

Solute Concentrations and Strains in Nanograined Materials and Nanoparticles

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In this presentation, we report a newly developed Gibbs-approach based adsorption isotherm for interface (including grain boundary and surface) segregation in nanograined polycrystals and nanoparticles. An excess interface thickness was introduced to describe the excess of interface atomic volume in comparison with the atomic volume in lattice. The interface bulk modulus was then determined with the excess interface thickness and a universal function. The newly developed adsorption isotherm is able to analyze simultaneously stresses, concentrations and their coupling behaviors in lattice and interface. The thermodynamic analysis shows that the apparent solute concentration is greatly enhanced in nanomaterials due to two factors. The first one is the large interface volume fraction in nanomaterials and interface segregation. The second is due to a considerable increase in the lattice concentration that is boosted by the concentration-induced stresses. The difference of concentration in lattice and interface changes the stress on lattice from compressive to tensile and thus enhances the concentration in lattice. The theoretical predictions have been verified by experimental data reported in the literature for H-Pd system. With the measured lattice strain and sample strain of the nanograined Pd, with an averaged grain size of 10 nm, versus the hydrogen gas partial pressure, we determined H concentrations and stresses in grains and grain boundaries and the intrinsic properties of grain boundaries, such as the grain boundary bulk modulus, the grain boundary excess thickness, the difference in chemical potential between grains and grain boundaries, etc. Applying the Gibbs-approach based adsorption isotherm to the experimental data of nominal H concentration in Pd nanoparticles, with a mean diameter of 3.6 nm, versus H₂ partial pressure, we determined the H-trap depth of Pd surface, the H concentrations and

stresses in both core and surface shell of the nanoparticles. The developed Gibbs-approach based adsorption isotherm is able to be applied to other material systems.

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