Photoanode driven photoelectrocatalytic system for CO_2 reduction to formic acid based on lattice-dislocated Bi nanosheets cathode

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Formula to calculation

Faradaic Efficiency (FE)[1]

Faraday efficiency has become an important evaluation parameter for ERC-HCOOH, which can be understood as the ratio between transferred the charge amount generating a product and the total amount of charge transferred through the circuit, directly reflecting the selectivity of the electrocatalyst to a target product.

For the liquid product:

$$FE = \frac{\alpha n F}{Q}$$

α is the quantity of electrons transferred to form the liquid product; n is the quantity of moles for the liquid product; F is the Faraday constant (96485 C mol^{-1}) and Q is the total number of the charge consumed during the reaction.

For gas product：

$$FE = \frac{Q_{gas}}{Q} = \frac{v \times y \times \alpha \times F \times P_0}{j \times R \times T_0}$$

v represents the flow rate of CO_2; y is the measured concentration of the gas product in 1mL sample loop based on the calibration of the GC with a standard gas; α is the number of electrons required to form a molecule of the gas product; F is the Faraday constant (96485 C mol^{-1}); P_0 is the standard atmosphere; R is the universal gas constant (8.314 J Mol^{-1} K^{-1}); T_0 is the absolute temperature; and j is the total current.

Mott-Schottky (MS)[2]

On the condition that a frequency of 1000 Hz and amplitude of 30 mV, the

Mott-Schottky plots of $BiVO_4$ and $C_xN_y/BiVO_4$ photoanode were recorded in a 0.01 M PBS (pH 7.4) under the dark condition.

From the intercept of these Mott-Schottky curves, flat band potential are calculated for all the samples using Equation：

$$\frac{1}{C^2} = 2/\left(e\varepsilon\varepsilon_0 N_d A^2\right).\left(E_{app} - E_{FB} - kT/e\right)$$

Where C is the capacitance at the semiconductor/electrolyte interface, $F\cdot cm^{-2}$; e is elementary charges, 1.60×10^{-19} C; ε is the relative dielectric constant, 68 for $BiVO_4$; ε0 is the permittivity of the vacuum, 8.85×10^{-12} $F\cdot m^{-1}$; N_D is the donor density, cm^{-3}; A is the surface area of photoanode, cm^2; E_{app} is the applied potential, E_{FB} is the flat band potential, V; k is Boltzmanns constant, 1.38×10^{-23} $F\cdot m^{-1}$; T is absolute temperature, K. At room temperature, kT/e is the temperature dependent term 25 mV and can be ignored. the density of calculated carriers (N_D) of $C_xN_y/BiVO_4$ reached 10.9×10^{22} cm^{-3}, which is substantially higher than pristine $BiVO_4$ photoanode (N_D= 7.1×10^{22} cm^{-3}).

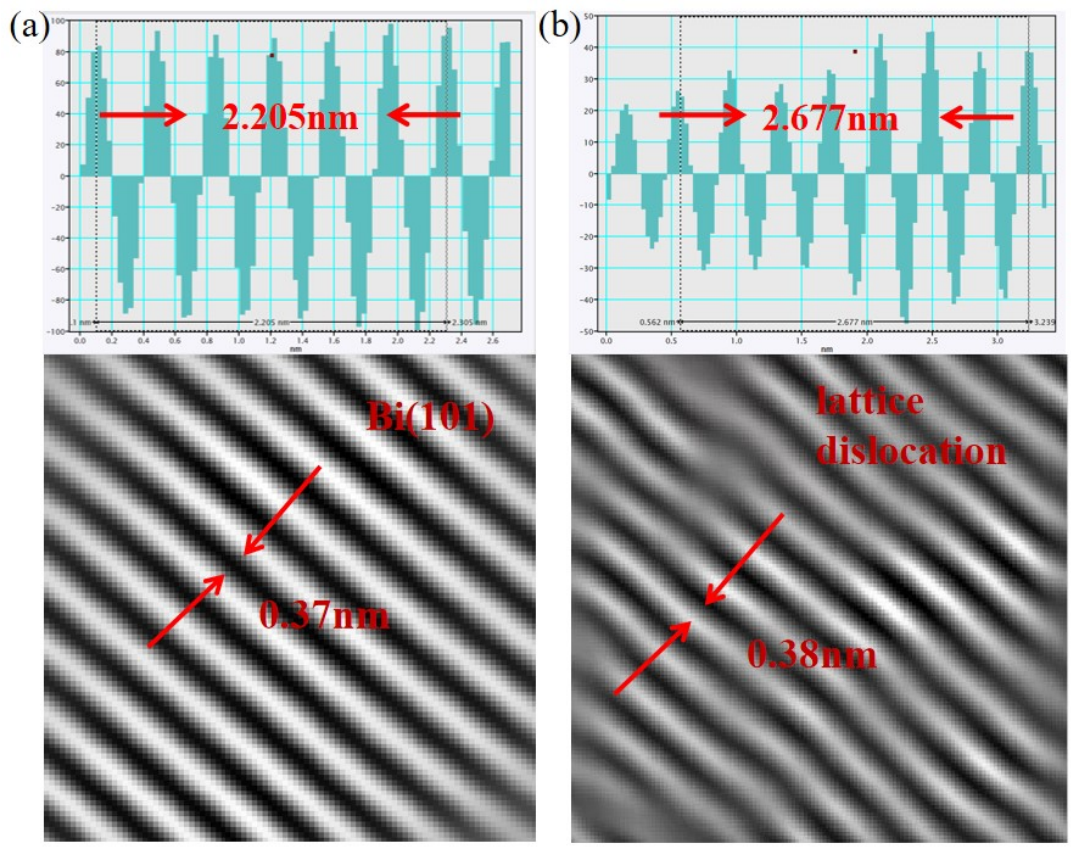

Fig. S1 Lattice distance of HR-TEM image of (a) Bi and (b) lattice disloction Bi

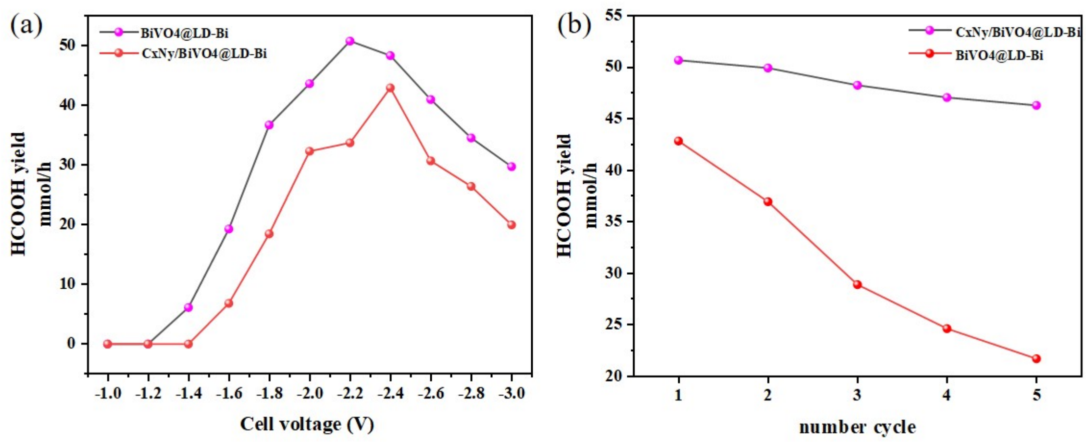

Fig. S2 (a) HCOOH yield in $BiVO_4$@LD-Bi system and CxNy/$BiVO_4$@LD-Bi system, (b) HCOOH yield corresponding to the number of cycles in $BiVO_4$@LD-Bi and $BiVO_4/C_xN_y$@LD-Bi systems.

References

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