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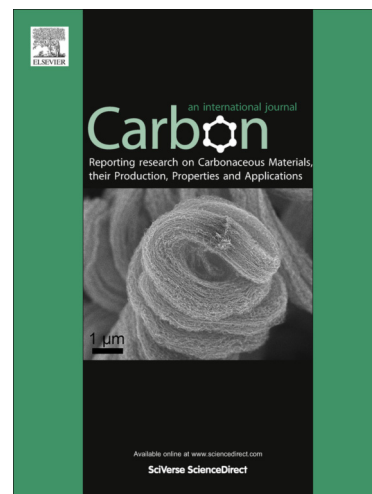
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NON-EQUILIBRIUM GRAIN BOUNDARIES WITH EXCESS ENERGY IN GRAPHENE

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Abstract. Exploring an approach to grain boundary (GB) mesoscopic structure in 3D polycrystals, we develop a model description for equilibrium and non-equilibrium states of GBs in graphene. Non-equilibrium states of GBs in graphene are analyzed for the first time. On the base of this model, dependence of total energy for symmetric GBs on the misorientation angle, $E(\theta)$, in graphene was calculated. It was found that for the same average misorientation angle the energy in a non-equilibrium state of a GB in graphene can significantly exceed the energy in the equilibrium state. In graphene, the GB energy depends to a greater extent on the deviation from the equilibrium state than on the misorientation angle. It is proposed to account for the presence of non-equilibrium GBs in the explanations of unusual physical properties of graphene.

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