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PROF. DR. OSMAN TURAN CULTURE AND CONVENTİON CENTER

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CONFERENCE OBJECTIVE

The 5th International Conference of Materials and Engineering Technology (TICMET'23) will be held on 13-16 November 2023 in partnership with Karadeniz Technical University, Hasan Kalyoncu University, and Gaziantep University.

The main purpose of TICMET'23 is to present the latest research and results of scientists related to materials and engineering technologies. This conference provides different field delegates with opportunities to exchange new ideas and application experiences, build business or research relationships, and find global partners for future collaboration. After this science feast, your abstract/full texts will be published in conference book with ISBNs and will be brought to the world of science literature with open access and significant contributions will be made to the scientific field.

In addition to the valuable speeches of the invited speakers, a special R&D session will be held at the Conference. It is expected that the R&D session will be a very productive session with the participation of academicians, industrialists and students from universities.

The conference organizing committee is pleased to invite prospective authors to send their original texts to TICMET'23. All papers will be reviewed and evaluated by the referees in the field, based on their technical and/or research content depth, accuracy, relevance to the conference, contributions, and readability. Selected papers presented at the conference will be published in conference book as an abstract and then will be proposed for publication in one of the following journals:

* IEEE Transactions on Engineering Management (SCI)
* Sigma Journal of Engineering and Natural Sciences (Sigma) (E-SCI)
* Acta Mechanica et Automatica (E-SCI)
* Journal of Sustainable Construction Materials and Technologies (JSCMT) (TR Dizin)
* Turkish Journal of Materials (TJOM)
* Turkish Journal of Electromechanics and Energy (TJOEE)
* International Journal of Materials and Engineering Technologies (TIJMET) (Dergipark)

(The publication of selected papers in journals is not guaranteed. The extended version of the selected papers recommended to the journals must be submitted to the journal by the corresponding author. Afterwards, the publications will be subjected to an additional refereeing process. No additional fees will be charged by the Journals)

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DFT STUDY OF HYDROGEN INTERACTION WITH NICKEL AND NICKEL ALLOYS

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Abstract

Interaction of nickel and nickel alloys with hydrogen is a topic of interest in hydrogen production and storage, and also due to the unwanted hydrogen embattlement in the nickel-containing alloys. The strength of the metal-hydrogen bond plays a crucial role in electrocatalysis or hydrogen sorption; therefore, correlating electronic structure and stability of metal hydrides is of broad interest for material design. We present a theoretical investigation of the interaction of nickel with hydrogen, concentrating on the influence of volume and chemical surroundings on the electronic structure and magnetism in the studied systems. Density functional theory calculations are done using the all-electron FPLAPW method, as included in the Wien2k program. In addition to various concentrations of hydrogen in the nickel, the influence of Hf and Pt on the structure, bulk modulus, and stability are examined. By augmenting these calculations with data from the NOMAD archive, we also search for structure-property relations and trends in numerous nickel-metal-hydride systems.

Keywords: Nickel, DFT, hydride, electronic structure.

1. Introduction

Nickel's primary use is as an alloying element in stainless steels, alloy steels, non-ferrous metals, and other corrosion-resistant alloys [1], industrial alkaline electrolysis, and automotive and aerospace materials [2]. Hydrogen interaction with Ni and Ni-containing metal alloys is a topic of interest in hydrogen production and storage. Nickel is an important destabilization element in metal hydrides used to tune their hydrogen storage properties [3]. Additionally, hydrogen embattlement of the nickel-containing alloys is an unwanted phenomenon [4,5]. The strength of the metal-hydrogen bond plays a crucial role in catalysis and electrocatalysis [6,7,8]; therefore, correlating alloy composition, electronic structure, and stability of metal hydrides is of broad interest for material design. This paper examines the influence of volume and chemical effects on the electronic structure and stability of nickel hydride.

2. Materials and Methods

Calculations were performed using a Full Potential (Linearized) Augmented Plane-Waves plus local orbitals (FP (L)APW + lo) method, as implemented in the Wien2k program package based

on the density functional theory [9]. The exchange and correlation effects were included within the generalized gradient approximation. The muffin-tin radii of 2.0 bohr for Ni and 1 bohr for H were adopted. Appropriate supercells were also adopted for the Ni-H system to simulate the concentration effect, while also supercells of formula $Ni_{15}XH$, X=Pt, Hf were constructed to simulate the influence of these metals. The Brillouin zone integration was achieved via a tetrahedron method. Criteria for the convergence of the integrated charge difference between the two successive iterations was set to less than 10^{-5} electrons. The unit cell volumes were optimized, and structures relaxed until the forces acting on atoms were less than 1 mRy/bohr. Additionally, the NOMAD database [10] was searched for Ni-containing bimetal hydrides, to further examine the structure-property relations in these materials.

3. Results and Discussion

First, we examine the influence of structural stress, i.e. volume change on the stability and electronic structure of NiH, by comparing the stability of NiH and Ni having various volumes. Table 1 displays calculated changes in the stability of nickel hydride in reference to nickel and hydrogen in their standard state, i.e. metal nickel and H_2 molecule [11].

Table 1. Hydride formation energy as a function of the volume change in the hydride and metal; % of volume change marks the deviation from the optimized volume for these structures

Volume change (%)	Hydride formation energy (kJ/mol^{-1})
-10	-12.13
-7.5	-13.55
-5.0	-12.30
-2.5	-12.14
0	-12.17
2.5	-11.44
5	-10.98
10	-10.38

We can observe a general trend that an increase in the cell volume leads to the destabilization of the hydride. This is also in line with some data-driven observations in metal hydride systems that demonstrated how the enthalpy of hydride formation decreases with the increase of the volume per atom in the metal/metal alloy, for various systems [12].

Additionally, fig.1. displays the density of states in nickel hydride for the systems having various volumes. The volume increase is reflected in the upward shift of the hydrogen states, as well as nickel d-states, toward the Fermi level. The same is seen for nickel metal. A recent study of tensile and compressive strain of various metal lattices showed that with volume increase the d-band center shifts up and the hydrogen solution energy decreases [4]. The Hammer-Nørskov d-band model is a known descriptor for catalysis[6]. It demonstrates that a stronger upward shift of the d-band center leads to a stronger binding energy of the hydrogen atom at the surface. Also, for the fcc crystals (Cu, Ni) it was demonstrated that tensile strain instead decreases the electrons transferring to the hydrogen atom[4], which is in line with the decreased stability we observed.

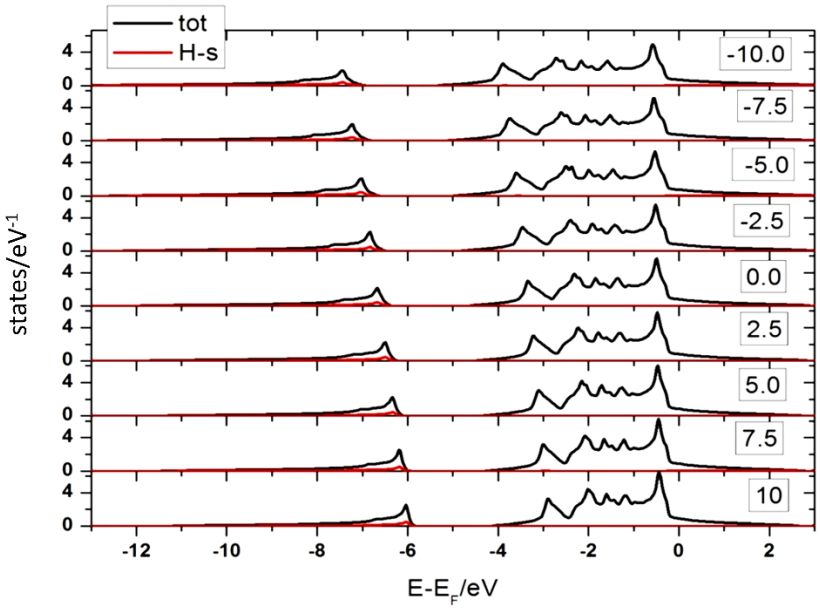

Figure 1. The density of states in NiH for various volumes; volume variations in reference to optimized NiH structure are shown in % at the right of each plot

However, in the case of hydrogen absorption volume of metal as well as the behavior of hydride with strain, also plays an additional important role. Additionally, the volume of the interstitial site itself in the metal lattice [4]. This is evident from Table 2, where the influence of hydrogen concentration in the metal lattice is discussed.

Table 2. Influence of concentration of hydrogen in the metal cell on the hydride stability, magnetization, and position of the d-band center

	Hydride formation energy (kJ/mol^{-1})	**E_d-E_F (eV)**	**Spin magnetic moment (μb)**
Ni	-	-1.83	0.66
$NiH_{0.065}$	-11.903	-1.81	0.60
$NiH_{0.25}$	+3.68	-1.71	0.46
NiH	-12.17	-1.60	0

An increase in the concentration of hydrogen in nickel leads to the deterioration of the magnetization, and the spin magnetic moment is zero for the nickel monohydride. A similar trend is observed for the other metal hydrides found in the NOMAD database – the higher H/M (ratio of hydrogen in metal) in general leads to a lower spin magnetic moment. At the same time, higher hydrogen concentration moves the d-band center closer to the Fermi level. Given that these results are all obtained for the optimized volumes of the hydrides, the influence of hydrogen concertation is one factor, while the other, which is also present, is the influence of the volume increase that is happening during the absorption of hydrogen.

To test the influence of chemical surroundings, we studied the supercells of $Ni_{16}H$ where one of the nickel atoms is replaced with Pt or Hf, fig.2. Volume was kept fixed to the optimized volume of the nickel hydride supercell.

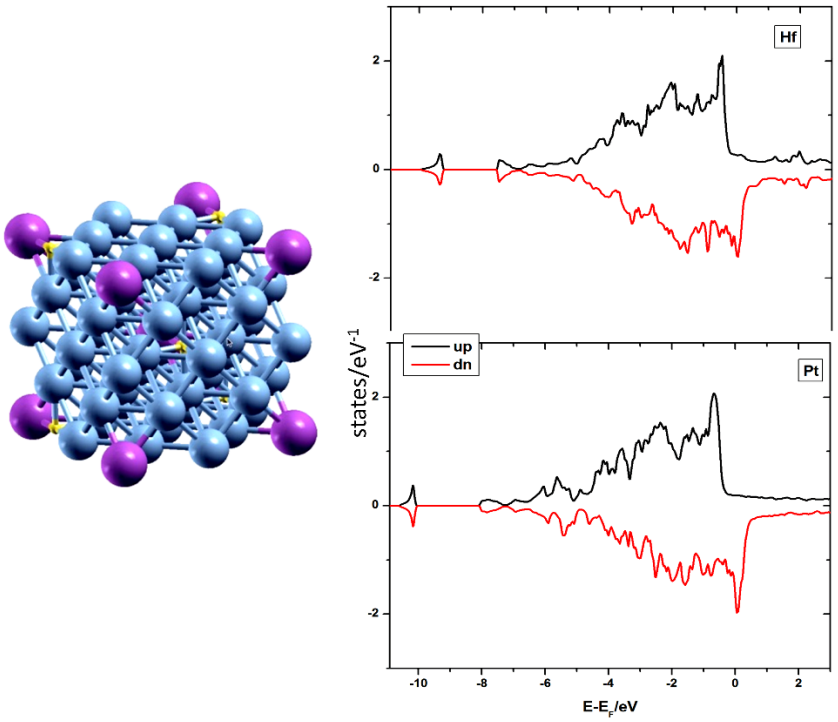

Figure 2. left: Supercell of $Ni_{15}XH$, X=Hf, Pt; right: DOS plot for Hf-substituted hydride (top) and Pt-substituted hydride (bottom)

By calculating the stability of these hydrides, both are found to be unstable in reference to bimetal alloys, while the relative stability of the Hf-containing one is higher than that of the Pt-containing one. The d-band center is closer to the Fermi level for Hf containing supercell. We see that in the case of the influence of chemical surroundings, the stability and position of the d-band center follow the Hammer-Nørskov d-band model; however, we cannot neglect the important influence of volume change due to the various natures of substituting atoms. These results are in line with a recent study on metal doping in Fe. The doping of Cr, Mo, or Ni was shown to cause the shift down of the d-band center of the Fe atom near the doping atom after the hydrogen solution, meanwhile, the hydrogen solution energy also increases[4]. In contrast, the doping of Zn, Al, Cu, or Ti results in the shift up of the d-band center of the Fe atom near the doping atom after the hydrogen solution, together with a decreased hydrogen solution energy, i.e. higher hydride stability[4]. The chemical nature of various dopants is a factor that is also correlated to the density, volume, and available interstitial sites in metal lattices. This is illustrated in a search for Ni-containing ternary metal hydrides that was done in the NOMAD database. Figure 3 displays results, i.e. dependence of volume per site and formation energy from the H/M for 23 various optimized hydrides found. Although some correlation can be seen, that an increase of hydrogen concentration in the metal leads to the decrease of volume per site, this is only a logical consequence of the incorporation of hydrogen atoms in an interstitial site. Future work is therefore planned to investigate further structure-property relation in nickel hydride when doped with various metals.

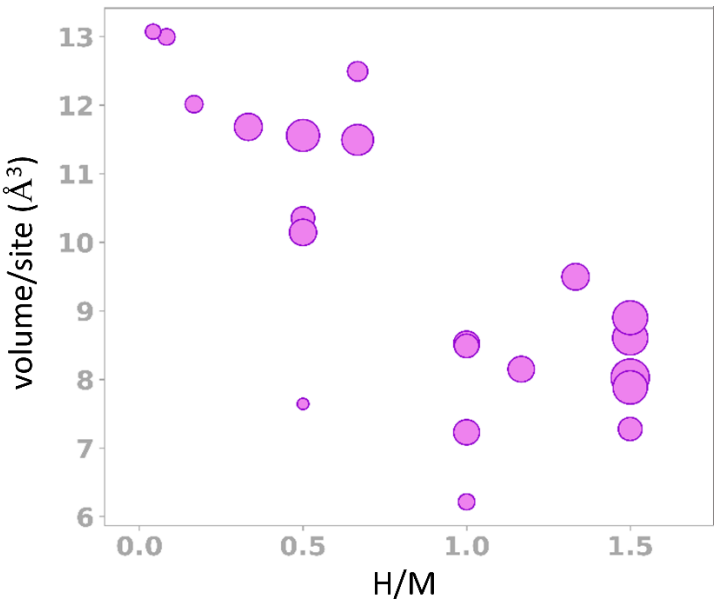

Figure 3. Dependence of volume per site in the crystal lattice from the ratio of hydrogen in metal for 23 unique ternary Ni-containing hydrides found in the NOMAD database [10]; the size of points is proportional to the formation energy of each hydride

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