Journal of Materials, Processing and Design (2026)
Clausius Scientific Press, Canada

DOI: 10.23977/jmpd.2026.100108
ISSN 2516-0923 Vol. 10 Num. 1

First-Principles Study on the Sensitization Mechanism of PdNi Alloy Based on Ni Doping for Hydrogen Sensing

Yichen Jin, Zejie Pan, Yuhao Chen, Binkai Yu, Jingrong Ye, Taiquan Wu[a], Wei Zhang[b]

College of Electrical Engineering, Zhejiang University of Water Resources and Electrical Power, Hangzhou, 310018, Zhejiang, China
[a]wutq@zuwe.edu.cn, [b]zhangw@zuwe.edu.cn

Keywords: PdNi alloy; hydrogen-sensing kinetics; first-principles; hydrogen adsorption; hydrogen diffusion

Abstract: Hydrogen-sensing Pd suffers from inherent defects such as structural distortion and response hysteresis, and PdNi alloy provides an effective solution to ameliorate the above problems. In this paper, first-principles simulations were employed to investigate the hydrogen-sensing reaction mechanism and hydrogen transfer kinetic characteristics. The hydrogen adsorption properties of different surfaces and sites, the hydrogen binding energy, as well as the diffusion behavior of hydrogen were analyzed. The results show that the (111) surface exhibits the optimal hydrogen adsorption performance; hydrogen in Pd and PdNi alloy preferentially occupy octahedral sites, and the embedding of hydrogen into tetrahedral sites is the main cause of excessive lattice expansion. Ni doping does not inhibit lattice expansion but reduces the hydrogen binding energy, which is conducive to avoiding excessive hydrogen dissolution. In hydrogen transfer kinetics, the path from tetrahedral sites to octahedral sites is the energy-optimal one. Ni doping significantly increases the diffusion energy barrier between tetrahedral sites, which can inhibit the α-β phase transition. An appropriate increase in Ni doping content can further reduce the energy barrier of the optimal path, improve the reversibility of phase transition and the stability. This study systematically reveals the hydrogen-sensing mechanism of Ni doping on Pd-based materials, and provides important theoretical support and guidance for the design and development of PdNi alloy with high activity and fast response.

1. Introduction

Hydrogen accounts for about 90% of the total mass in the universe and has an extremely high energy density (120~142 MJ/kg, three times that of fossil fuels), making it a potential alternative energy source for the future.[1] However, during the processes of production, storage, transportation and utilization, hydrogen is flammable and explosive, and its safety issues have become one of the core bottlenecks restricting its commercial application.[2] As a core device for real-time monitoring of hydrogen leakage, accurate early warning of concentration and intelligent judgment of safety status, hydrogen sensors provide important technical support for ensuring the safe operation of the entire hydrogen energy industry chain.[3-4] At room temperature, metallic Pd can undergo a reversible chemical reaction with H_2 to form palladium hydride, a process that leads to a significant

increase in the resistivity of Pd. Pd-based hydrogen sensors developed based on this characteristic play an indispensable detection role in the field of hydrogen safety identification and prevention.[5]

Pure Pd as a hydrogen-sensing material has inherent problems such as structural distortion and response hysteresis, which limit its practical application effect.[5] Recent studies have shown that adding metals such as nickel, silver, gold and magnesium to palladium can improve the test range and stability of hydrogen sensors.[6] For example, Wang et al. prepared a highly sensitive hydrogen sensor using PdAu thin film as the hydrogen-sensing material by micro-electro-mechanical system (MEMS) technology, which exhibits a good response rate to hydrogen with a concentration range of 5 ppm to 3%, and has excellent selectivity, repeatability and long-term stability compared with other gases.[7] Chung et al. immobilized PdMg nanoparticles on commercial filter membranes, and the obtained nanowire network structure can inhibit phase transition and exhibit significant device stability, high response amplitude and fast response time at a concentration range of 10~40000 ppm.[8] Among numerous structurally stable Pd-based alloys,[9] PdNi alloy has attracted extensive attention due to its durability and fast response.[10-11]

Although a large number of experimental studies on the structure, activity and tolerance of PdNi hydrogen sensors have been carried out, the existing research lacks an in-depth understanding of the hydrogen-sensing activity and hydrogen mass transfer process inside PdNi alloy, especially the modification mechanism of Ni doping.[12] In this study, first-principles simulations were used to explore the variation laws of the hydrogen-sensing process of Pd and PdNi alloy step by step starting from the hydrogen adsorption crystal plane and site effects of Pd metal. Meanwhile, the diffusion paths and energy barrier characteristics of hydrogen atoms in Pd lattice and Ni-doped Pd lattice were analyzed to systematically reveal the hydrogen-sensing reaction mechanism and hydrogen transfer kinetic characteristics of PdNi alloy, aiming to provide a clear direction and solid theoretical foundation for the design and development of PdNi alloy hydrogen-sensing materials with high activity.

2. Computational Methods

This study adopted the Vienna Ab-initio Simulation Package (VASP) based on Density Functional Theory (DFT).[13] The Projector Augmented Wave (PAW) method was used to describe the ion-core interaction, and the Perdew-Burke-Ernzerh (PBE) functional under the Generalized Gradient Approximation (GGA) was applied to describe the exchange-correlation interaction of valence electrons.[14] The cutoff energy of the plane wave basis set was set to 400 eV. The van der Waals interaction was corrected based on Grimme's DFT-D3 method.[15] The self-consistent convergence of electronic energy was set to be lower than 10^{-5} eV, and the convergence of atomic force in geometric optimization was set to 0.02 eV/Å. The Climbing Image-Nudged Elastic Band (CI-NEB) method was used to calculate the hydrogen diffusion kinetic process and search for the transition state, with a convergence criterion of 0.05 eV/Å. The hydrogen dissolution model adopted a metal unit cell structure, and Pd_4 and Pd_3Ni models were constructed respectively. $10\times10\times10$ and $1\times1\times1$ Monkhorst-Pack k-point grids were used for the unit cell and supercell calculation, respectively, to sample the Brillouin zone; the hydrogen diffusion kinetic model adopted a metal supercell, a $3\times3\times3$ Pd supercell structure (containing 108 Pd atoms) was established, and Ni-doped supercell models $Pd_{107}Ni$ and $Pd_{106}Ni_2$ were constructed. The hydrogen atom adsorption energy(ΔE_{ad})was calculated using Formula (1), where E_{total}, E_{ad} and E_{sub} represent the total energy of the fully relaxed adsorption system, hydrogen atom and adsorption substrate, respectively. The binding energy(ΔE_b)after hydrogen atom embedding was calculated using Formula (2), where E_{total}, E_H and E_{bulk} represent the total energy of the metal hydride solid solution, total hydrogen atoms and hydrogen-free metal after full structural relaxation, respectively.

$$\Delta E_{ad} = E_{total} - E_{ad} - E_{sub} \quad (1)$$

$$\Delta E_b = E_{total} - E_H - E_{bulk} \quad (2)$$

3. Results and Analysis

3.1 Hydrogen Adsorption for Pd-based Metals

A Pd surface model was established by first-principles simulation to study the hydrogen adsorption of different surface (Pd(100), Pd(110), Pd(111)) and different sites, and the results are shown in Figure 1. The hydrogen adsorption behavior of Pd metal exhibits a significant crystal plane effect: the Pd(110) plane has the worst hydrogen adsorption performance with an adsorption energy range of -0.33~-0.73 eV; the Pd(111) has the optimal hydrogen adsorption performance with an adsorption energy range of -0.19~-0.96 eV. This result indicates that in the preparation of Pd-based hydrogen-sensing materials, the material should be made to expose the Pd(111) crystal plane as much as possible to ensure the high active adsorption capacity for hydrogen and improve the hydrogen capture capacity and overall hydrogen-sensing activity of the hydrogen-sensing material. Meanwhile, there are obvious differences in the hydrogen adsorption capacity of different sites on the Pd metal surface, and hydrogen molecules tend to adsorb on the H, B, hcp and fcc sites of the Pd. Except for the T site, the Pd(111) can provide stronger adsorption capacity such as B, hcp and fcc, which further proves that the Pd(111) is the most suitable surface for Pd as a hydrogen-sensing material. Tian et al. revealed that H_2 adsorption has a significant surface effect through first-principles simulation, among which the Pd(111) has the largest adsorption energy and the most charge transfer, which is conducive to the formation of PdH_x and the rapid change of resistivity.[16] Based on the molecular orbital analysis of H_2 adsorption, Nakatsuji et al. confirmed that Pd electrons transfer from the δu (d-d*) molecular orbital to the H_2 antibonding orbital, and electrons in the H_2 bonding orbital transfer back to the σg(5s-5s) orbital of Pd, proposing that the orbital hybridization and electron exchange between Pd and H_2 weaken the H-H bond.[17]

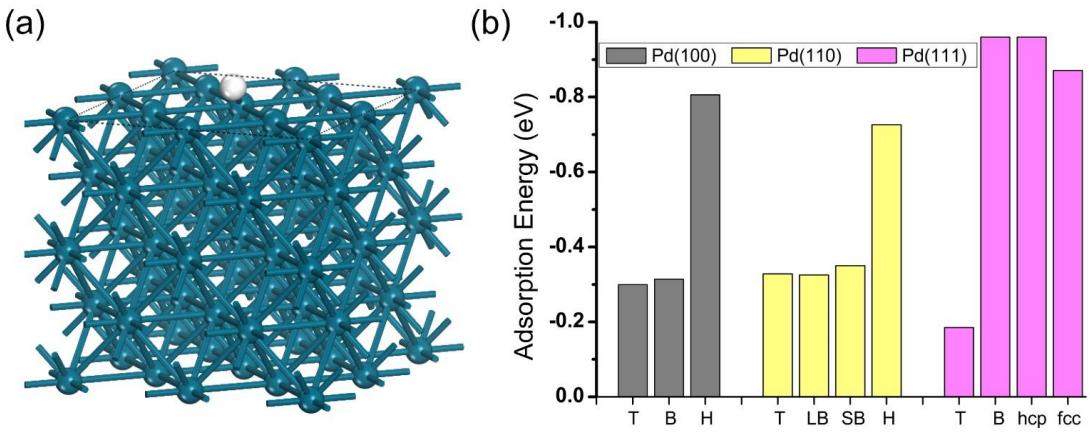

Figure 1. (a) Hydrogen adsorption model of Pd(001) plane; (b) Variation of hydrogen adsorption energy at different crystal planes and sites of Pd metal.

On the basis of the study on the hydrogen adsorption characteristics of Pd metal, first-principles simulation was further used to explore the differences in hydrogen adsorption between pure Pd metal and PdNi alloy, and it was found that the hydrogen adsorption of both mainly exists in two forms: tetrahedral site adsorption and octahedral site adsorption. As shown in Figure 2, for both Pd and PdNi alloy systems, hydrogen atoms can be stably embedded in the tetrahedral and octahedral

sites in the unit cell, and the embedding space of tetrahedral sites is smaller than that of octahedral sites. When all tetrahedral sites are fully occupied, a single metal unit cell can embed a maximum of 8 hydrogen atoms, namely Pd_4H_8 and Pd_3NiH_8, while the octahedral sites can only embed a maximum of 4 hydrogen atoms, namely Pd_4H_4 and Pd_3NiH_4. The calculation results show that the metal hydride solid solution can still remain stable in the fully embedded state, and Pd-based metals are also often used as hydrogen storage materials.[18]

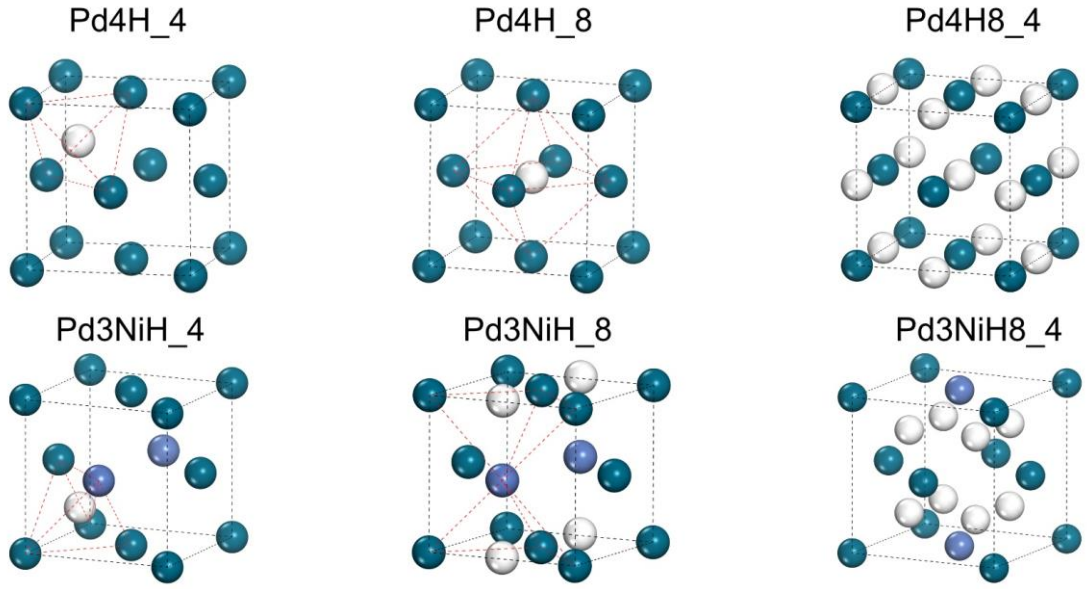

Figure 2. Hydrogen embedding at tetrahedral sites, octahedral sites and hydrogen full adsorption structure diagrams of Pd (upper figure) and PdNi (lower figure).

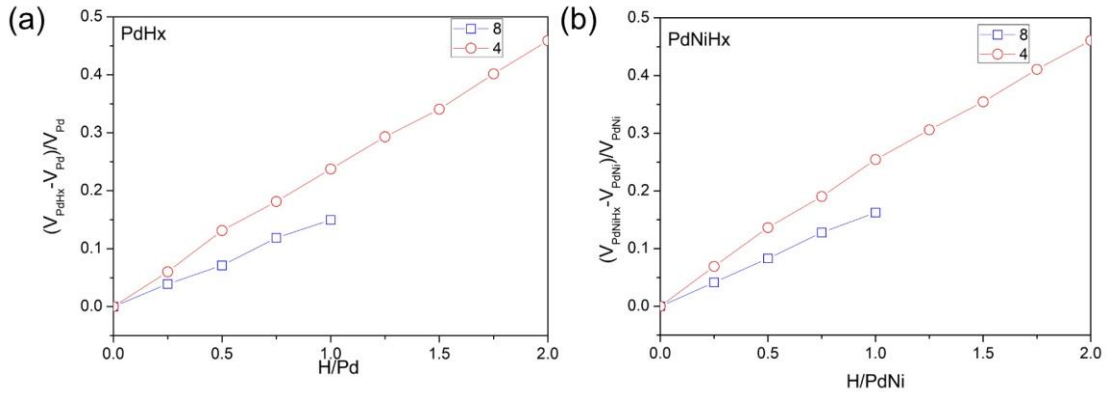

Figure 3. Volume expansion change trends of (a) PdH_x and (b) $PdNiH_x$.

During the hydrogen absorption and desorption cycle, the continuous volume change of Pd-based metals is the main cause of structural damage.[5, 19] In Figure 3, we analyzed the volume changes of Pd and PdNi after hydrogen embedding in detail. First, in the hydrogen-free state, the volume of Pd unit cell doped with Ni (Pd_3Ni) shrinks by 6.5%, mainly due to the fact that the Pd-Ni bond length is shorter than the Pd-Pd bond length, leading to lattice contraction. With hydrogen embedding, the volume of both Pd and PdNi expands with the increase of hydrogen embedding amount, but the expansion amount is closely related to the embedding site. When all octahedral sites are occupied, the unit cells of Pd and PdNi expand by 15% and 16% respectively; when all tetrahedral sites are occupied, the unit cells of Pd and PdNi expand by 46% together. A comparison shows that Ni doping cannot inhibit lattice expansion, and the volume change trend of PdNi is

basically the same as that of pure Pd. It is also found that the volume expansion after hydrogen occupation of tetrahedral sites is significantly larger than that of octahedral sites. Therefore, excessive hydrogen embedding leading to the filling of tetrahedral sites and severe volume expansion is the main cause of the deactivation of hydrogen-sensing materials.[20]

In Figure 4, we further studied the variation of the average binding energy of hydrogen atoms under different hydrogen contents. For pure Pd materials, a single Pd unit cell can store a maximum of 4 hydrogen atoms at octahedral sites, and its hydrogen binding energy shows a decreasing trend with the increase of the number of hydrogen atoms, with a variation range of -0.24~-0.27 eV; the tetrahedral sites can store a maximum of 8 hydrogen atoms, and the hydrogen binding energy shows a significant decreasing trend when the number of hydrogen atoms is more than 4, with a variation range of -0.25~+0.2 eV. It can be seen that the stability of tetrahedral sites decreases with the increase of hydrogen embedding, and the hydrogen desorption phenomenon becomes prominent [21]; meanwhile, the hydrogen binding energy of octahedral sites is always higher than that of tetrahedral sites, indicating that octahedral sites are the stable sites for hydrogen dissolution in Pd, and hydrogen atoms will preferentially fill the octahedral sites and then the tetrahedral sites, with a significant decrease in binding energy during the secondary filling, which is consistent with the results of other studies.[22]

The variation trend of hydrogen binding energy of PdNi alloy is consistent with that of pure Pd material, with the binding energy of octahedral sites ranging from -0.21 to -0.24 eV and that of tetrahedral sites ranging from -0.18 to 0.1 eV. Compared with PdAg, the binding energy of a single hydrogen atom embedded in PdNi (0.22 eV) is smaller than that in PdAg (0.35 eV), mainly because the ionic radius of Ag is larger than that of Ni, and the unit cell contraction of PdAg is smaller than that of PdNi.[6] However, similar to Pd, hydrogen atoms in PdNi alloy also preferentially fill the octahedral sites and then the tetrahedral sites. The key difference is that the hydrogen binding energy of octahedral sites in PdNi alloy is lower than that in pure Pd metal, which reduces the overall hydrogen adsorption energy of PdNi alloy, and the decrease of adsorption energy is conducive to avoiding excessive hydrogen dissolution in metal materials, which is an important reason why PdNi alloy improves the response hysteresis problem of pure Pd.[23]

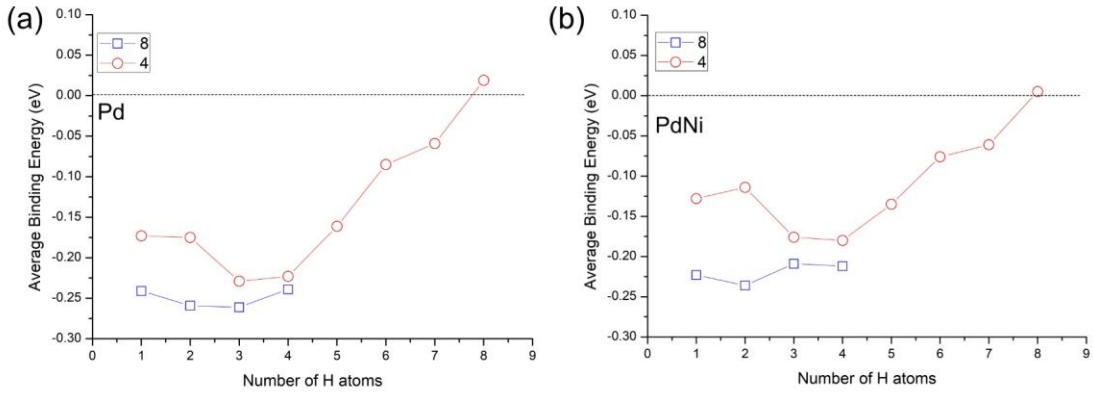

Figure 4. Variation trends of embedded hydrogen binding energy with hydrogen content in the unit cells of pure Pd metal (left figure) and PdNi alloy (right figure).

3.2 Hydrogen Transfer Kinetics

The hydrogen mass transfer kinetic process inside Pd-based metals is an important factor affecting the hydrogen-sensing activity of the material.[24] Theoretical research has clarified that the diffusion paths of hydrogen atoms in the metal lattice mainly include three types (Figure 5): Path 1 is the diffusion from tetrahedral sites to octahedral sites, Path 2 is the diffusion from tetrahedral

sites to tetrahedral sites, and Path 3 is the diffusion from octahedral sites to octahedral sites.[25] To avoid the influence of excessive lattice deformation on the calculation results, a supercell model was used to calculate the variation of hydrogen atom diffusion free energy under different diffusion paths, and the results are shown in Figures 6 and 7.

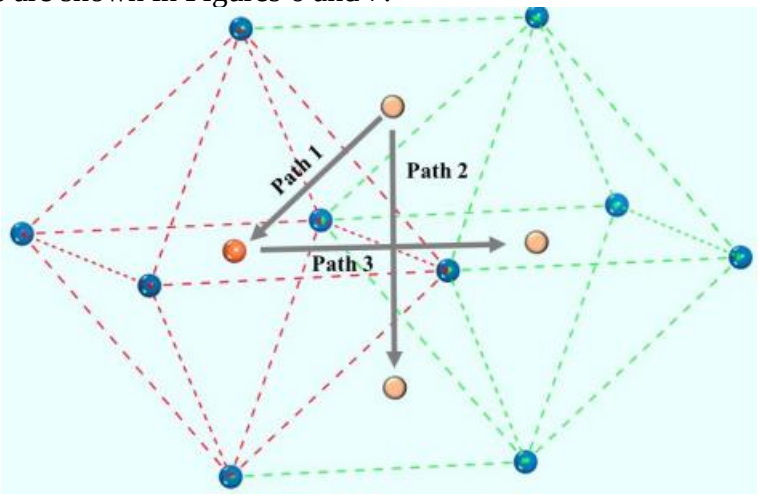

Figure 5. Schematic diagram of hydrogen atom diffusion paths inside the Pd-based metal lattice.

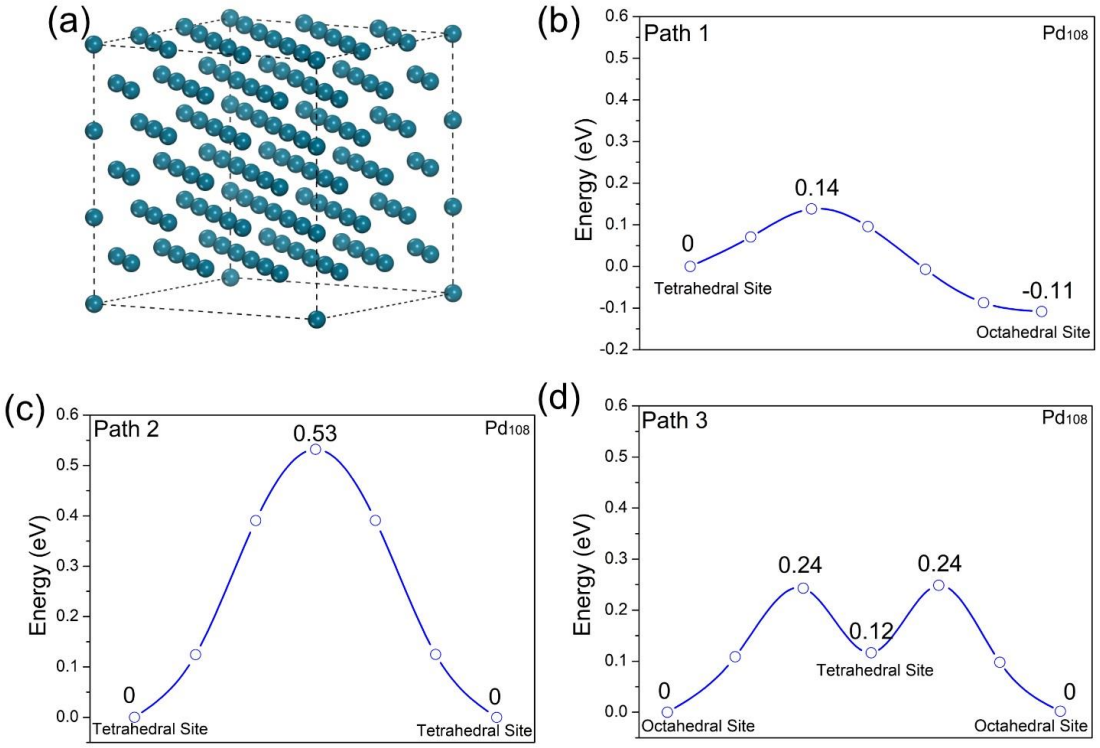

Figure 6. Variation trend of free energy of hydrogen atoms under different diffusion paths in the Pd metal lattice.

As shown in Figure 6, the calculation results show that the hydrogen atom diffusion energy barriers of Path 1, Path 2 and Path 3 are 0.14 eV, 0.53 eV and 0.24 eV respectively, among which Path 3 is a combination of two Path 1 (i.e., octahedral sites → tetrahedral sites → octahedral sites). The results indicate that the hydrogen atom diffusion energy barrier in the Pd lattice is low and the process is easy to occur, among which Path 1 is the energy-optimal path, that is, hydrogen atoms

tend to diffuse from tetrahedral sites to octahedral sites, and the diffusion reaction is an exothermic process, which is also the main factor affecting the transformation between the α and β phases of Pd hydrogen solid solution.[26] It can be seen from Figure 5 that hydrogen diffusion in Path 1 passes through a triangular plane composed of three Pd atoms, while Path 3 passes through a plane composed of two Pd atoms. Obviously, the activity space of the Pd_3 plane is larger than that of the Pd_2 plane, making the diffusion process of Path 1 easier to proceed.[27-28]

To study the effect of Ni doping on hydrogen mass transfer kinetics, we further investigated the changes in hydrogen atom mass transfer kinetics in two Ni-doped alloy systems ($Pd_{107}Ni_1$ and $Pd_{106}Ni_2$). To better reflect the effect of Ni, the hydrogen mass transfer behavior was arranged near Ni elements, and the results are shown in Figure 7.

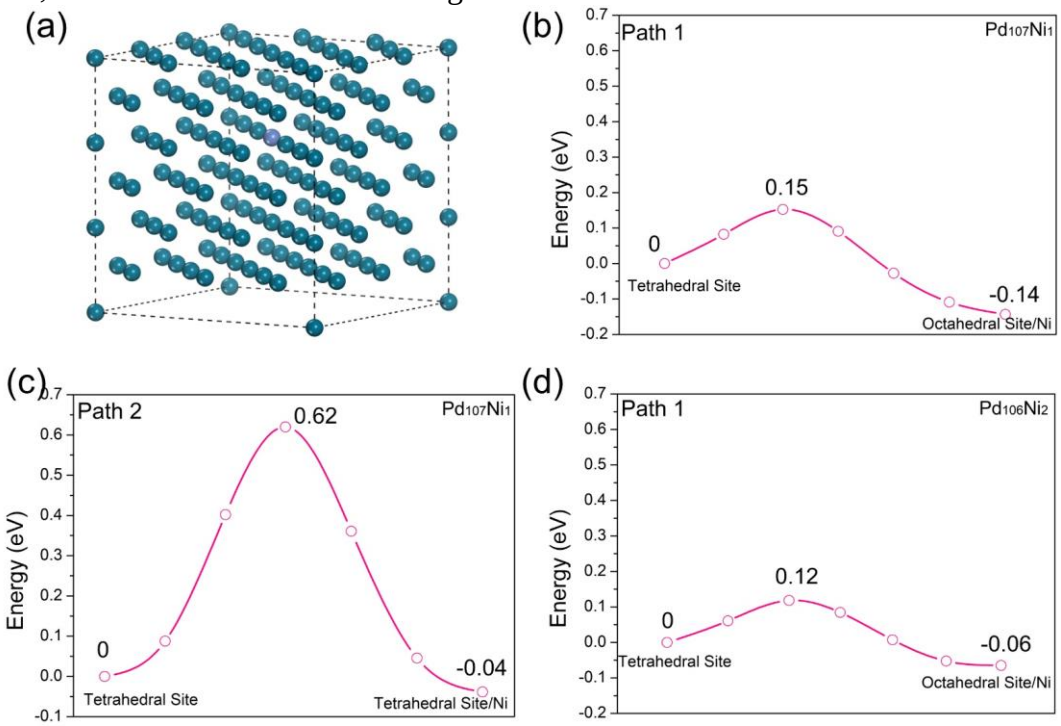

Figure 7. Variation trend of free energy of hydrogen atoms under different diffusion paths in the Pd metal lattice.

For the $Pd_{107}Ni_1$ system, the hydrogen atom diffusion energy barriers of Path 1 and Path 2 are 0.15 eV and 0.62 eV respectively, and Path 1 is still the energy-optimal path, and the hydrogen atom diffusion along this path is still an exothermic process (Path 3 is a combination of two Path 1). Compared with pure Pd, the hydrogen diffusion energy barrier of the $Pd_{107}Ni_1$ system is increased to a certain extent, mainly because the local contraction of the alloy lattice after Ni doping leads to a decrease in the internal activity space of hydrogen atoms; among them, the energy barrier of Path 2 increases significantly (from 0.53 eV to 0.62 eV), which is due to the fact that the Ni-Pd bond length is shorter than the Pd-Pd bond, resulting in a decrease in the hydrogen activity space in the tetrahedral sites. Therefore, Ni doping on the one hand ensures the diffusion activity from tetrahedral sites to octahedral sites, and on the other hand makes the hydrogen atom diffusion along Path 2 more difficult to realize. These two changes are beneficial to the improvement of the hydrogen-sensing activity of Pd-based metals. It can be seen from the previous research that the occupation of tetrahedral sites is the main cause of excessive expansion of the metal lattice, and weakening the diffusion kinetics between tetrahedral sites can ensure that hydrogen atoms are mainly embedded in octahedral sites and inhibit the α-β phase transition.

We further studied the effect of increased Ni doping content on hydrogen mass transfer kinetics,

and the results are shown in Figure 7(d). For the $Pd_{106}Ni_2$ system, compared with pure Pd and $Pd_{107}Ni_1$ systems, the diffusion energy barrier of hydrogen atoms along the optimal path (Path 1) is slightly reduced to 0.12 eV, but the significant change of this system is the reduction of reaction exotherm, with a reaction energy of only -0.06 eV. It can be seen that an appropriate increase in Ni doping concentration can improve the mass transfer kinetics of hydrogen atoms between tetrahedral and octahedral sites, further enhance the reversibility of the α-β phase transition, and effectively improve the stability of hydrogen-sensing materials.[9] The main reason for the reduction of reaction heat is that the adsorption capacity of Ni to H is lower than that of Pd, leading to a decrease in the energy release during the hydrogen atom diffusion process.

4. Conclusions

In summary, this paper systematically studied the hydrogen-sensing performance of pure Pd metal and PdNi alloy from three aspects: hydrogen adsorption characteristics, hydrogen binding energy and hydrogen atom diffusion behavior by using first-principles simulations, and proposed the sensitization mechanism of Ni doping. On the one hand, in metal surface adsorption, hydrogen adsorption has significant crystal plane and site effects, the (111) surface has the most stable hydrogen adsorption, and the adsorption sites include B, hcp and fcc. In metal internal adsorption, the hydrogen adsorption inside both pure Pd metal and PdNi alloy is mainly dominated by tetrahedral and octahedral sites; hydrogen embedding into tetrahedral sites is the main cause of lattice expansion, with a lattice expansion of 46% in the fully embedded state, and Ni doping does not inhibit lattice expansion. On the other hand, by comparing the internal hydrogen binding energy, octahedral sites are the stable sites for hydrogen storage, and hydrogen atoms are preferentially filled; Ni doping reduces the hydrogen embedding binding energy, which is conducive to inhibiting excessive hydrogen dissolution. Finally, there are three hydrogen mass transfer paths inside Pd-based metals, and Path 1 (tetrahedral sites to octahedral sites) is the energy-optimal path in both Pd and PdNi lattices, with a diffusion energy barrier of only 0.14 eV for Pd, which is slightly increased to 0.15 eV after Ni doping. Ni doping significantly increases the energy barrier required for Path 2 (tetrahedral sites to tetrahedral sites), which is the main reason for inhibiting the α-β phase transition; when the Ni content is increased, the diffusion energy barrier of Path 1 is reduced to 0.12 eV, which enhances the reversibility of the α-β phase transition and effectively improves the stability of hydrogen-sensing materials. This study reveals the hydrogen-sensing reaction and hydrogen mass transfer kinetic mechanism of PdNi alloy, and provides a clear theoretical basis and research direction for the subsequent regulation of Ni doping ratio and the design of PdNi alloy hydrogen-sensing materials with high activity and fast response.

Acknowledgment

The work was supported in part by the Student Innovation and Entrepreneurship Training Program at Zhejiang University of Water Resources and Electric Power under Grant No. S202411481091, the Nanxun Scholars Program for Young Scholars of ZJWEU under the Grant No. RC2024021016, and a Project Supported by Scientific Research Fund of Zhejiang Provincial Education Department under Grant No.Y20245691.

References

[1] Abe, J. O.; Popoola, A. P. I.; Ajenifuja, E.; Popoola, O. M. Hydrogen Energy, Economy and Storage: Review and Recommendation. International Journal of Hydrogen Energy 2019, 44, 15072-15086.
[2] Buttner, W. J.; Post, M. B.; Burgess, R.; Rivkin, C. An Overview of Hydrogen Safety Sensors and Requirements. International Journal of Hydrogen Energy 2011, 36, 2462-2470.

[3] Zhang, Y.; Su, Y. Q.; Chen, J. S.; Zhang, Y. B.; He, M. G. Progress and Prospect of Hydrogen Sensor Research. Chinese Science Bulletin 2023, 68, 204-219.
[4] Chauhan, P. S.; Bhattacharya, S. Hydrogen Gas Sensing Methods, Materials, and Approach to Achieve Parts Per Billion Level Detection: A Review. International Journal of Hydrogen Energy 2019, 44, 26076-26099.
[5] Lee, E.; Lee, J. M.; Koo, J. H.; Lee, W.; Lee, T. Hysteresis Behavior of Electrical Resistance in Pd Thin Films During the Process of Absorption and Desorption of Hydrogen Gas. International Journal of Hydrogen Energy 2010, 35, 6984-6991.
[6] Ke, X.; Kramer, G. J. Absorption and Diffusion of Hydrogen in Palladium-Silver Alloys by Density Functional Theory. Physical Review B 2002, 66, 184304.
[7] Gong, J.; Wang, Z.; Tang, Y.; Sun, J.; Wei, X.; Zhang, Q.; Tian, G.; Wang, H. MEMS-Based Resistive Hydrogen Sensor with High Performance Using a Palladium-Gold Alloy Thin Film. Journal of Alloys and Compounds 2023, 930, 167398.
[8] Hassan, K.; Uddin, A. S. M. I.; Chung, G.-S. Mesh of Ultrasmall Pd/Mg Bimetallic Nanowires as Fast Response Wearable Hydrogen Sensors Formed on Filtration Membrane. Sensors and Actuators B: Chemical 2017, 252, 1035-1044.
[9] Sun, L.; Chen, M.; Peng, X.; Xie, B.; Han, M. The Effects of Ni Contents on Hydrogen Sensing Response of Closely Spaced Pd–Ni Alloy Nanoparticle Films. International Journal of Hydrogen Energy 2016, 41, 1341-1347.
[10] Xue, Y.; Zhang, H.; Zhang, Y. X.; Chen, W. J.; Lin, Z. C.; Xiao, C. L.; Yu, Y. Study on Improving the Anti-Interference Performance of Pd-Ni Alloy Hydrogen Sensors. Journal of Test and Measurement Technology 2023, 37, 386-393.
[11] Liu, G.; Shu, L.; Yan, D.; Peng, L.; Fan, L.; Wu, W. High Durability for PdNi Nano-Film Hydrogen Sensor. International Journal of Hydrogen Energy 2024, 50, 1146-1156.
[12] Wang, B.; Sun, L.; Schneider-Ramelow, M.; Lang, K.-D.; Ngo, H.-D. Recent Advances and Challenges of Nanomaterials-Based Hydrogen Sensors. Micromachines 2021, 12(11), 1429. https://doi.org/10.3390/mi12111429
[13] Kresse, G.; Furthmüller, J. Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set. Physical Review B 1996, 54, 11169-11186.
[14] Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. Physical Review Letters 1996, 77, 3865-3868.
[15] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. The Journal of Chemical Physics 2010, 132, 154104.
[16] Gao, Y.; Lu, Q.; Yan, P.; Tian, P.; Zhu, M.; Xiao, B.; Xuan, F. Theory-Guided Design of Pd/C Nanocomposite for H_2 Sensing at Room-Temperature. Applied Surface Science 2022, 581, 152367.
[17] Nakatsuji, H.; Hada, M. Interaction of a Hydrogen Molecule with Palladium. Journal of the American Chemical Society 1985, 107, 8264-8266.
[18] Li, G.; et al. Hydrogen Storage in Pd Nanocrystals Covered with a Metal–Organic Framework. Nature Materials 2014, 13, 802-806.
[19] Liu, Q.; Yao, J.; Wang, Y.; Sun, Y.; Ding, G. Temperature Dependent Response/Recovery Characteristics of Pd/Ni Thin Film Based Hydrogen Sensor. Sensors and Actuators B: Chemical 2019, 290, 544-550.
[20] Yun, S.; Oyama, S. T. Correlations in Palladium Membranes for Hydrogen Separation: A Review. Journal of Membrane Science 2011, 375, 28-45.
[21] Sonwane, C. G.; Wilcox, J.; Ma, Y. H. Solubility of Hydrogen in PdAg and PdAu Binary Alloys Using Density Functional Theory. The Journal of Physical Chemistry B 2006, 110, 24549-24558.
[22] Long, D.; Li, M.; Meng, D.; He, Y.; Yoon, I. T.; Ahuja, R.; Luo, W. Accounting for the Thermo-Stability of PdH_x (x = 1–3) by Density Functional Theory. International Journal of Hydrogen Energy 2018, 43, 18372-18381.
[23] Wadell, C.; Nugroho, F. A. A.; Lidström, E.; Iandolo, B.; Wagner, J. B.; Langhammer, C. Hysteresis-Free Nanoplasmonic Pd–Au Alloy Hydrogen Sensors. Nano Letters 2015, 15, 3563-3570.
[24] Bian, H.; Kang, H.; Zhong, W.; Zhao, J.; Liang, T. Hydrogen Diffusion into Pd(100) Subsurface: Role of Co-Adsorbed Bicomponent Species on Surface. Applied Surface Science 2020, 533, 147448.
[25] Ishimoto, T.; Koyama, M. Theoretical Study of Tetrahedral Site Occupation by Hydrogen in Pd Nanoparticles. The Journal of Chemical Physics 2018, 148, 034705.
[26] Noh, J.-S.; Lee, J. M.; Lee, W. Low-Dimensional Palladium Nanostructures for Fast and Reliable Hydrogen Gas Detection. Sensors 2011, 11(1), 825-852.
[27] https://doi.org/10.3390/s110100825
[28] Senftle, T. P.; Janik, M. J.; van Duin, A. C. T. A ReaxFF Investigation of Hydride Formation in Palladium Nanoclusters Via Monte Carlo and Molecular Dynamics Simulations. The Journal of Physical Chemistry C 2014, 118, 4967-4981.