Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information for

Effect of $C_6H_5NO_2$ on diamond synthesis by FeNi catalyst under high temperature and high pressure

Zhenghao Cai [a], Ming Li[a], Liangchao Chen [b,*], Shuai Fang [a], Zhiwen Wang [a], Hongyu Zhao [a], Hongan Ma [a,*] and Xiaopeng Jia [a,*]

a. State Key Lab of Super-hard Materials, Jilin University, Changchun 130012, Jilin, China. E-mail: maha@jlu.edu.cn, jiaxp@jlu.edu.cn; Fax: +86 431 85168881; Tel: +86 431 85168881.

b. Key Laboratory of Material Physics of Ministry of Education and School of Physical Engineering, Zhengzhou University, Zhengzhou 450001, Henan, China. E-mail: chenlc@zzu.edu.cn; Tel: +86-371-67780665.

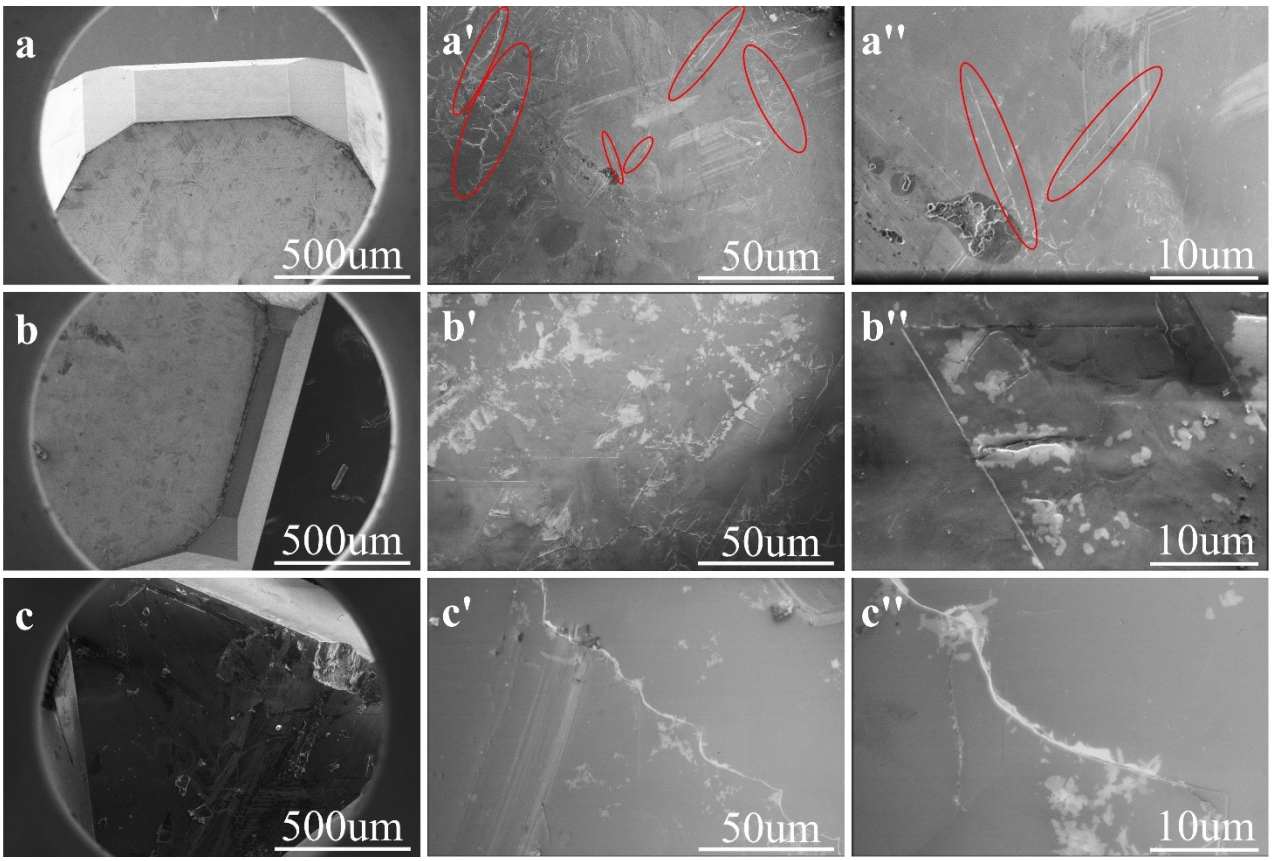

Fig. S1 SEM images of the diamond crystals grown from the Fe-Ni-C system with: (a) 0.1 wt%, (b) 0.2% wt%, (c) 0.8wt% $C_6H_5NO_2$ additive; (a', a'') partial magnification of (a), (b', b'') partial magnification of (b) and (c', c'') partial magnification of (c).

The concentration of nitrogen in C-center form (N_C) and nitrogen in A-center form (N_A) are calculated by following formula：[1-4]

N_C/ppm = 25.0 α_C; α_C = 1.1 α_{1130} – 0.2 α_{1282};

N_A/ppm= 16.5 α_A; α_A = 1.1 α_{1282} – 0.2 α_{1130};

α_{1130} and α_{1282} were absorption coefficients calculated as follows：

α_{1130} = μ (1130cm^{-1})/μ (2000cm^{-1}) ×12.3;

α_{1282} = μ (1282cm^{-1})/μ (2000cm^{-1}) ×12.3;

μ (1130cm^{-1}), μ (2000cm^{-1}) and μ (1282cm^{-1}) were absorption intensity could be calculated according to the recorded value A in FTIR spectra:

μ (1130 cm^{-1}) = A (1130cm^{-1}) – A (1370cm^{-1}),

μ (2000cm^{-1}) = A (2000cm^{-1}) – A (1370cm^{-1}),

μ (1282 cm^{-1}) = A (1282cm^{-1}) – A (1370cm^{-1}).

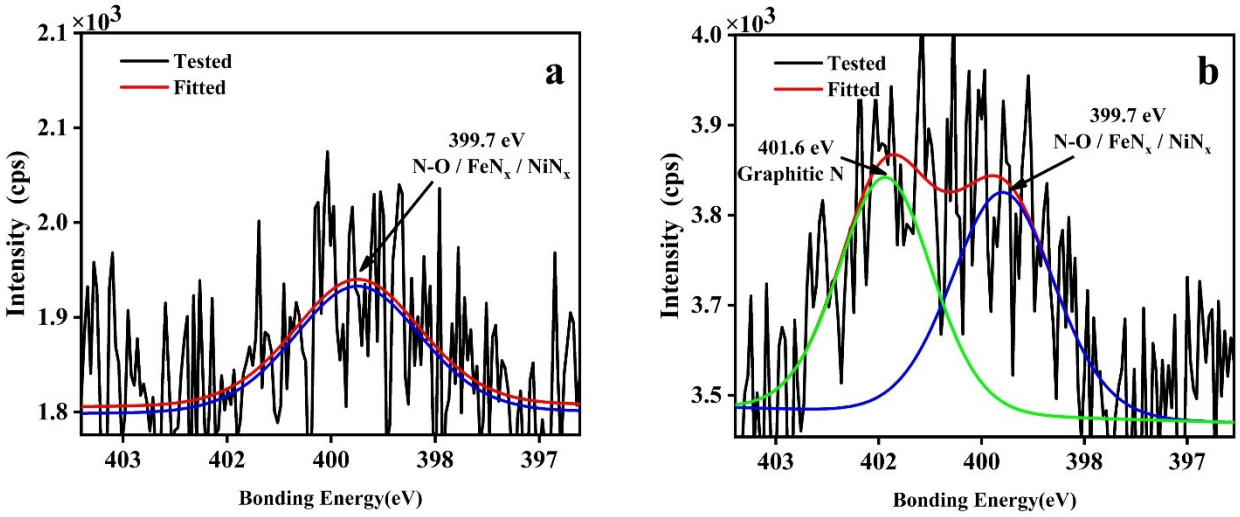

Fig. S2 High-resolution N 1s XPS spectrum of the diamonds synthesized in the FeNi–C system without $C_6H_5NO_2$ (a) and with 1.6wt.% $C_6H_5NO_2$ additive (b).

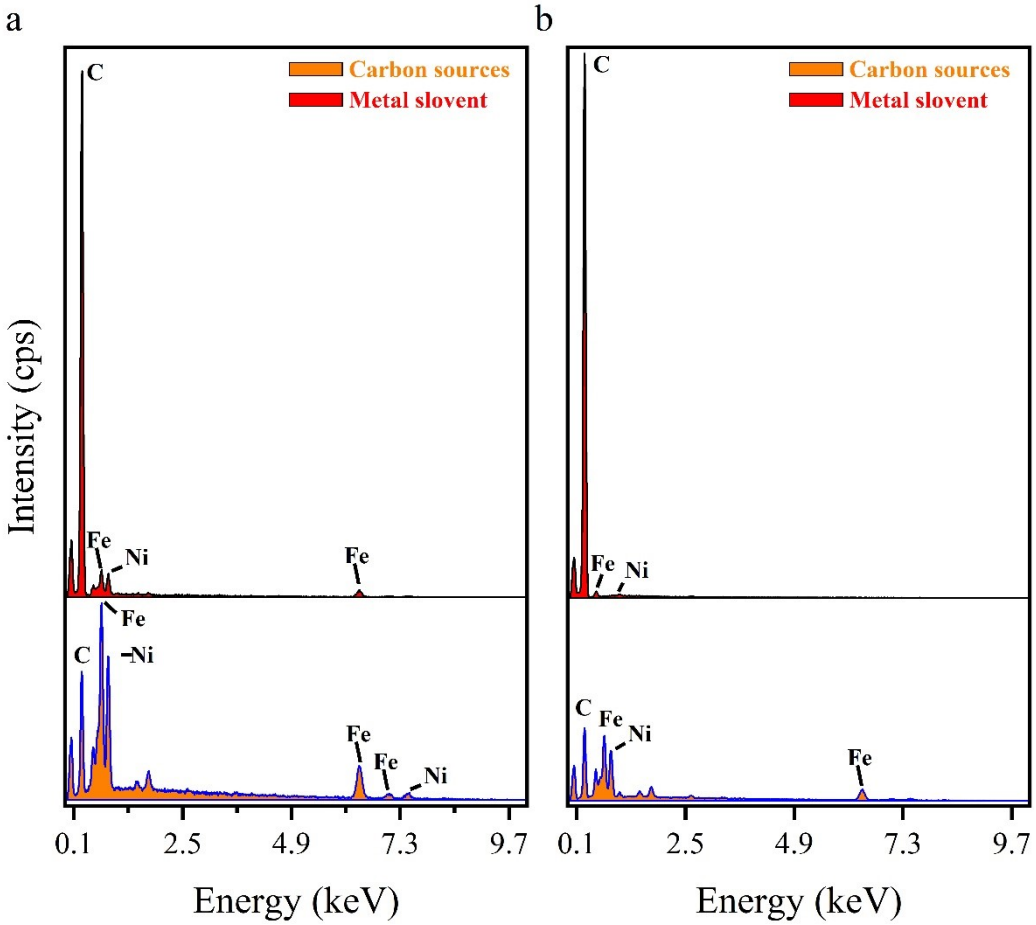

Fig. S3 Energy spectrum test results of carbon sources (The upper part of the figure) and metal solvent (the bottom of the figure): a) without doping; b) doped with 0.8% $C_6H_5NO_2$.

Reference：

(1) Boyd, S. R.; Kiflawi, I.; Woods, G. S., Infrared absorption by the B nitrogen aggregate in diamond. *Philosophical Magazine Part B* **1995,** 72, 351-361.

(2) Chepurova, A. A.; Dereppe, J. M.; Fedorov, I. I.; Chepurov, A. I., The change of Fe-Ni alloy inclusions in synthetic diamond crystals due to annealing. *Diamond and Related Materials* **2000,** 9, 1374-1379.

(3) Huang, G.-F.; Jia, X.-P.; Li, Y.; Hu, M.-H.; Li, Z.-C.; Yan, B.-M.; Ma, H.-A., Growth of gem-grade nitrogen-doped diamond crystals heavily doped with the addition of $Ba(N_3)_2$. *Chinese Physics B* **2011,** 20, (7), 5.

(4) Kiflawi, I.; Mayer, A. E.; Spear, P. M.; Van Wyk, J. A.; Woods, G. S., Infrared absorption by the single nitrogen and A defect centres in diamond. *Philosophical Magazine B* **2006,** 69, (6), 1141-1147.