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The capillarity equation at the nanoscale: size effects on gas bubbles in metals.

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Gas bubbles in materials are relevant in several technological applications. A usual way to estimate the amount of gas in a bubble is to assume equilibrium, i. e. the gas pressure P satisfy the Young-Laplace capillarity equation $P=2\gamma/R$, with γ the surface energy of the host material, R the bubble radius, and the relation between P and density extracted form an equation of state (EOS) for He. In this work we show that at the nanoscale this picture is no longer correct

Both the P-density relation and the capillarity pressure need to be modified to describe nanoscale gas bubbles embedded in metals, scale at which the width of the interface region cannot be neglected. We focus in particular on the case of He in Fe.

In contrast to the common assumption that pressure inside a gas or fluid bubble is constant, we bring the concept of Tolman's length from the field of colloidal particles that provides a curvature dependence for the interface energy that becomes relevant at the nano scale. Pressure and density can no longer be defined as global quantities determined by an EOS, but they become functions of position because the bubble develops a core-shell structure. To highlight the origin of this effect we solve the bubble problem first using continuum mechanics and then using empirical potentials to find a quantitative measure of this effect.

The fact that the pressure becomes a function of position calls for a new equation of state for He at the nanoscale that accounts for these interface effects (see A. Caro et al. Appl. Phys. Lett. 103, 213115 (2013). We derive an expression to predict pressure, and from it density and the amount of He in nanoscale bubbles. We find that conditions for equilibrium are found for values of pressure or density at variance by a factor of 2 compared to the traditional way of using the capillarity equation and a bulk He EOS.