Simulations of the thermodynamic and physical properties of liquid Al-Zn-Li alloys in terms of free volume theory and molecular dynamics techniques

M.Sc. Eng. **Marcela Trybuła**
Supervisor: Associate Professor **Władysław Gąsior**, D.Sc., Ph.D.

The main goals of the PhD thesis are as follows:

1. Theoretical description of thermodynamic (enthalpy of mixing, entropy and Gibbs free energy) and physical (density, viscosity and surface tension) properties using free volume theory and molecular dynamics techniques.
2. Development new parameters coming from ab initio molecular dynamics calculations for improvement free volume theory.
3. Modelling interatomic potentials for ternary metallic systems.
4. Extension the applied theory on ternary alloys using symmetrical and asymmetrical models.
5. Experimental measurement of the lithium activity- the electromotive force measurement for three constant Al to Zn ratio using concentration cell method.
6. Experimental investigation of the three physical properties by Roach-Henein method.