Supplementary information for

Theoretical study of the substitutional solute effect on the interstitial carbon in nickel-based alloy

Xun Zhang[a,b], Cui-Lan Ren[a,c,*], Han Han[a], Xiang-Xi Ye[a], Eugenia Kuo[d], Cheng-Bin Wang[a,c], Wei Zhang[a,c], Li Jiang[a], Gregory Lumpkin[d], Ping Huai[a] and Zhi-Yuan Zhu[a,c,*]

[a] Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China, E-mail: rencuilan@sinap.ac.cn, zhuzhiyuan@sinap.ac.cn

[b] University of Chinese Academy of Sciences, Beijing 100049, China

[c] Key Laboratory of Interfacial Physics and Technology, Chinese Academy of Sciences, Shanghai 2018004

[d] Australian Nuclear Science and Technology Organization, Lucas Heights, New South Wales 2234, Australia

1. Local effect of vacancy on the formation energy of carbon in nickel.

Table S1. The formation energy of carbon in pure nickel and carbon locates at 1-3 NN of vacancy in nickel, unit in eV.

C in nickel		C-V in nickel		
Oct site	Tet site	1NN	2NN	3NN
0.74	2.44	–	–	–
–	–	0.65	0.6	0.73

2. The carbon content effect on their behaviors in nickel.

The C-M binding is expressed by the following equation, $E_b^C = E_{107M+M+nC} - E_{107ni+N} - n * E_{108Ni+C} + n * E_{108Ni}$, where $E_{107M+M+nC}$ is the energy of supercell containing 107 Ni atoms, one M atom and n C atoms, $E_{107ni+N}$ is the energy of supercell containing 107 Ni atoms and one M atom, $E_{108Ni+C}$ is the energy of supercell containing 108 Ni atoms and single carbon atom, E_{108Ni} is the energy of defect-free nickel supercell with 108 Ni atoms, and n is the number of carbon atom.

Table S2. The formation energy of carbon (E_f^C) in pure Ni and Ni-M (M represent Ti, Cr) systems, the binding energy (E_b^{M-C}) of carbon in Ni-M systems.

n	$\boldsymbol{E_f^C}$/eV	$\boldsymbol{E_f^C}$($\boldsymbol{E_b^{M-C}}$)/eV	
	Ni-nC	Ni-Ti-nC	Ni-Cr-nC
1	0.74	1.06 (0.32)	0.67 (-0.07)
2	0.83	1.07 (0.65)	0.72 (-0.05)
3	0.93	1.09 (1.04)	0.73 (-0.03)

3. **The 1NN carbon binding energy as a function of metal solute size factor in the C-M-Ni systems.**

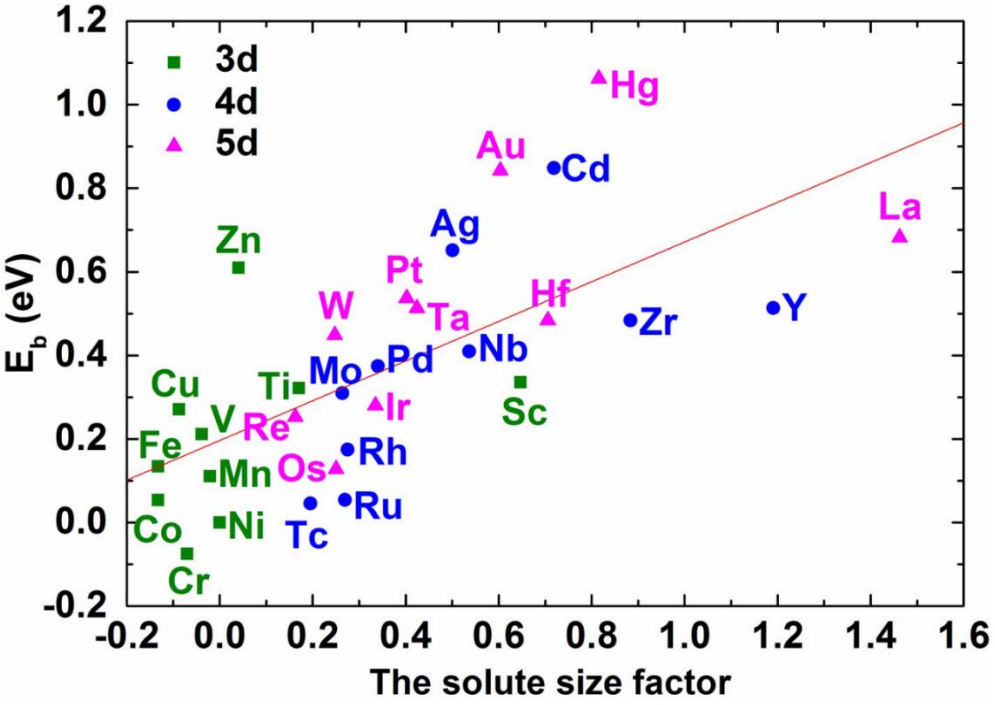

Fig. S1. The C-M-Ni binding energy for carbon at 1NN as a function of the metal solute size factor.

4. The PDOS for C and Ni atom in C-Ni system.

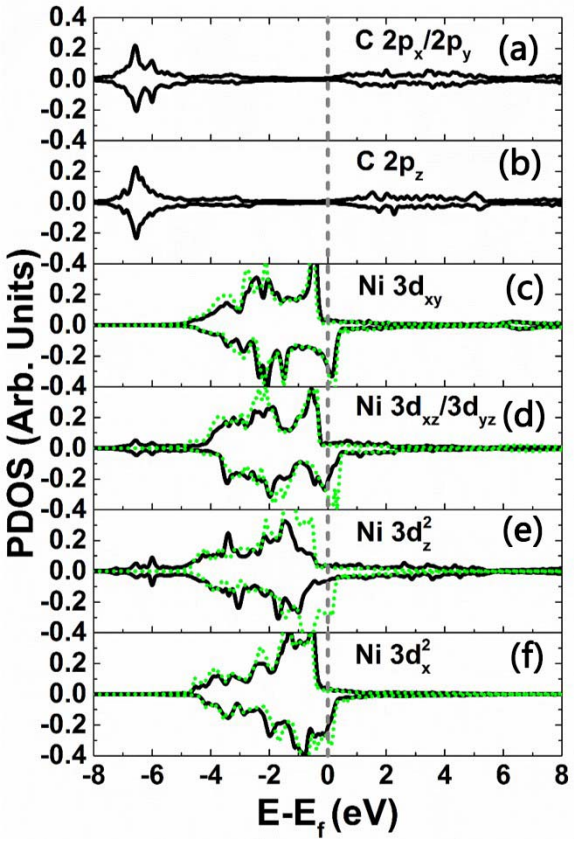

Fig. S2. PDOS for C and Ni atom in C-Ni system. The Fermi level is fixed at 0 eV (the dashed gray line). The PDOS of pure Ni system is also indicated by the dashed green line for a comparison.