Mapping the binding energy of $\text{H}$ inside amorphous and crystalline transition metals using the effective medium theory

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June 12, 2020

Abstract

The effective medium theory (EMT), as developed by Norskov and Nordlander et al., is used to determine the location and binding energy of impurities inside crystalline, as well as amorphous transition metals and amorphous transition metal alloys. The example probed is that of $\text{H}$ inside $\text{V}$ and Fe/V-alloys. The electron density distribution of the crystalline metals is approximated as the linear combination of atomic electron densities, that are given by a single gaussian centered around each atom in the lattice. Furthermore, a method is proposed to apply the insights derived from EMT in well defined crystal lattices to amorphous transition metals without internal long range order. Hereby, the binding energy of $\text{H}$ inside the metal is correlated to the metal’s average valence electron density. For crystalline transition metals, it is found, that despite the simplicity of the applied model, structural properties, like the tetrahedral binding sites of $\text{H}$ inside bcc metals, can be correctly reproduced. They are hereby shown to be a direct result of the lattice geometry, independent of the precise spatial structure of the electronic bands. Clear trends are found in the changes of $\text{H}$ ground state binding energy versus average valence electron density, that are different for transition metals of bcc, hcp and fcc-lattices. They suggest, that the value of the lowest electron density found in the system, which in the investigated transition metals corresponds to the ground state binding energy, corresponds more to the structural type of the lattice than to the average of the valence electron density.

1 Introduction

$\text{H}$ has long been known to cause embrittlement in various construction steels [1]. Lately, it has gained increased attention, as $\text{H}$ can be used to store energy without emitting greenhouse gases in the process. Its small physical size and simple structure make it also a versatile tool to probe the internal structure of various materials and put theoretical models to the test, be it of the host material structure or the nature of these material’s binding behaviour. One such theory commonly used to describe material structures is hereby the density functional theory (DFT) [2, 3], which makes use of the fact, that all of the information needed to describe the ground state behaviour of any material system is described by the spatial electron distribution inside it. These calculations however are generally very complicated and time consuming. This is why, in 1977, the effective medium theory (EMT) was introduced by Norskov et al. [1]. This approach to the EMT made use of previous DFT calculations to simplify considerations of binding energy of impurities inside transition metals and applied them to $\text{H}$ specifically. It was improved in the following years and can be used to describe qualitative trends and even quantitative estimates for a great range of phenomena, like chemisorption on transition metal surfaces, absorption of $\text{H}$ in interstitial sites as well as diffusion behaviour and interactions with other impurities and defects [1, 4, 5, 6, 7, 8], while greatly simplifying the calculations needed. In this report, the latest version of EMT, as showcased in [5, 6], is broken down and applied to the case of crystalline $\text{V}$, before an attempt is made to generalise it to amorphous transition metals and transition metal alloys in the example of different $\text{V}$ and Fe mixes.

Section 2 quickly summarises the version of EMT used in this report and explains the calculations done in section 3. Section 3, hereby introduces the parameters used in the specific cases and discusses