Abstract Submitted for the OSF16 Meeting of The American Physical Society

Analysis of Debye Scattering of 2-D and 3-D Simulated Carbon Crystals for Comparison with Electron Diffraction Patterns of Graphitic Stardust LINDSAY LESH, ERIC MANDELL, ALEXEY ZAYAK, Bowling Green State University — The objective of this research is to understand the structure of graphitic stardust found in primitive meteorites (e.g. the Murchison meteorite). The meteoritic carbon formations of interest exhibit a core-rim structure, where the core – with a density less than that of the graphitic rim – comprises the majority of the grain. There is reason to hypothesize that the cores of these grains are the result of the rapid freezing (quenching) of a liquid carbon droplet. In order to understand these structures, simulated 3-D carbon crystals were rapidly quenched from a gaseous state using the molecular dynamics (MD) simulation software, GROMACS. The resulting condensates from these simulations have been analyzed using radial distribution function (RDF) calculations and Debye scattering calculations. In addition, it was necessary to understand how individual layers of differently shaped graphene sheets affect Debye scattering. Therefore, the Debye formula was also applied to simulated 2-D crystals – different sized apex-angled triangular shaped graphene sheets - using the research software, Mathematica. The Debye scattering patterns from the 2-D and 3-D crystals were then compared with the experimental electron diffraction data from the stardust.

> Lindsay Lesh Bowling Green State University

Date submitted: 02 Sep 2016

Electronic form version 1.4