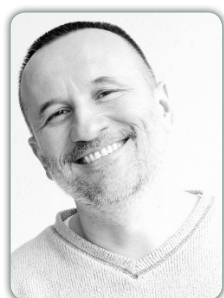


24th World Nano Conference

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Chemical thermodynamics for nano-systems

Nano-systems are systems containing at least one phase with at least one of its dimensions below 100 nm. The equilibrium of nano-phases depend not only on pressure, temperature and composition but also on the number of atoms in the nano-phases, as an additional state parameter. That is why the phase rule of Gibbs is changed for nano-Calphad: the maximum number of possible co-existing nano-phases equals the number of components + three (3=pressure, temperature and number of atoms in nano-phases). As the phase rule is changed, all rules to construct and to read phase diagrams of nano-systems will change. This point is usually missing in the majority of published nano-phase diagrams. When macro-phase equilibria are calculated, the role of interfaces is negligible. However, for equilibria of nano-systems the role of interfaces is significant. The type and amount of interfaces in multi-phase nano-systems depend on the shape, size and arrangement of nano-phases. That is why when phase equilibrium is calculated for nano-systems, also the equilibrium size, shape and arrangement of nano-phases should be calculated. This point is usually missing in the majority of published nano-phase diagrams. To calculate solid/liquid equilibrium between solid and liquid nano-phases, the concentration and temperature dependence of the solid-liquid interfacial energy should be taken into account. This point is usually missing in the majority of published nano-phase diagrams. Systems containing nano-phases are usually unstable due to the positive interfacial energy between them. Thus, the conditions of negative interfacial energy are crucial for stabilization of nano-systems. For equilibrium calculation of nano-systems, the chemical potential of components should be known as function of size, shape and arrangement of nano-phases. The new equations presented here prove that the Kelvin paradigm is mistaken, i.e. the thermodynamic nano-effect is due not to the increased curvature of nano-phases, it is rather due to the increased specific surface area of nano-phases. This forms the basis of a new paradigm presented here after Gibbs.

Recent Publications

1. A Yakymovych et al. (2018) The nano heat effect of replacing macro-particles by nano-particles in drop calorimetry: the case of core/shell metal/oxide nano-particles. RSC Adv. 8(16):8856-8869.
2. G Kaptay (2017) On the negative surface tension of solutions and on spontaneous emulsification. Langmuir. 33(40):10550-10560.
3. G Kaptay (2017) A new paradigm on the chemical potentials of components in multi-component nano-phases within multi-phase systems. RSC Adv. 7(65):41241-41253.
4. J Korozs and G Kaptay (2017) Derivation of the Butler equation from the requirement of the minimum Gibbs energy of a solution phase, taking into account its surface area. Coll. Surf. A: Physicochemical and Engineering Aspects. 533:296-301.
5. A Dezso and G Kaptay (2017) On the configurational entropy of nanoscale solutions for more accurate surface and bulk nano-thermodynamic calculations. Entropy. 19(6):248.

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Biography

George Kaptay obtained his higher education in St Petersburg, Russia as Metallurgical Engineer. Since 1988 he has been with the University of Miskolc, Hungary. In 2007 he established the Department of Nanotechnology and has been serving as its Head and Professor. He was elected a corresponding Member of the Hungarian Academy of Sciences in 2016. He is also the president of the Hungarian Society of Materials (MAE). He established a new research institute in 2006 on nanotechnology (BAY-NANO), which is now a part of a larger BAY-ENG unit within the Bay Zoltan Ltd on Applied Research. Since 2017 he is a leader of the MTA-ME Materials Science Research Group. He is also the president of the Scientific Council of the University of Miskolc. His main scientific interest is modelling thermodynamic and thermophysical properties, interfacial energies, forces and phenomena, including the equilibrium of macro- and nano-systems

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