Supplementary Information (SI) for Catalysis Science & Technology.
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Supporting Information for

Analysis of Ammonia Synthesis Pathways from Nitrogen-Hydrogen Plasma on Ni-Based Catalyst: A Combined Experimental and Simulation Study

Baiqiang Zhang*[1], Jia Wang[1], Yongqi Liang[1], Guangzhen Shi[1], Yuhui Chen[1], Yuxiang Zhang[1], Gang Chen[1], Tan Wu[1], Nobusuke Kobayashi[2], Bo Wu*[3]

1 Henan International Joint Laboratory of Energy Efficient Conversion and Utilization, School of Energy and Power Engineering, Zhengzhou University of Light Industry, China

2 Environmental and Renewable Energy Systems, Gifu University, Japan

3 Engineering Research Center of Advanced Functional Material Manufacturing of Ministry of Education, School of Ecology and Environment, Zhengzhou University, China

Figure S1. Temperature profile of the flat-plate reactor.

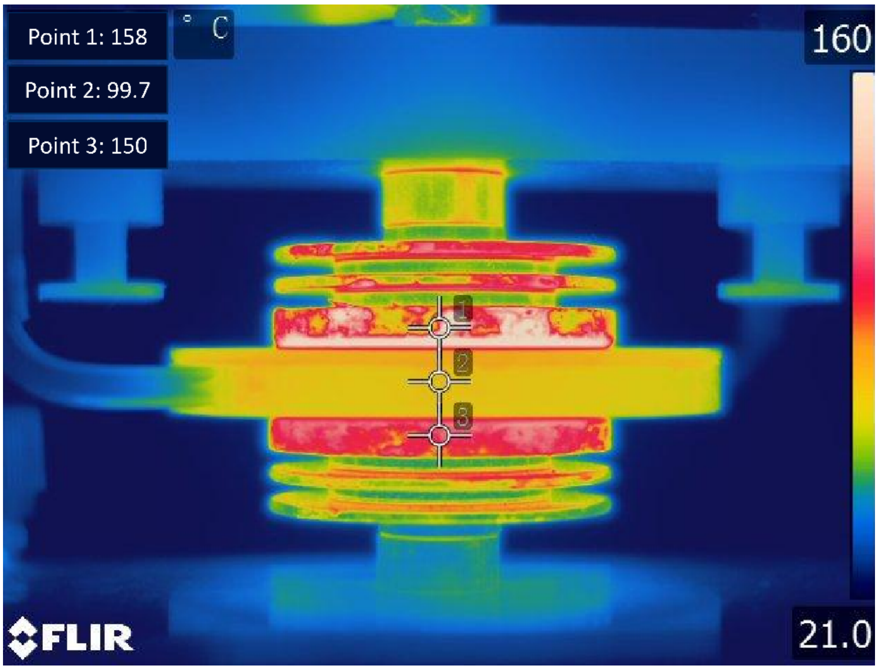

Figure S1. Temperature profile of the flat-plate reactor

Text S1 Reaction rate calculation process.

The reaction rate of the E-R reaction N + H(s) → NH(s) at 373 K was calculated using the Eq. S1.

$$k_{ads} = (\tau_{ads} S_T)^{-1} = \left[\frac{\Lambda^2}{D} + \frac{V}{A}\frac{2(2-\gamma_{ads})}{\bar{v}\gamma_{ads}}\right]^{-1} S_T^{-1} \tag{S1}$$

Based on references[1,2] and the catalyst particle size (0.1 mm), the diffusion length (Λ) is set to 0.1 mm. The diffusion coefficient (D) is approximately proportional to $T^{3/2}$ and inversely proportional to pressure(P) [2]. At 373 K and 1 atm, the diffusion coefficient for N_2 and H_2 is calculated as 10.9×10^{-5} m^2s^{-1}. *V/A* represents the ratio of the reactor volume to its effective surface area, which is 0.088 cm here. For the estimation of the effective surface area, a roughness factor of 2 is assumed [3]. $\bar{v}$ represents the mean thermal velocity of atoms and free radicals (as presented in Eq. S2), where *k* is Boltzmann's constant, *T* is the thermodynamic temperature with 373 K, and *m* is the mass of the atom or molecule. According to Hong's study [2], the adsorption coefficient (γ_{ads}) for the reaction N + H(s) → NH(s) is taken as 1×10^{-2}. S_T is the total surface site density, which was assigned a value of 10^{15} cm^{-2} according to the theory of Carrasco [4].

$$\bar{v} = \sqrt{\frac{8kT}{\pi m}} \tag{S2}$$

References

1 J. Sun, Q. Chen, X. Zhao, H. Lin and W. Qin, *Plasma Sources Sci. Technol.*, 2022, **31**, 094009.

2 J. Hong, S. Pancheshnyi, E. Tam, J. J. Lowke, S. Prawer and A. B. Murphy, *J. Phys. D: Appl. Phys.*, 2017, **50**, 154005.

3 Y. C. Kim and M. Boudart, Recombination of oxygen, nitrogen, and hydrogen atoms on silica, https://pubs.acs.org/doi/pdf/10.1021/la00060a016, (accessed January 4, 2026).

4 E. Carrasco, M. Jiménez-Redondo, I. Tanarro and V. J. Herrero, *Phys. Chem. Chem. Phys.*, 2011, **13**, 19561.

Figure S2. EEDF under different reduced electric fields（N_2:H_2=1:1, 373 K, 1 atm）.

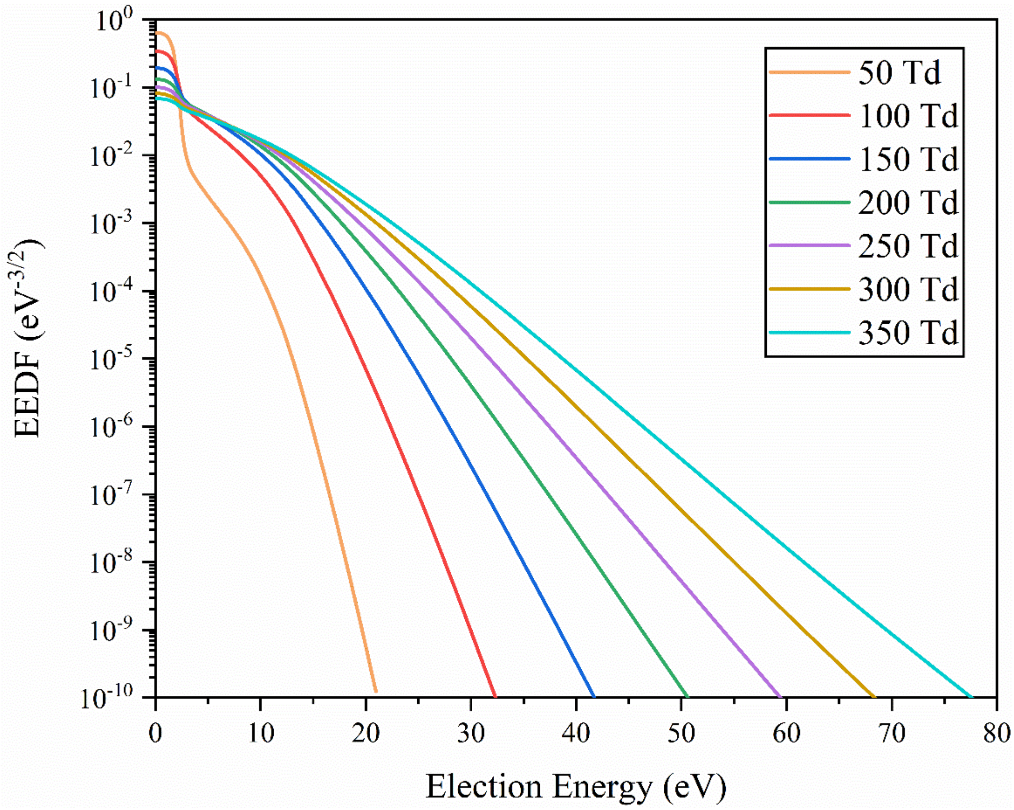

Figure S2. EEDF under different reduced electric fields（N_2:H_2=1:1, 373 K, 1 atm）

Figure S3. The variation of the mean electron energy with the reduced electric field.

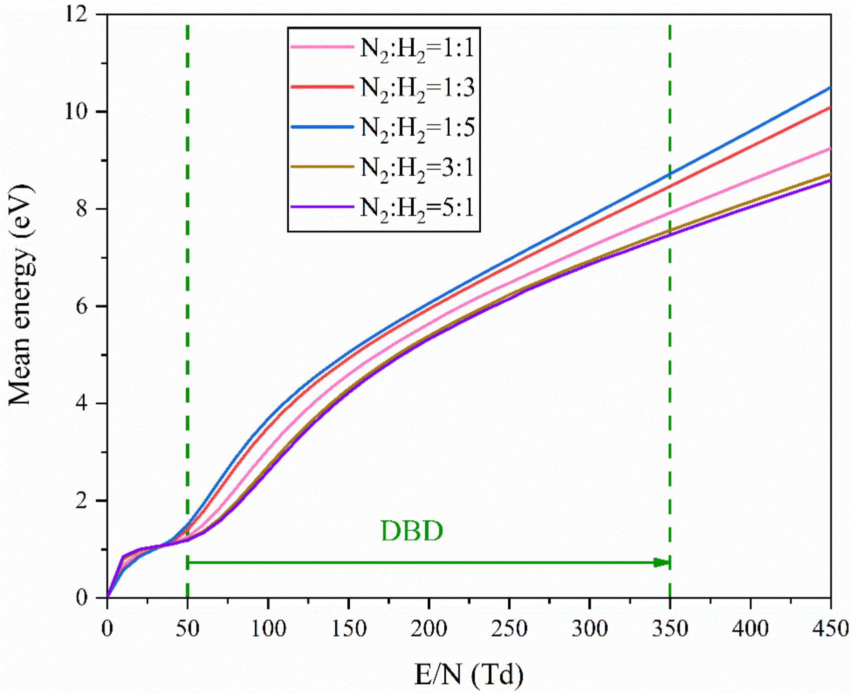

Figure S3. The variation of the mean electron energy with the reduced electric field