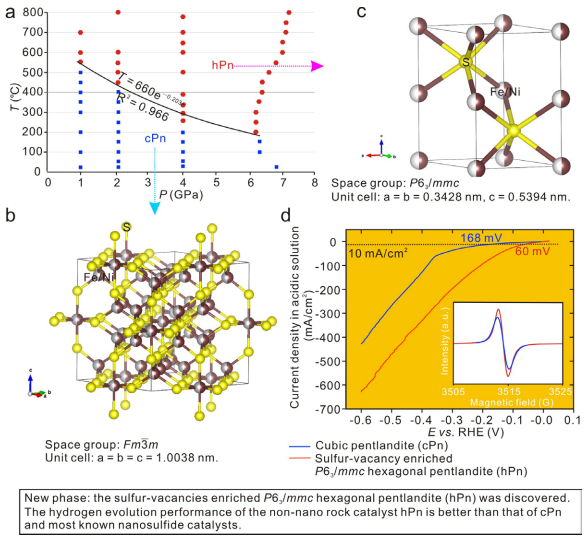
Goldschmidt 2025 Abstract
https://doi.org/10.7185/gold2025.26717

The efficient catalytic performance of a new mineral phase hexagonal pentlandite during hydrogen evolution reaction and its implication for natural hydrogen

YUEGAO LIU

Institute of Deep-sea Science and Engineering, Chinese Academy of Sciences

Cubic pentlandite [$(Ni,Fe)_9S_8$], the most important mineral in magmatic nickel deposits, can be used as a functional material for solar cells [1] and lithium-sulfur batteries [2], and has efficient catalytic properties during hydrogen evolution reaction [3]. Cubic pentlandite (cPn) can be transformed to a hexagonal form (hPn) at elevated pressure (Fig. 1a)[4]. The space group of hPn is $P6_3/mmc$, and the unit cell parameters are: a = b = 3.428 Å and c = 5.394 Å (Fig. 1c). The hPn with a diameter of 0.2–2 um as a catalyser exhibits an overpotential of 60 mV at 10 mA cm^{-2} (Fig. 1d) under 0.5 M acidic conditions without any loss in activity for approximately 50 h, which is the most efficient known non-nano natural single mineral electrocatalyst for hydrogen evolution reaction [4]. Two important reasons for the improvement of hydrogen evolution performance of hPn relative to cPn are as follows: (1) the hydrogen adsorption free energy of high coordination metal atoms in hPn is closer to zero; (2) hPn has more sulfur vacancies than cPn (Fig. 1d)[4]. Pentlandite is an important accessory mineral of peridotite. Its existence contributes to the serpentinization of natural olivine to produce hydrogen. Therefore, this study also provides inspiration for the mechanism of the generation of gold hydrogen (such as modern subduction zones). There is a "dark oxygen" phenomenon on the seabed of the Pacific Ocean, which is believed to be the generation of oxygen by the electrolysis of water catalyzed by Ni-Co-Mn polymetallic nodules [5]. The catalytic process of Ni-Co-Mn polymetallic nodules should also produce a large amount of hydrogen.



New phase: the sulfur-vacancies enriched $P6_3/mmc$ hexagonal pentlandite (hPn) was discovered. The hydrogen evolution performance of the non-nano rock catalyst hPn is better than that of cPn and most known nanosulfide catalysts.

References:

[1] Dai, Lim, Wang, Hu, Chen, Chen, Chen, Bao, Shen, Li, 2018. Advanced Functional Materials 28, 1704443.

[2] Chang, Lu, Tung, Tuan, 2013. ACS nano 7, 9443–9451.

[3] Konkena, Puring, Sinev, Piontek, Khavryuchenko, Dürholt, Schmid, Tüysüz, Muhler, Schuhmann, Apfel, 2016. Nature Communications 7, 1–8.

[4] Liu, Cai, Zhu, Zheng, Li, Chen, Li, Sun, Chou, Yu, Mei, Wang, 2024. Small 13, 2311161.

[5] Sweetman, Smith, de Jonge, Hahn, Schroedl, Silverstein, Andrade, Edwards, Lough, Woulds, Homoky, Koschinsky, Fuchs, Kuhn, Geiger, Marlow, 2024.. Nature Geoscience 17, 737–739.