

THE STUDY OF FORMATION OF METAL–CARBON NANOPARTICLES IN SHOCK WAVES: KINETICS AND MECHANISMS OF NUCLEATION AND GROWTH OF METAL NUCLEI AND CARBON SHELL FORMATION

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Abstract: Experimental and simulation study of the formation of iron nanoparticles during thermal decomposition of iron pentacarbonyl $\text{Fe}(\text{CO})_5$, carbon (soot) nanoparticles during ethylene C_2H_4 pyrolysis, and iron nanoparticles encapsulated into carbon shell during the heating of a mixture of $\text{Fe}(\text{CO})_5 + \text{C}_2\text{H}_4$ in argon behind reflected shock waves was carried out. Microstructure of these nanoparticles was investigated with the help of a high-resolution field-emission scanning electron microscope Zeiss Ultra plus (Ultra 55). The detailed kinetic modeling of the processes of thermal decomposition of iron pentacarbonyl molecules and condensation of iron atoms with the formation of iron nanoparticles, the formation of carbon (soot) particles during ethylene pyrolysis, and the joint process of formation of iron and carbon particles and iron particles encapsulated in a carbon shell was conducted.

Keywords: encapsulated nanoparticles; nanoparticle microstructure; field-emission scanning electron microscope; shock waves; kinetic modeling

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References

- Hermann, I. K., R. N. Grass, and W. J. Stark. 2009. High-strength metal nanomagnets for diagnostics and medicine: Carbon shells allow long-term stability and reliable linker chemistry. *Nanomedicine* 4:787–798.
- Xu, Y., M. Mahmood, Z. Li, E. Dervishi, S. Trigwell, V. P. Zharov, N. Ali, V. Saini, A. R. Biris, D. Lupu, D. Boldor, and A. S. Biris. 2008. Cobalt nanoparticles coated with graphitic shells as localized radio frequency absorbers for cancer therapy. *Nanotechnology* 19(43):435102.
- Ermakov, A. E., M. A. Uimin, A. A. Mysik, V. S. Gaviko, E. S. Lokteva, S. A. Kachevskii, A. O. Turakulova, and V. V. Lunin. 2009. The synthesis, structure, and properties of carbon-containing nanocomposites based on nickel, palladium, and iron. *Russ. J. Phys. Chem. A* 83(7):1187–1193.
- Zhao D.-L., X. Li, and Z.-M. Shen. 2009. Preparation and electromagnetic and microwave absorbing properties of Fe-filled carbon nanotubes. *J. Alloy. Compd.* 471:457–460.
- Liu, Q., B. Cao, C. Feng, W. Zhang, S. Zhu, and D. Zhang. 2012. High permittivity and microwave absorption of porous graphitic carbons encapsulating Fe nanoparticles. *Compos. Sci. Technol.* 72:1632–1636.
- Tyagi, S., P. Verma, H. B. Baskey, R. C. Agarwala, V. Agarwala, and T. C. Shami. 2012. Microwave absorption study of carbon nanotubes dispersed hard/soft ferrite nanocomposite. *Ceramics International* 38:4561–4571.
- David, B., N. Pizurova, O. Schneeweiss, P. Bezdicka, and I. Morjan, R. Alexandrescu. 2004. Preparation of iron/graphite core–shell structured nanoparticles. *J. Alloy. Compd.* 378:112–116.
- Tokoro, H., S. Fujii, S. Muto, and S. Nasu. 2006. Fe–Co and Fe–Ni magnetic fine particles encapsulated by graphite carbon. *J. Appl. Phys.* 99:08Q512.
- Fan, N., X. Ma, Zh. Ju, and J. Li. 2008. Formation, characterization and magnetic properties of carbon-encapsulated iron carbide nanoparticles. *Mater. Res. Bull.* 43:1549–1554.
- Bystrzejewski, M., K. Pyrzynska, A. Huczko, and H. Lange. 2009. Carbon-encapsulated magnetic nanopar-

- ticles as separable and mobile sorbents of heavy metal ions from aqueous solutions. *Carbon* 47(4):1201–1204.
11. Ning, L., L. Xiaojie, W. Xiaohong, Y. Honghao, M. Fei, and S. Weighing. 2009. Preparation and magnetic behavior of carbon-encapsulated iron nanoparticles by detonation method. *Compos. Sci. Technol.* 69:2554–2558. 1
 12. Ning, L., L. Xiaojie, W. Xiaohong, Y. Honghao, Zh. Chengjiao, and W. Haitao. 2010. Synthesis and characterization of carbon-encapsulated iron/iron carbide nanoparticles by a detonation method. *Carbon* 48:3858–3863.
 13. Atkinson, J. D., M. E. Fortunato, S. A. Dastgheib, M. Rostam-Abadi, M. J. Rood, and K. S. Suslick. 2011. Synthesis and characterization of iron-impregnated porous carbon spheres prepared by ultrasonic spray pyrolysis. *Carbon* 49:587–598.
 14. Tsurin, V. A., A. Y. Yermakov, M. A. Uimin, A. A. Mysik, N. N. Shchegoleva, V. S. Gaviko, and V. V. Maikov. 2014. Synthesis, structure, and magnetic properties of iron and nickel nanoparticles encapsulated into carbon. *Phys. Solid State* 56(2):287–301.
 15. Lee, K., M. Kim, and H. Kim. 2010. Catalytic nanoparticles being facet-controlled. *J. Mater. Chem.* 20:3791–3798.
 16. He, Z., J.-L. Maurice, A. Gohier, C. S. Lee, D. Pribat, and C. S. Cojocar. 2011. Iron catalysts for the growth of carbon nanofibers: Fe, Fe₃C or both? *Chem. Mater.* 23:5379–5387.
 17. Gurentsov, E. V., and A. V. Eremin. 2015. Synthesis of metal-carbon nanoparticles in pulsed UV-photolysis of Fe(CO)₅-CCl₄ mixtures at room temperature. *Tech. Phys. Lett.* 41(6):547–550.
 18. Agafonov, G. L., V. N. Smirnov, and P. A. Vlasov. 2010. Shock tube and modeling study of soot formation during pyrolysis of propane, propane/toluene and rich propane/oxygen mixtures. *Combust. Sci. Technol.* 182:1645–1671.
 19. Agafonov, G. L., V. N. Smirnov, and P. A. Vlasov. 2011. Shock tube and modeling study of soot formation during the pyrolysis and oxidation of a number of aliphatic and aromatic hydrocarbons. *Proc. Combust. Inst.* 33:625–632.
 20. Agafonov, G. L., V. N. Smirnov, and P. A. Vlasov. 2012. Effect of iron pentacarbonyl on soot formation behind shock waves. *Combust. Sci. Technol.* 184(10-11):1838–1861.
 21. Smirnov, V. N. 2008. Termicheskaya dissotsiatsiya gazo-obraznykh gibridov i metallorganicheskikh soedineniy i reaktsii produktov ikh raspada [Thermal dissociation of the gas-phase hydrides and organometallic compounds and the reactions of their decomposition products]. Moscow: N. N. Semenov Institute of Chemical Physics. D.Sc. Thesis. 490 p.
 22. Agafonov, G. L., I. V. Bilera, P. A. Vlasov, Yu. A. Kolbanovskii, V. N. Smirnov, and A. M. Tereza. 2015. Soot formation during the pyrolysis and oxidation of acetylene and ethylene in shock waves. *Kinet. Catal.* 56(1):12–30.
 23. Agafonov, G. L., I. V. Bilera, P. A. Vlasov, I. V. Zhil'tsova, Yu. A. Kolbanovskii, V. N. Smirnov, and A. M. Tereza. 2016. Unified kinetic model of soot formation in the pyrolysis and oxidation of aliphatic and aromatic hydrocarbons in shock waves. *Kinet. Catal.* 57(5):557–572.
 24. Wen, J. Z., C. F. Goldsmith, R. W. Ashcraft, and W. H. Green. 2007. Detailed kinetic modeling of iron nanoparticle synthesis from the decomposition of Fe(CO)₅. *J. Phys. Chem. C* 111:5677–5688.

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