



Thermodynamic and physical properties of liquid alloys. Theory vs experiment

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Interdyscyplinarne studia doktoranckie z zakresu inżynierii materiałowej z wykładowym językiem angielskim

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Projekt współfinansowany ze środków Unii Europejskiej w ramach Europejskiego Funduszu Społecznego

Schedule

1. Aims and results:

- theoretical ideas:

free atom theory (macroscopic level)

classical and ab initio calculation (atomic level)

Bathia - Thornton theory (microscopic level)

- experimental ideas:

EMF study of liquid Al-Li-Zn alloys

2. Future plans

Results → theory

free atom theory (macroscopic level)

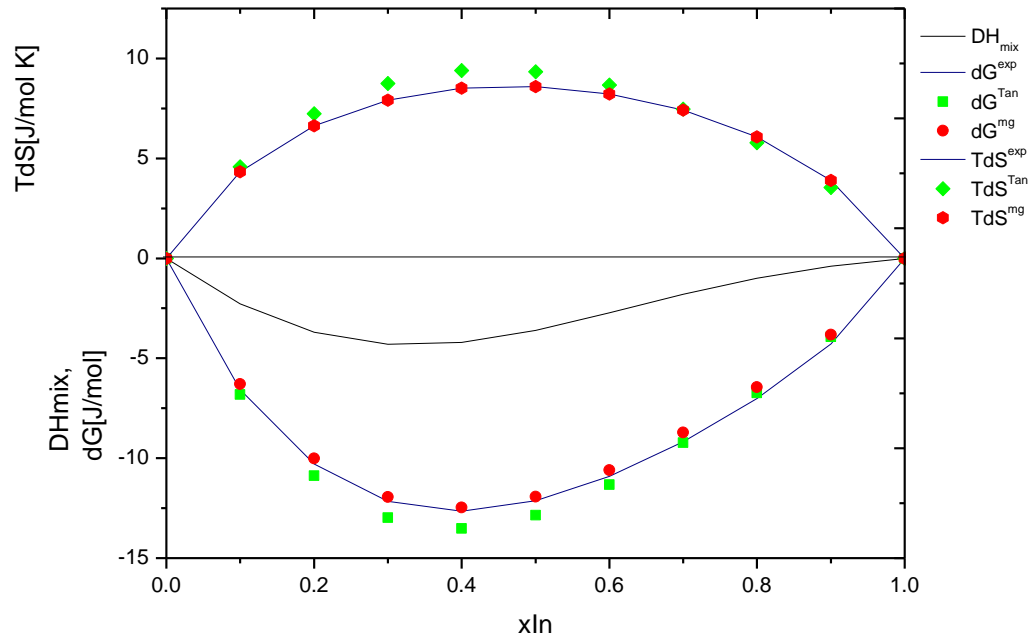


thermodynamics

excess functions
(Gibbs free energy,
entropy) from enthalpy mixing



Metallic solutions



negative enthalpy of mixing, i.e. AgIn

Results → theory

free atom theory (macroscopic level)



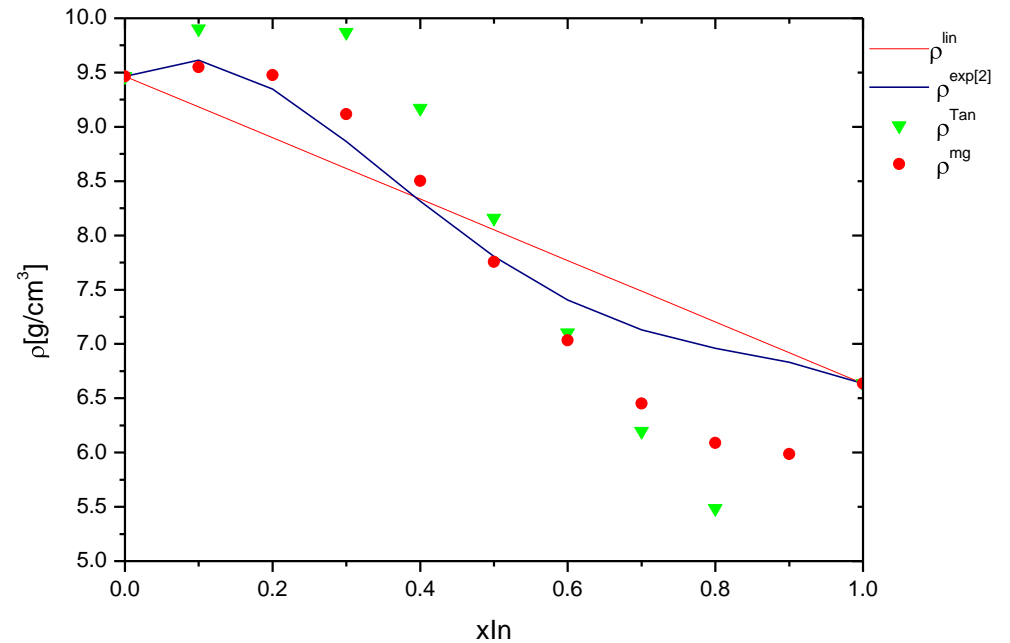
Metallic solutions



physics

density, viscosity from thermodynamics

Negative enthalpy of mixing, i.e. AgIn



classical and ab initio calculation (atomic level)

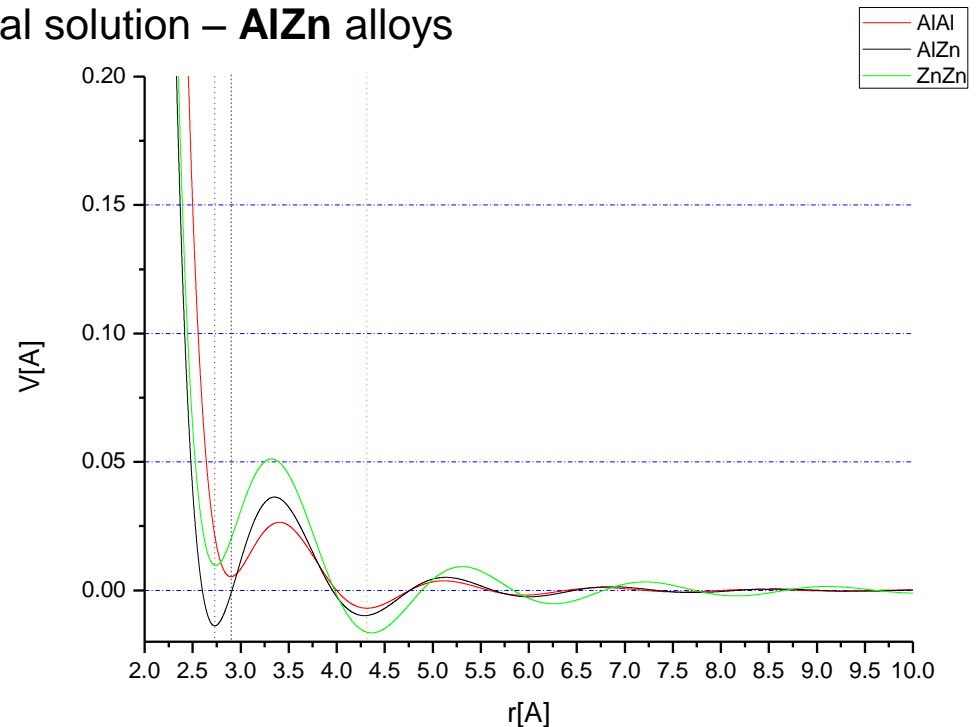
Metallic solution positive deviation from ideal solution – **AlZn** alloys

LAMMPS code: EOPP potential,
cubic box - fcc lattice

Thermodynamic quantities: total energy,
enthalpy, pressure

Dynamic properties: volume (density), viscosity and diffusion coefficient

Structural properties: surface tension, radial distribution function, $g(r)$



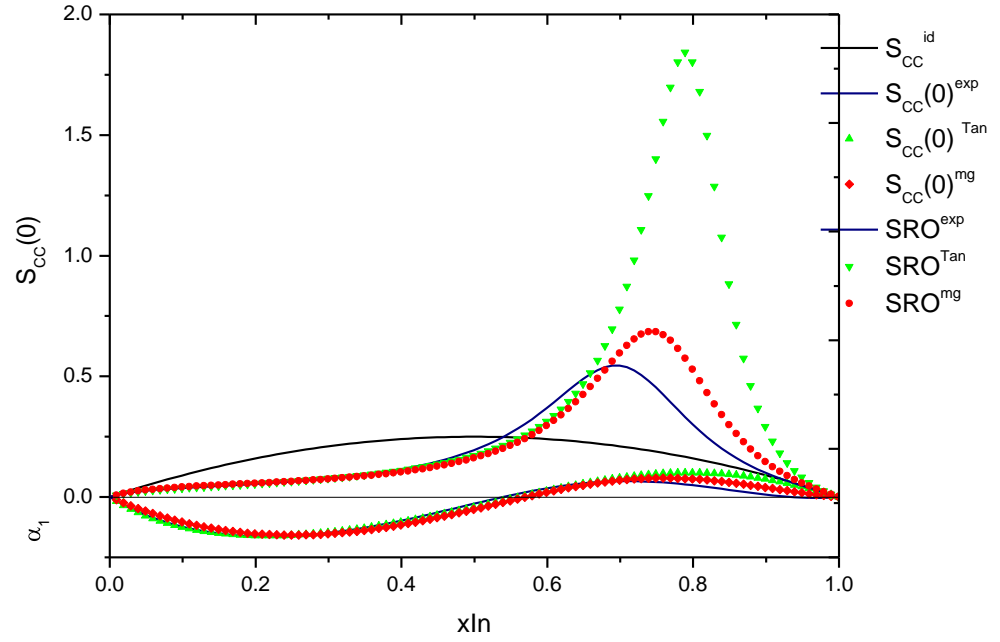
Bathia - Thornton theory (microscopic level)

↓
Structural information

Warren-Cowley short range order parameter (α)
– ordering/demixing properties of liquid alloys

Concentration- concentration fluctuations function - $S_{cc}(0)$

Metallic solution with negative enthalpy of mixing – AgIn

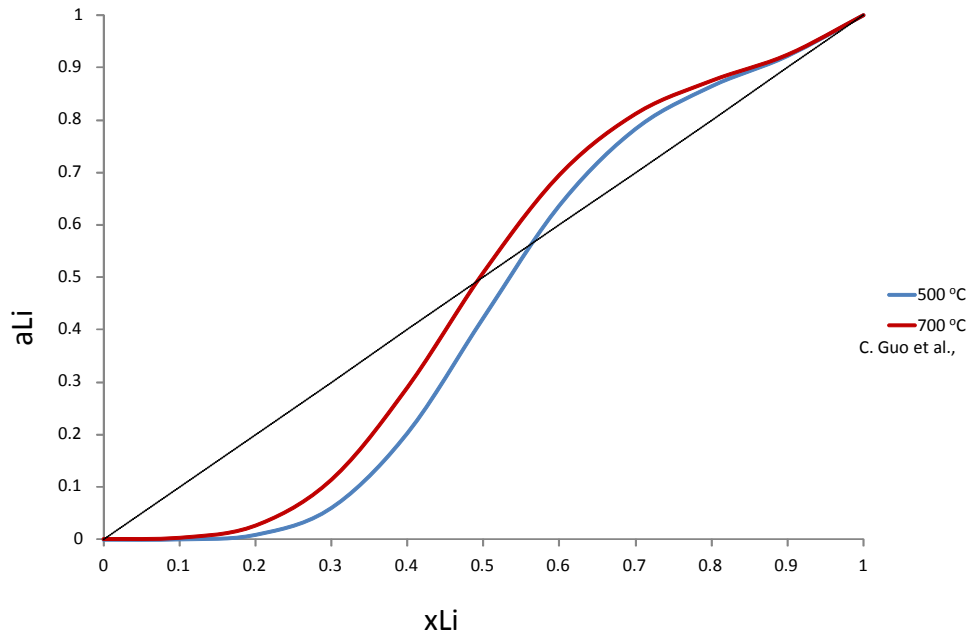


EMF study of liquid Al-Li-Zn alloys

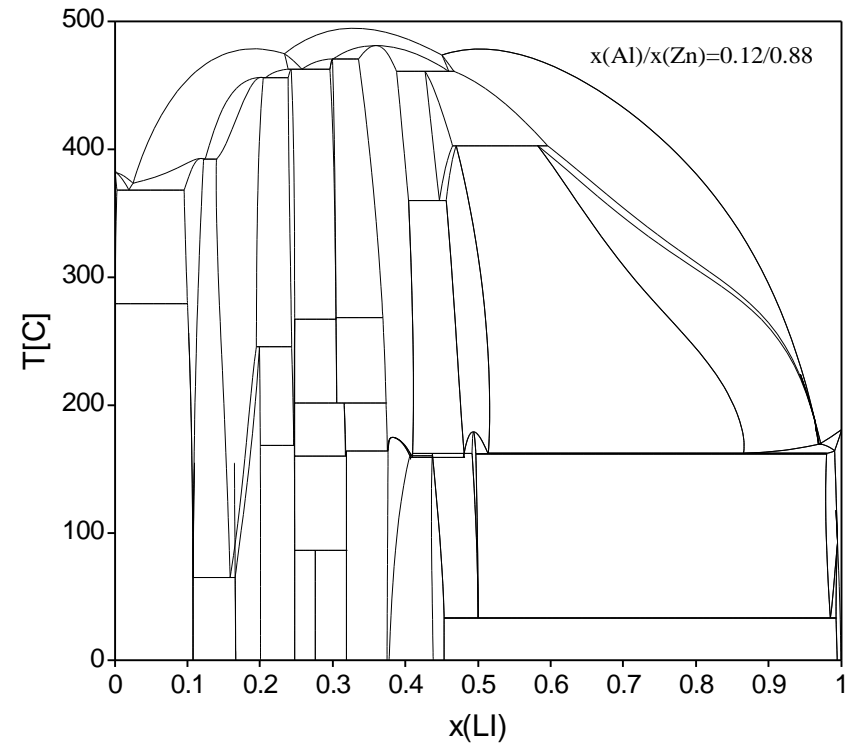
Al/Zn- eutectic composition (0.12/0.88)

Lithium concentration changed from 0.1 to 0.9

activity of lithium



Modelled phase diagram

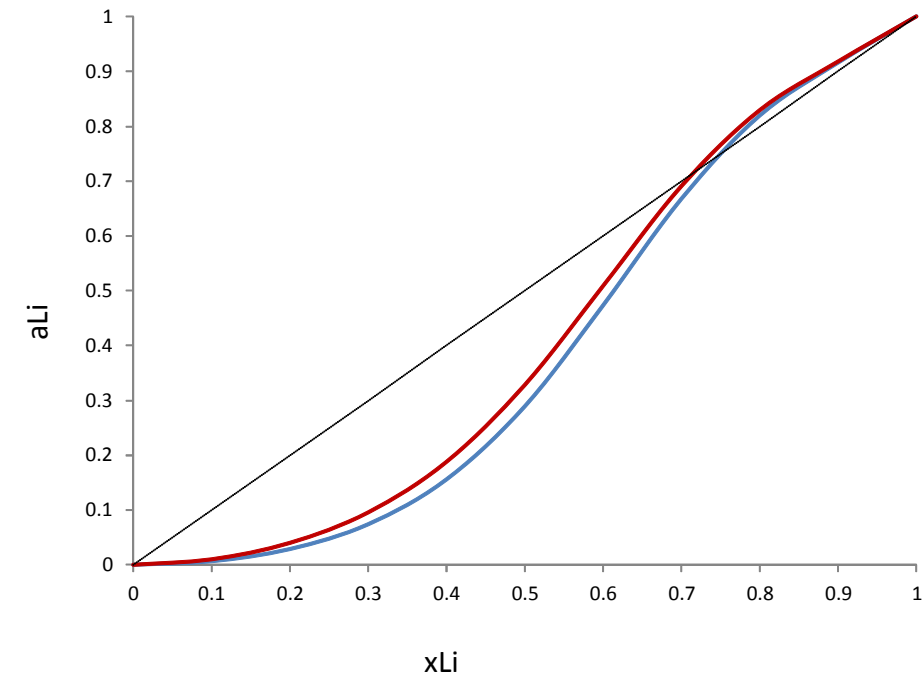


EMF study of liquid Al-Li-Zn alloys

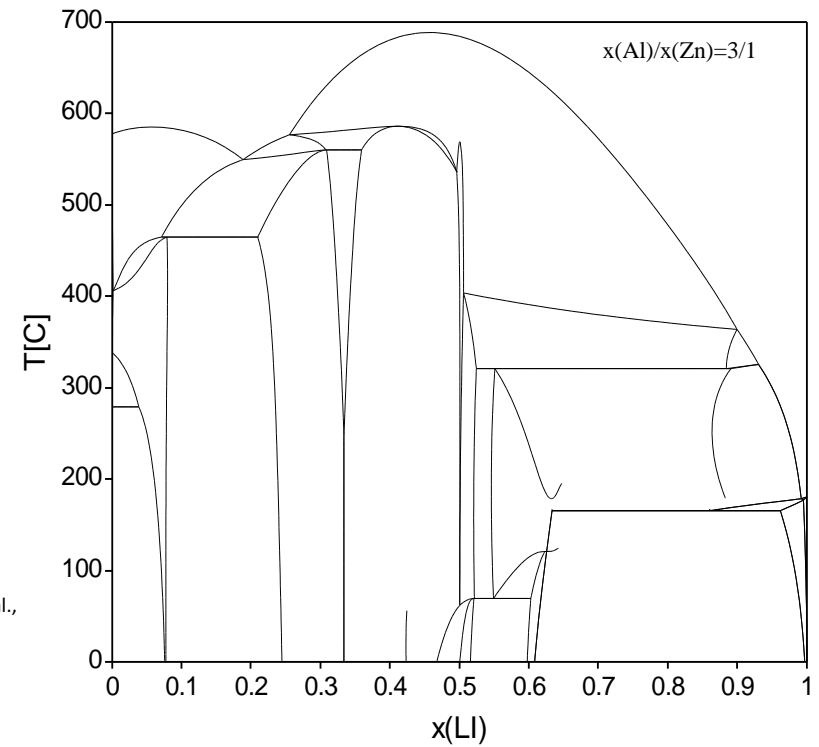
Al/Zn- 3/1

Lithium concentration changed from 0.1 to 0.9

activity of lithium



Modelled phase diagram



700 °C
800 °C
C. Guo et al.,

Summary

- ✓ Free atom theory (modelling of thermodynamic and physical properties of liquid alloys)
 - Improvement of model proposed by Tanaka (new correction factor)
 - Better agreement with experimental data achieved
- ✓ MD calculations
 - Attempt to define a potential for AlZn alloys
- ✓ Bahtia and Hargrove theory
 - Investigation of AgIn microscopic structure
- ✓ Experimental research
 - EMF studies of Al-Li-Zn alloys – determination of Li activity

Future plans

- ✓ Extension of a free volume model on:
 - multicomponent metallic systems
 - modelling of viscosity
 - pseudopotential theory
 - anharmonic oscillations
- ✓ Classical and Ab initio Molecular Dynamics calculations for liquid alloys
- ✓ Application of Bathia - Thornton theory for multicomponent solutions
- ✓ Application of Roach and Henein method – measurement of physical properties of liquid Al-Li-Zn



KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI



INSTYTUT METALURGII
I INŻYNIERII MATERIAŁOWEJ
im. Aleksandra Krupkowskiego
Polskiej Akademii Nauk

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FUNDUSZ SPOŁECZNY



Thank You

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