

Effect of the ordering potential on the structure of liquid alloys

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Abstract. The concept of “ordering or alloying potential” (J. Hafnerⁱ: from Hamiltonians to phase diagrams: Springer Berlin 1987 and R. N. Singh and F. Sommerⁱⁱ Rep. Prog. Phys. **60** (1997) 57–150) enables the understanding of the different kind of alloys: hetero-coordinated one’s leading to compounds, homo-coordinated ones leading to miscibility gap systems and substitutional alloys. The ordering potential is based on the comparison of identical atom interionic potentials (V_{11} and V_{22}) and different atom interionic potential (V_{12}) It allows the description of the demixing properties of some alloys. In order to understand the concepts, we developed our calculations by using a Lennard-Jones potential, the atomic structure being calculated by molecular dynamics simulation. We obtained surprising and unexpected results putting in evidence the time of simulation and the strength of the ordering potential.

1 Introduction

The ordering potential is defined by the difference between identical atoms interionic potentials and unlike atoms interionic potential:

$$V_{\text{ord}}(\mathbf{r}) = c_1 c_2 [V_{11}(\mathbf{r}) + V_{22}(\mathbf{r}) - 2V_{12}(\mathbf{r})]$$

Knowing how the atoms interact together is crucial to understand most physical properties of the condensed matter. It is easy to understand that if the mean homocoordinated potential is deeper than the heterocoordinated atoms potential, each atom will prefer to be surrounded by identical atoms, this preference can go to demixion if the temperature decreases. Nevertheless the situation is not so simple since:

- The hardness of the potential may be different (slope of the potential in the hard core region).
- The depth of the potential may be different.
- The size of the atoms may be different (first intersection of the potential with $V=0$).

It is necessary to fix some of these parameters by using an adapted potential. We first chose the same hardness (same potentials in the repulsive part) and the same size.

The only difference is the depth of the potential chosen so as to have the same minimum for V_{11} and V_{22} . The potential V_{12} is the only different function.

In this work, we have used the Lennard-Jones (LJ) potential for a binary system:

$$V_{\alpha\beta}(\mathbf{r}) = 4\varepsilon_{\alpha\beta} \left[\left(\frac{\sigma_{\alpha\beta}}{r} \right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r} \right)^6 \right]$$

So, the mean density of particles ρ at the temperature T , the concentrations c_1 and c_2 , and the two sets of parameters $\varepsilon_{\alpha\beta}$ and $\sigma_{\alpha\beta}$ (α and $\beta=1, 2$) define the thermodynamic state of LJ-system.

2) Calculations

The studied system is the so-called “symmetrical binary fluid” for which the concentrations c_1 and c_2 are equal, and for which LJ-parameters are:

$$\sigma_{11} = \sigma_{22} = \sigma_{12} = \sigma, \quad \varepsilon_{11} = \varepsilon_{22} = \varepsilon \quad \text{and} \quad \varepsilon_{12} = \lambda\varepsilon.$$

