

Electronic Supporting Information A

Hysteresis phenomenon in the reaction system of nanocrystalline iron with mixture of ammonia and hydrogen

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List of symbols used in the text

Symbol	Unit	Definition
α		solid solution of α -Fe with nitrogen, sublattice of Fe <i>bcc</i>
γ		solid solution of γ -Fe with nitrogen, sublattice of Fe <i>fcc</i>
γ'		γ' -Fe ₄ N _{1-x} , sublattice of Fe <i>fcc</i>
μ	kJ	chemical potential
N_g		nitrogen in a gas phase
N_s		nitrogen on a surface of solid phase
N_b		nitrogen in a bulk of solid phase
x		mole fraction
θ		surface coverage degree
ΔH_a	kJ/mol	enthalpy of adsorption of nitrogen molecules on the surface of iron
ΔH_{cb}	kJ/mol	enthalpy of formation of the bond between the surface iron atom and nitrogen, Fe _s -N
ΔG	kJ/mol	Gibbs energy
ΔG_{seg}	kJ/mol	Gibbs energy of segregation
E_s	kJ/mol	Surface energy of nanocrystallite
Fe _s -		unoccupied surface iron atom , free adsorption site for nitrogen molecule
Fe _s -N		surface iron atom bonded with nitrogen
Γ	J/m ²	density of the surface energy
P	Pa ^{-0.5}	nitriding potential
superscript n or r		as appropriate for nitriding ⁿ or reduction ^r process

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Symbol	Unit	Definition
superscript or subscript α or γ or γ'		designation of α -Fe α , γ -Fe γ , γ' -Fe ₄ N γ' phases
subscript 0 or max		as appropriate for the minimum and maximum of nitriding potential at which phase exist
square bracket []		transition state