A new discrete methodology for dynamic fracture simulations of rGO-enriched nanoceramics

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In this study the new principles for simulations of microstructure-related dynamic fracture of ceramics/graphene composites [1,2] have been developed employing discrete cell complexes [3–5] and tools of modern graph theory [4]. It became a continuation of the previous works [4,5] where the new tools such as configurational entropy and structural indices were introduced for a more informative complex structure characterisation. The topological conditions determine the critical damage value for coalescence of many nanocracks into a single network of fractured grain boundaries and strongly depend on the composite microstructure. We determined the configurations of graphene plates corresponding to the maximum stability of the composites electrical properties to cracking processes. The calculations draw the conclusion about the advantages of the geometry of elongated rGO inclusions in the form of strips covering several grain boundaries.

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[1] Sheinerman A G, Morozov N F and Gutkin M Y 2019 *Mechanics of Materials* **137** 103126

[2] Kurapova O Y, Glukharev A G, Glumov O V, Kurapov M Y, Boltynjuk E V and Konakov V G 2019 *Electrochimica Acta* **320** 134573

[3] Šeruga D, Kosmas O and Jivkov A P 2020 *International Journal of Solids and Structures* **198** 136–148

[4] Borodin E N and Jivkov A P 2020 *Philosophical Magazine* **100** 467–485

[5] Zhu S, Borodin E N and Jivkov A P 2020 *Materials & Design* **198** 1093522