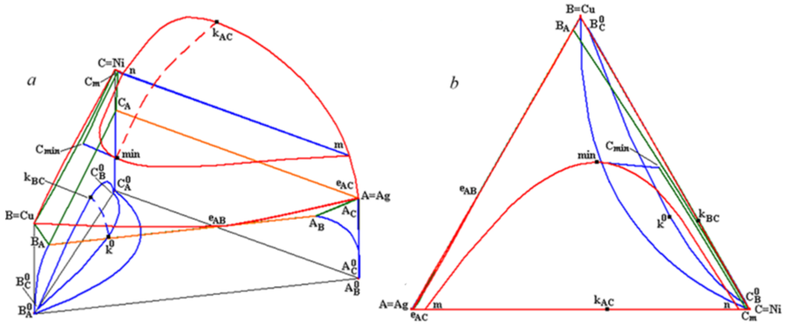


**Figure 4.** 3D model of the Ag–Cu–Ni T–x–y diagram (a) and its x–y projection (b)

## Conclusion

Based on published experimental and calculated data (binary systems, x-y liquidus projection, reactions scheme, four isothermal sections), a spatial computer model of the T-x-y Ag-Cu-Ni diagram is constructed. The results obtained were compared with those published in the Atlas [1] and some papers [3-4].

## References

1. Atlas of Phase Diagrams for Lead-Free Soldering compiled by: COST 531 /A. Dinsdale [et al.], European Science Foundation. – Brno, Czech Republic: Vydavatelstvi Knihar, 2008. – Vol. 1. – 289 p.
2. Parfenova M. D., Vorob'eva V. P., Lutsyk V. I. 3D computer model of the Ag–Cu–Ni T–x–y diagram: verification of sections in the atlas of phase diagrams for lead-free soldering. Proceedings of the National Academy of Sciences of Belarus. Chemical Series, 2021, vol. 57, no. 1, pp. 15–24 (in Russian). https://doi.org/10.29235/1561-8331-2021-57-1-15-24
3. X. J. LIU, C. P. WANG, 2 F. GAO, I. OHNUMA, K. ISHIDA. Thermodynamic Calculation of Phase Equilibria in the Sn-Ag-Cu-Ni-Au System // Journal of ELECTRONIC MATERIALS, Vol. 36, No. 11, 2007, 1429-1441.
4. Liu X.J., Gao F., Wang C.P., Ishida K. Thermodynamic Assessments of the Ag-Ni Binary and Ag-Cu-Ni Ternary Systems // J. Electron. Materials. 2008. V. 37. No 2. P. 210-217.

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