

Accepted Manuscript

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PII: S1350-4177(17)30399-1

DOI: <http://dx.doi.org/10.1016/j.ultsonch.2017.09.007>

Reference: ULTSON 3855

To appear in: *Ultrasonics Sonochemistry*

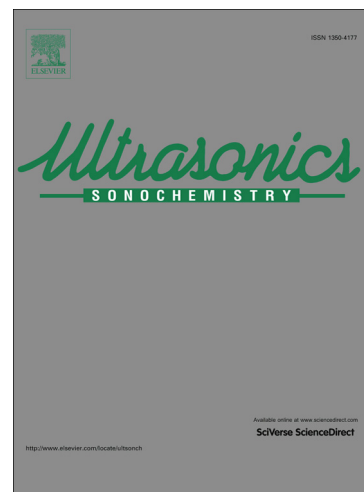
Received Date: 11 June 2017

Revised Date: 3 September 2017

Accepted Date: 3 September 2017

Please cite this article as: Y. Gai, W. Wang, D. Xiao, Y. Zhao, Ultrasound coupled with supercritical carbon dioxide for exfoliation of graphene: simulation and experiment, *Ultrasonics Sonochemistry* (2017), doi: <http://dx.doi.org/10.1016/j.ultsonch.2017.09.007>

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Ultrasound coupled with supercritical carbon dioxide for exfoliation of graphene: simulation and experiment

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Abstract

Ultrasound coupled with supercritical CO₂ has become an important method for exfoliation of graphene, but behind which a peeling mechanism is unclear. In this work, CFD simulation and experiment were both investigated to elucidate the mechanism and the effects of the process parameters on the exfoliation yield. The experiments and the CFD simulation were conducted under pressure ranging from 8 MPa to 16 MPa, the ultrasonic power ranging from 12W to 240W and the frequency of 20 kHz. The numerical analysis of fluid flow patterns and pressure distributions revealed that the fluid shear stress and the periodical pressure fluctuation generated by ultrasound were primary factors in exfoliating graphene. The distribution of the fluid shear stress decided the effective exfoliation area, which, in turn, affected the yield. The effective area increased from 5.339cm³ to 8.074cm³ with increasing ultrasonic power from 12W to 240W, corresponding to the yield increasing from 5.2% to 21.5%. The pressure fluctuation would cause the expansion of the interlayers of graphite. The degree of the expansion increased with the increase of the operating pressure but decreased beyond 12 MPa. Thus, the maximum yield was obtained at 12MPa. The

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