Thermodynamic Models based on DFT data for Hydrogen Supersaturation and Defects Stabilization

Tuesday, April 12, 2022 10:50 AM (30 minutes)

In this presentation, I will review some of the thermodynamic models that have been built to understand the formation of Super-Abundant Vacancies (SAV). In case of tungsten, when exposed to H/D plasmas, Super Saturated Layers (SSL) form by clustering of SAV in the first 10 nm of the top sample [1]. The stability of SAV is driven by the chemical potential of hydrogen, which is a central quantity in most of the models dealing with SAV. The chemical potential of a hydrogen gas with an ideal behavior is known analytically. In case of a real gas at high pressure, the chemical potential of hydrogen and deuterium was fitted against experimental data versus the pressure and the temperature [2]. But under plasma irradiation, the chemical potential cannot be established in a simple way. I will present one of our recent works that proposes such a correlation between the flux, the incident energy of the impinging ions, the temperature, and the chemical potential of hydrogen in the sub-surface of the material [3]. Then, in order to open the discussion, I will comment some experimental results from the literature with regard to the models that exist.

References:

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